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Relaxation at finite temperatures

The weak coupling theory of chapter 17 is the workhorse of quantum optics and serves very well in practice, also at nonzero temperatures. From the viewpoint of the theory one might wonder about the structure at fixed small, but nonzero, coupling strength, which needs to go beyond the analysis of the weak coupling theory. Much effort has been invested to achieve this goal, basically by trying to identify corrections within time-dependent perturbation theory. Unfortunately, since the long-time behavior must be extracted, the details quickly become unwieldy and one has to rely on ad hoc approximations.

Over recent years a novel approach has been pursued which investigates the pole structure of the analytic continuation of the resolvent of H_λ across the real axis through complex dilations; compare with section 17.3. The techniques are demanding but simplify substantially at finite temperatures when the Hamiltonian is replaced by the Liouvillean and, since its spectrum is the full real line, complex dilations are replaced by complex translations which can be handled more easily. From the pole structure a fairly complete picture of the long-time dynamics can be extracted with the potential of computing systematically higher corrections to the weak coupling theory.

The finite temperature relaxation is a digression into the realm of time-dependent statistical mechanics with small deviations from thermal equilibrium. While this is of independent interest and has important applications in quantum optics and condensed matter, our goal is merely to illustrate the power of complex translations and make the connection to the weak coupling theory.

For completeness we recall once again the set-up. In the dipole approximation and N-level approximation the Hamiltonian is

$$H_\lambda = H_{\mathrm{at}} + H_{\mathrm{f}} + \lambda Q \cdot E_\varphi = H_0 + \lambda H_{\mathrm{int}}, \qquad (18.1)$$

see (17.10). H_{at} acts on $\mathbb{C}^N$. Diverging from our previous convention, the energies ε_j are labeled as $\varepsilon_1 \leq \varepsilon_2 \ldots \leq \varepsilon_N$ allowing for possible degeneracies. Q is the

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dipole operator as an $N \times N$ matrix. The field energy H_{f}, and the electric field $E_\varphi = E_\varphi(0)$ are operators on Fock space $\mathcal{F}$. For finite temperatures we need some extra structure, which will be explained below.

The photon field is at temperature $T > 0$. It will be more convenient to work with the inverse temperature and set $\beta = 1/k_{\mathrm{B}}T$. In the initial state the atom and its nearby photons are out of equilibrium and the goal is to understand how the coupled system relaxes back to global equilibrium. In the weak coupling theory one disentangles the effective dynamics of the atom and regards the field as driven by the atomic source. At fixed λ such a distinction becomes hazy and a more global view is adopted with the separation deduced in the small-λ limit.

The analysis of thermal relaxation relies on the following strategy. One introduces coordinates which encode the finite energy excitations away from equilibrium. Doing this properly relies on tools from the representation theory of C^*-algebras which for our context was mostly developed in the 1960–70s. For noninteracting photons the representation of Araki and Woods (1963) is of a sufficiently concrete form and also allows the incorporation of the coupling to the atom. Note that at zero coupling the spectrum of finite energy excitation covers the full real axis $\mathbb{R}$, since $\omega(k) = |k|$ and energy can be either below or above its equilibrium value. The energy differences of the atom are embedded in this spectrum as discrete eigenvalues. As the coupling is turned on, they become resonances which are uncovered by a complex downward translation of the photon excitation spectrum. The location of the resonance poles and the corresponding eigenspaces can be handled through standard analytic perturbation theory.

To convince the reader that the Araki–Woods Liouvillean correctly describes the finite energy excitation, we need some background material on quantum systems at finite temperature. We conform with established notation which to some extent deviates from our previous conventions.

18.1 Bounded quantum systems, Liouvillean

We start with an abstract quantum system on a separable Hilbert space $\mathcal{H}$ equipped with the scalar product $\langle \cdot, \cdot \rangle$. We assume that the Hamiltonian H is bounded from below and has a purely discrete spectrum such that

$$\mathrm{tr}[\mathrm{e}^{-\beta H}] < \infty \qquad (18.2)$$

for arbitrary $\beta > 0$. The algebra of observables, $\mathcal{A}$, is the set of all bounded operators on $\mathcal{H}$, denoted by $B(\mathcal{H})$. A general quantum state is given through the density matrix ρ, satisfying $\rho \geq 0$, $\mathrm{tr}\rho = 1$. In particular $\rho \in \mathcal{T}_1(\mathcal{H})$, denoting the two-sided ideal of trace class operators on $\mathcal{H}$. In the Heisenberg picture the time

evolution is given through

$$\alpha_t(a) = e^{itH} a e^{-itH} \tag{18.3}$$

as acting on $a \in B(\mathcal{H})$. The dual Schrödinger picture provides the time evolution of states as

$$\rho \mapsto \rho_t = \alpha_{-t}(\rho) = e^{-itH} \rho e^{itH}. \tag{18.4}$$

We want the evolution of density matrices to look like the evolution of vectors on a Hilbert space and, for this purpose, introduce the two-sided ideal of Hilbert–Schmidt operators $\mathcal{T}_2(\mathcal{H})$. A bounded operator a belongs to $\mathcal{T}_2(\mathcal{H})$ if and only if $\mathrm{tr}[a^*a] < \infty$. $\mathcal{T}_2(\mathcal{H})$ becomes a Hilbert space under the scalar product

$$\langle a|b \rangle = \mathrm{tr}[a^*b], \quad a, b \in \mathcal{T}_2(\mathcal{H}). \tag{18.5}$$

It will be useful to represent $\mathcal{A} = B(\mathcal{H})$ as an algebra of operators on $\mathcal{T}_2(\mathcal{H})$. $\mathcal{T}_2(\mathcal{H})$ carries a left representation through

$$\ell(a)\kappa = a\kappa \in \mathcal{T}_2(\mathcal{H}). \tag{18.6}$$

Later on we will need also the right antirepresentation defined through

$$r(a)\kappa = \kappa a^* \in \mathcal{T}_2(\mathcal{H}). \tag{18.7}$$

This representation is antilinear since $r(za)\kappa = z^*r(a)\kappa$ for $z \in \mathbb{C}$.

We transcribe states and dynamics to $\mathcal{T}_2(\mathcal{H})$. To every element $\kappa \in \mathcal{T}_2(\mathcal{H})$ a state ρ is associated through

$$\rho = \langle \kappa|\kappa \rangle^{-1} \kappa\kappa^*. \tag{18.8}$$

The expectation of $a \in B(\mathcal{H})$ is given by

$$\langle a \rangle_\rho = \mathrm{tr}[\rho a] = \langle \kappa|\kappa \rangle^{-1} \langle \kappa|\ell(a)\kappa \rangle. \tag{18.9}$$

The time evolution becomes

$$\langle \alpha_t(a) \rangle_\rho = \langle \kappa|\kappa \rangle^{-1} \mathrm{tr}[\kappa^*\alpha_t(a)\kappa] = \langle \kappa|\kappa \rangle^{-1} \langle \kappa|\ell(\alpha_t(a))\kappa \rangle \tag{18.10}$$

and for $\kappa, \sigma \in \mathcal{T}_2(\mathcal{H})$

$$\begin{aligned} \langle \kappa|\ell(\alpha_t(a))\sigma \rangle &= \mathrm{tr}[\kappa^*\alpha_t(a)\sigma] = \mathrm{tr}[(e^{-itH}\kappa e^{itH})^* a (e^{-itH}\sigma e^{itH})] \\ &= \langle \alpha_{-t}(\kappa)|\ell(a)\alpha_{-t}(\sigma) \rangle = \langle e^{-it\mathcal{L}}\kappa|\ell(a)e^{-it\mathcal{L}}\kappa \rangle. \end{aligned} \tag{18.11}$$

The last identity defines the Liouvillean $\mathcal{L}$. Clearly

$$\mathcal{L}\kappa = [H, \kappa] \tag{18.12}$$

and $\kappa_t = \alpha_{-t}(\kappa)$ is governed by the Schrödinger-like equation

$$i\frac{d}{dt}\kappa_t = \mathcal{L}\kappa_t. \tag{18.13}$$

The Liouvillean is a symmetric operator as can be seen from

$$\langle \kappa | \mathcal{L}\sigma \rangle = \text{tr}[\kappa^*[H, \sigma]] = \text{tr}[([H, \kappa])^* \sigma] = \langle \mathcal{L}\kappa | \sigma \rangle. \tag{18.14}$$

To work concretely with the left, respectively right, representation of $\mathcal{A}$ and the Liouvillean $\mathcal{L}$ it is convenient to identify $\mathcal{T}_2(\mathcal{H})$ with $\mathcal{H} \otimes \mathcal{H}$ through the isomorphism

$$I_C : \mathcal{T}_2(\mathcal{H}) \to \mathcal{H} \otimes \mathcal{H}. \tag{18.15}$$

In a suitable basis C is simply complex conjugation. More abstractly C is an anti-unitary involution on $\mathcal{H}$, i.e.

$$C^2 = 1 \quad \text{and} \quad \langle C\psi, C\varphi \rangle = \langle \varphi, \psi \rangle. \tag{18.16}$$

Then with κ defined through $\kappa\psi = \psi_1 \langle \psi_2, \psi \rangle$ one sets

$$I_C\kappa = \psi_1 \otimes C\psi_2 \in \mathcal{H} \otimes \mathcal{H} \tag{18.17}$$

which extends by linearity. Note that

$$I_C\ell(a)\kappa = I_C a\kappa = a\psi_1 \otimes C\psi_2 = (a \otimes 1)I_C\kappa. \tag{18.18}$$

Thus I_C intertwines with the left representation ℓ of $\mathcal{A}$ on $\mathcal{H} \otimes \mathcal{H}$ given by

$$\ell(a) = a \otimes 1. \tag{18.19}$$

Similarly

$$I_C r(a)\kappa = I_C(\kappa a^*) = \psi_1 \otimes Ca\psi_2 = 1 \otimes CaCI_C\kappa \tag{18.20}$$

and

$$r(a) = 1 \otimes CaC \quad \text{on} \quad \mathcal{H} \otimes \mathcal{H}. \tag{18.21}$$

In particular for the Liouvillean

$$I_C\mathcal{L}\kappa = H\psi_1 \otimes C\psi_2 - \psi_1 \otimes CH\psi_2 = H\psi_1 \otimes C\psi_2 - \psi_1 \otimes (CHC)C\psi_2$$
$$= (H \otimes 1 - 1 \otimes CHC)(\psi_1 \otimes C\psi_2) = (H \otimes 1 - 1 \otimes CHC)I_C\kappa \tag{18.22}$$

and

$$L = I_C\mathcal{L}I_C^{-1} = H \otimes 1 - 1 \otimes CHC \quad \text{on} \quad \mathcal{H} \otimes \mathcal{H}. \tag{18.23}$$

If H is invariant under time-reversal, we may choose $C = T$, with time-reversal T, and $CHC = THT = H$. Then the Liouvillean is given by

$$L = H \otimes 1 - 1 \otimes H \tag{18.24}$$

as an operator on $\mathcal{H} \otimes \mathcal{H}$. Clearly the spectrum of L consists of the energy differences $\{E_i - E_j \mid i, j = 0, 1, \dots\}$, where E_i, $i = 0, 1, \dots$, are the eigenvalues of H.

18.2 Equilibrium states and their perturbations, KMS condition

Of the many possible quantum states thermal equilibrium plays a special role. It is defined by the density matrix

$$\rho_\beta = Z^{-1} e^{-\beta H}, \quad Z = \text{tr}[e^{-\beta H}]. \tag{18.25}$$

As an element of $\mathcal{T}_2(\mathcal{H})$ we set

$$\kappa_\beta = Z^{-1/2} e^{-\beta H/2}. \tag{18.26}$$

Then $\rho_\beta = \kappa_\beta \kappa_\beta^*$. Since ρ_β is strictly positive, $\langle a^* a \rangle_\beta = \text{tr}[\rho_\beta \, a^* a] = 0$ for $a \in \mathcal{A}$ implies $a = 0$. Equivalently,

$$\ell(a)\kappa_\beta = 0 \quad \text{implies} \quad a = 0, \tag{18.27}$$

which means that κ_β is separating for the algebra $\ell(\mathcal{A})$. In principle, one should allow for additional conservation laws like total charge or total number of particles. However, this is ignored here since the Hamiltonian (18.1) does not have such a structure.

For the photon field in infinite space the spectrum of H is continuous and $Z^{-1} e^{-\beta H}$ as such makes no sense. On the other hand, the atom is a small perturbation. Thus the equilibrium state of the coupled system relative to that of the uncoupled system remains meaningful even at infinite volume and is the object of thermal perturbation theory.

We consider

$$H = H_0 + I. \tag{18.28}$$

H_0 is the unperturbed reference system and I is the perturbation, assumed to be bounded, $\|I\| < \infty$. By the Golden–Thompson inequality

$$Z_\beta = \text{tr}[e^{-\beta H}] = \text{tr}[e^{-\beta(H_0 + I)}] \leq \text{tr}[e^{-\beta H_0} e^{-\beta I}]$$
$$\leq e^{\beta\|I\|} \text{tr}[e^{-\beta H_0}] = e^{\beta\|I\|} Z_\beta^0. \tag{18.29}$$

Thus if $Z_\beta^0 < \infty$, as assumed, then $\rho_\beta = Z_\beta^{-1} e^{-\beta H} \in \mathcal{T}_1(\mathcal{H})$.

The Liouvillean of the reference system is given by

$$\mathcal{L}_0 = \ell(H_0) - r(H_0) \tag{18.30}$$

and the Liouvillean of the perturbed system by

$$\mathcal{L} = \ell(H) - r(H). \tag{18.31}$$

Under the isomorphism I_C the Liouvilleans become

$$L = I_C \mathcal{L} I_C^{-1} = (H_0 + I) \otimes 1 - 1 \otimes C(H_0 + I)C = L_0 + W,$$
$$L_0 = H_0 \otimes 1 - 1 \otimes C H_0 C, \quad W = I \otimes 1 - 1 \otimes C I C. \tag{18.32}$$

We also define the Radon–Nikodym operators, $\mathcal{L}_\ell$ and $\mathcal{L}_r$, through

$$\mathcal{L}_\ell = \mathcal{L}_0 + \ell(I), \quad \mathcal{L}_r = \mathcal{L}_0 - r(I). \tag{18.33}$$

Then, with $\kappa_\beta = (Z_\beta)^{-1/2} e^{-\beta H/2}$, $\kappa_\beta^0 = (Z_\beta^0)^{-1/2} e^{-\beta H_0/2}$, we have

$$e^{-\beta \mathcal{L}_\ell/2} \kappa_\beta^0 = e^{-\beta(\ell(H_0) + \ell(I) - r(H_0))/2} \kappa_\beta^0 = e^{-\beta(H_0 + I)/2} \kappa_\beta^0 e^{\beta H_0/2}$$
$$= (Z_\beta/Z_\beta^0)^{1/2} (Z_\beta)^{-1/2} e^{-\beta H/2} = (Z_\beta/Z_\beta^0)^{1/2} \kappa_\beta \tag{18.34}$$

and by a similar calculation

$$e^{\beta \mathcal{L}_r/2} \kappa_\beta^0 = (Z_\beta/Z_\beta^0)^{1/2} \kappa_\beta. \tag{18.35}$$

κ_β^0 is in the domain of the operators $e^{-\beta \mathcal{L}_\ell/2}$ and $e^{\beta \mathcal{L}_r/2}$ and their action maps unperturbed to perturbed equilibrium,

$$\kappa_\beta = (Z_\beta^0/Z_\beta)^{1/2} e^{-\beta \mathcal{L}_\ell/2} \kappa_\beta^0, \quad \kappa_\beta = (Z_\beta^0/Z_\beta)^{1/2} e^{\beta \mathcal{L}_r/2} \kappa_\beta^0. \tag{18.36}$$

The thermal state $e^{-\beta H}$ is related to the unitary time evolution e^{-itH} through analytic continuation to $\beta = it$, which gives rise to a very powerful analytic structure of equilibrium time correlations known as the Kubo–Martin–Schwinger (KMS) boundary condition. We define the time correlations as

$$\langle a \alpha_t(b) \rangle_\beta = F_{ab}(t), \quad \langle \alpha_t(b) a \rangle_\beta = G_{ab}(t). \tag{18.37}$$

They are linked through

$$\langle a \alpha_t(b) \rangle_\beta = Z_\beta^{-1} \mathrm{tr}[e^{-\beta H} a e^{itH} b e^{-itH}] = Z_\beta^{-1} \mathrm{tr}[e^{-\beta H} e^{(\beta + it)H} b e^{-(\beta + it)H} a]$$
$$= \langle \alpha_{-i\beta + t}(b) a \rangle_\beta, \tag{18.38}$$

which is the *KMS condition*. It states that $F_{ab}(t)$ is the boundary value of a function $G_{ab}(z)$ which is analytic in the strip $\mathcal{S}_{-\beta} = \{z \mid -\beta < \mathrm{Im} z < 0\}$ such that

$$\lim_{\eta \uparrow \beta} G_{ab}(t - i\eta) = F_{ab}(t). \tag{18.39}$$

Equivalently, $G_{ab}(t)$ is the boundary value of a function $F_{ab}(z)$ analytic in the strip $\mathcal{S}_\beta$ such that

$$\lim_{\eta \uparrow \beta} F_{ab}(t + i\eta) = G_{ab}(t). \qquad (18.40)$$

A state which satisfies either of these boundary conditions is called a KMS state with respect to the time evolution α_t. In our set-up, the only KMS state is ρ_β. The KMS condition is used as a defining property for equilibrium states in infinitely extended systems. In general, for the same group of automorphisms there could then be several KMS states. Physically they represent distinct thermodynamic phases.

18.3 Spectrum of the Liouvillean and relaxation

As discussed in section 17.5, at zero temperature the relaxation to the ground state can be reduced to a scattering problem, see Proposition 17.5. As a simplification, at finite temperature it suffices to have sufficiently strong spectral properties of the Liouvillean. We have in mind now a situation where the size of the black-body cavity is huge on the atomic scale. Therefore the relevant mathematical idealization is to have the photon field infinitely extended. The algebra $B(\mathcal{H})$ must be replaced then by a suitable algebra $\mathcal{A}$ of quasi-local observables. Its construction will be explained in the following. At the moment we focus on the abstract structure. Thus we have given the C^*-algebra $\mathcal{A}$ and a one-parameter group α_t of $*$-automorphisms as the dynamics. The distinguished state on $\mathcal{A}$ is the KMS state ω_β at inverse temperature β. Its time correlations are defined by

$$F_{ab}(t) = \omega_\beta(a\alpha_t(b)), \quad G_{ab}(t) = \omega_\beta(\alpha_t(b)a) \qquad (18.41)$$

and they satisfy the KMS boundary condition

$$G_{ab}(t - i\beta) = F_{ab}(t), \quad F_{ab}(t + i\beta) = G_{ab}(t); \qquad (18.42)$$

compare with (18.39), (18.40). Note that ω_β is necessarily time-invariant, since $\omega_\beta(1\alpha_t(b)) = \omega_\beta(\alpha_t(b)1)$ and by the KMS condition

$$F_{1b}(t) = F_{1b}(t + i\beta). \qquad (18.43)$$

Let us define the $*$-algebra $\mathcal{A}^0$ through smoothing in time with a test function of compact support in Fourier space,

$$\mathcal{A}^0 = \left\{ a_f = \int dt f(t)\alpha_t(a) \,|\, a \in \mathcal{A}, \, \widehat{f} \in C_{00}(\mathbb{R}) \right\}. \qquad (18.44)$$

For $b \in \mathcal{A}^0$, $z \mapsto F_{1b}(z)$ is an entire function bounded as $|F_{1b}(z)| \leq \|\alpha_z(b)\| \leq \|\alpha_{i\,\mathrm{Im}z}(b)\|$. By (18.43) F_{1b} is periodic with period $i\beta$. Hence F_{1b} is bounded and

thus constant by Liouville's theorem, which implies

$$\omega_\beta(\alpha_t(b)) = \omega_\beta(b) \tag{18.45}$$

for all $t \in \mathbb{R}$.

We assume that $\mathcal{A}$ is a simple C^*-algebra, which means that the only two-sided $*$-ideals of $\mathcal{A}$ are either $\{0\}$ or $\mathcal{A}$ itself. The KMS condition then ensures that for every $a \in \mathcal{A}$

$$\omega_\beta(a^*a) = 0 \quad \text{implies} \quad a = 0. \tag{18.46}$$

To prove (18.46) we define $\mathcal{N} = \{a \in \mathcal{A} \,|\, \omega_\beta(a^*a) = 0\}$ with the goal of establishing that $\mathcal{N}$ is a two-sided $*$-ideal. Clearly, if $\omega_\beta(a^*a) = 0$ and $b \in \mathcal{A}$, then

$$\omega_\beta(a^*b^*ba) \leq \omega_\beta(a^*b^*bb^*ba)^{1/2}\omega_\beta(a^*a)^{1/2} = 0 \tag{18.47}$$

by the Schwarz inequality. Hence $\mathcal{A}\mathcal{N} \subset \mathcal{N}$. To show the converse one chooses $b \in \mathcal{A}$. By the KMS condition

$$\omega_\beta(b^*a^*ab) = \omega_\beta((b^*a^*a)b) = \omega_\beta(\alpha_{-\mathrm{i}\beta}(b)b^*a^*a) = 0 \tag{18.48}$$

by the Schwarz inequality as before. Thus $\mathcal{N}\mathcal{A} \subset \mathcal{N}$ and $\mathcal{N}$ is a two-sided $*$-ideal. Since $\mathcal{A}$ is simple, (18.46) follows.

Next we need the analog of $\mathcal{T}_2(\mathcal{H})$ and of the Liouvillean, which is the content of the Gelfand–Naimark–Segal (GNS) construction. The GNS Hilbert space $\mathcal{H}_\beta$ is defined as the completion of $\mathcal{A}$ equipped with the scalar product

$$\langle a|b\rangle = \omega_\beta(a^*b). \tag{18.49}$$

By the argument above $\langle a|a\rangle = 0$ implies $a = 0$, as it should. In our context $\mathcal{H}_\beta$ is a separable Hilbert space. We set $\Omega_\beta = 1$ and define the left representation of $\mathcal{A}$ through

$$\ell(a)b = ab. \tag{18.50}$$

Thereby $\ell(\mathcal{A}) \subset B(\mathcal{H}_\beta)$. In addition we define

$$\mathrm{e}^{-\mathrm{i}t\mathcal{L}}a = \alpha_t a \tag{18.51}$$

on $\mathcal{H}_\beta$. Since $\langle b|\mathrm{e}^{-\mathrm{i}t\mathcal{L}}a\rangle = \omega(b^*\alpha_t a) = \omega(\alpha_{-t}b^*a) = \langle \mathrm{e}^{\mathrm{i}t\mathcal{L}}b|a\rangle$ and since $\langle \mathrm{e}^{-\mathrm{i}t\mathcal{L}}b|\mathrm{e}^{-\mathrm{i}t\mathcal{L}}a\rangle = \omega(\alpha_t(b^*a)) = \langle b|a\rangle$ by time-invariance of ω_β, $\mathrm{e}^{-\mathrm{i}t\mathcal{L}}$ is a strongly continuous unitary group on $\mathcal{H}_\beta$. By Stone's theorem it has a self-adjoint generator, which by definition is the Liouvillean $\mathcal{L}$.

The initial state of interest is a local perturbation of the equilibrium state ω_β. It can be written as

$$\rho(a) = \omega_\beta(b^*ab), \quad b \in \mathcal{A}, \quad \omega_\beta(b^*b) = 1. \tag{18.52}$$

In the GNS representation ρ corresponds to the state given by the vector $b \in \mathcal{H}_\beta$. More generally, a perturbed state can be written as

$$\rho(a) = \sum_{n=1}^{\infty} p_n \omega_\beta(b_n^* a b_n) \tag{18.53}$$

with $b_n \in \mathcal{A}$, $\omega(b_n^* b_n) = 1$, $p_n \geq 0$, $\sum_{n=1}^{\infty} p_n = 1$. States of the form (18.53) are called normal. A state not covered by this class would be a two-temperature state of the photon gas, for example, where the temperature to the far right differs from that to the far left. In fact, its long-time behavior would be rather different from that of the initial states discussed here.

Let ρ be a normal state with time evolved $\rho_t(a) = \rho(\alpha_t(a))$. By relaxation to equilibrium we mean

$$\lim_{t \to \infty} \rho_t(a) = \omega_\beta(a) \tag{18.54}$$

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

Proposition 18.1 (Relaxation to equilibrium as a spectral property). *Suppose the Liouvillean $\mathcal{L}$ has a purely absolutely continuous spectrum except for a nondegenerate eigenvalue at 0. Then for all $a \in \mathcal{A}$*

$$\lim_{t \to \pm\infty} \rho_t(a) = \omega_\beta(a). \tag{18.55}$$

Proof: Since ω_β is time invariant, the (unique) zero eigenvector of $\mathcal{L}$ is Ω_β. By assumption the spectral measure of $\langle \psi | e^{-it\mathcal{L}} \varphi \rangle$ has the point mass $\langle \psi | \Omega_\beta \rangle \langle \Omega_\beta | \varphi \rangle$ at zero and is otherwise absolutely continuous. Therefore by the Riemann–Lebesgue lemma

$$\lim_{t \to \infty} \langle \psi | e^{-it\mathcal{L}} \varphi \rangle = \langle \psi | \Omega_\beta \rangle \langle \Omega_\beta | \varphi \rangle \tag{18.56}$$

for all $\psi, \varphi \in \mathcal{H}_\beta$.

In view of the structure of normal states it suffices to study

$$\begin{aligned}
\omega_\beta(b^* \alpha_t(a) c) &= \omega_\beta\big(\alpha_{-i\beta}(c) b^* \alpha_t(a)\big) \\
&= \langle \ell(b) \ell(\alpha_{i\beta}(c^*)) \Omega_\beta | \ell(\alpha_t(a)) \Omega_\beta \rangle \\
&= \langle \ell(b) \ell(\alpha_{i\beta}(c^*)) \Omega_\beta | e^{-it\mathcal{L}} \ell(a) \Omega_\beta \rangle.
\end{aligned} \tag{18.57}$$

We assume that $a, b, c \in \mathcal{A}^0$, see (18.44). Then $\ell(b) \ell(\alpha_{i\beta}(c^*)) \Omega_\beta, \ell(a) \Omega_\beta \in \mathcal{H}_\beta$. Therefore from (18.56)

$$\begin{aligned}
\lim_{t \to \infty} \omega_\beta(b^* \alpha_t(a) c) &= \langle \ell(b) \ell(\alpha_{i\beta}(c^*)) \Omega_\beta | \Omega_\beta \rangle \langle \Omega_\beta | \ell(a) \Omega_\beta \rangle \\
&= \omega_\beta(\alpha_{-i\beta}(c) b^*) \omega_\beta(a) \\
&= \omega_\beta(b^* c) \omega_\beta(a),
\end{aligned} \tag{18.58}$$

which, upon inserting in (18.53), implies the limit (18.55). Note that the KMS condition is used twice, in the first identity of (18.57) and in the last identity of (18.58).   □

Proposition 18.1 suggests that relaxation to equilibrium can be established in two steps: (i) One has to find for the equilibrium state a sufficiently concrete representation of the algebra of local observables and of the Liouvillean. (ii) The spectral properties of the Liouvillean must be studied. For (i) the natural representation is the Araki–Woods representation of the free photon gas in infinite volume. It will be taken up in the following section. The coupled system is constructed through perturbation series. For the dynamics the time-dependent Dyson series is used and for the thermal state the thermal perturbation theory of section 18.2. Of course, the convergence of both series relies on the atom being modeled as an N-level system and on the explicit control of the free photon gas. Only through the convergence of the perturbation series are we assured of the correct representation spaces for the interacting system. Nevertheless, we skip this important point completely and jump to the spectral analysis of the interacting Liouvillean.

18.4 The Araki–Woods representation of the free photon field

For photons in a cavity Λ, the spectrum of allowed momenta is discrete, $\mathrm{tr}[\exp[-\beta H_{\mathrm{f},\Lambda}]] < \infty$, and the rules of thermal equilibrium for bounded quantum systems are applicable, through which the time-correlations of local observables in the form $\omega_\beta^\Lambda(a\alpha_t^\Lambda(b))$ are defined. A macroscopic cavity with its surface kept at a uniform temperature is extremely well approximated by the infinite-volume limit $\Lambda \uparrow \mathbb{R}^3$. For the Hamiltonian (18.1) the infinite-volume limit of time-correlations can be established. Rather than going through the construction, we merely state the final answer, which will serve as a basis for the study of relaxation.

We work in the momentum space representation. Without risk of confusion we set $k = (k, \lambda) \in \mathbb{R}^3 \times \{1, 2\}$ and $\sum_{\lambda=1,2} \int \mathrm{d}^3 k = \int \mathrm{d}k$, $\delta(k - k') = \delta_{\lambda,\lambda'} \delta(k - k')$. The bosonic field operators are

$$a(f) = \int \mathrm{d}k f(k) a(k) = \sum_{\lambda=1,2} \int \mathrm{d}^3 k f(k, \lambda) a(k, \lambda), \quad a^*(f) = \int \mathrm{d}k f(k) a^*(k)$$

(18.59)

with $f \in \mathcal{S}_0(\mathbb{R}^3 \times \{1, 2\})$, the Schwartz space of functions that decrease rapidly and vanish at $k = 0$. Observe that our convention for the complex conjugation of the test function f differs from that in (13.59), (13.60). Let us also introduce the complex conjugation $\tau f(k) = f(k)^* = \big(f(k, 1)^*, f(k, 2)^*\big)$. Its second

quantization is the anti-unitary time-reversal operator T on $\mathcal{F}$ with the properties

$$T\Omega = \Omega, \quad Ta^{\sharp}(f)T = a^{\sharp}(\tau f), \quad T = T^* = T^{-1}. \qquad (18.60)$$

Note that $(a^*(f))^* = a(\tau f)$ and $\langle f, g \rangle_{\mathfrak{h}} = \int \mathrm{d}k (\tau f) g$. The boson fields satisfy the canonical commutation relations (CCR),

$$[a^*(f), a^*(g)] = 0 = [a(f), a(g)], \qquad (18.61)$$

$$[a(\tau f), a^*(g)] = \langle f, g \rangle_{\mathfrak{h}}. \qquad (18.62)$$

Let $\mathcal{P}$ denote the polynomial $*$-algebra generated by

$$\{a^*(f), a(g) \mid f, g \in \mathcal{S}_0(\mathbb{R}^3)^2\}. \qquad (18.63)$$

On $\mathcal{P}$ the time evolution α_t^{f} is defined through

$$\alpha_t^{\mathrm{f}}(a^*(k)) = \mathrm{e}^{\mathrm{i}t\omega(k)} a^*(k), \quad \alpha_t^{\mathrm{f}}(a(k)) = \mathrm{e}^{-\mathrm{i}t\omega(k)} a(k). \qquad (18.64)$$

The equilibrium state $\omega_{\beta}^{\mathrm{f}}$ of the photon field at inverse temperature β is a quasi-free state on $\mathcal{P}$. Set

$$\rho_{\beta}(k) = \frac{1}{\mathrm{e}^{\beta\omega(k)} - 1}. \qquad (18.65)$$

Then the two-point function is given by

$$\omega_{\beta}^{\mathrm{f}}\big(a^*(\tau f) a(g)\big) = \langle f, \rho_{\beta} g \rangle_{\mathfrak{h}} \qquad (18.66)$$

and all other moments by

$$\omega_{\beta}^{\mathrm{f}}\Big(\prod_{i=1}^{n} a^*(\tau f_i) \prod_{j=1}^{m} a(g_j)\Big) = \delta_{mn} \det\{\langle f_i, \rho_{\beta} g_j \rangle_{\mathfrak{h}}\}_{i,j=1,\dots,n}. \qquad (18.67)$$

$\omega_{\beta}^{\mathrm{f}}$ satisfies the KMS condition as can be seen directly from

$$\begin{aligned}
\omega_{\beta}^{\mathrm{f}}\big(a(k) a^*(k')\big) &= \delta(k - k') + \omega_{\beta}^{\mathrm{f}}\big(a^*(k') a(k)\big) \\
&= \mathrm{e}^{\beta\omega(k)} \rho_{\beta}(k) \delta(k - k') \\
&= \omega_{\beta}^{\mathrm{f}}\big(\alpha_{-\mathrm{i}\beta}^{\mathrm{f}}(a^*(k')) a(k)\big).
\end{aligned} \qquad (18.68)$$

Through the GNS construction the data $(\mathcal{P}, \alpha_t^{\mathrm{f}}, \omega_{\beta}^{\mathrm{f}})$ determine a separable Hilbert space $\mathcal{H}_{\beta}^{\mathrm{f}}$, a left representation ℓ of $\mathcal{P}$ on $\mathcal{H}_{\beta}^{\mathrm{f}}$, a vector $\Omega_{\beta}^{\mathrm{f}} \in \mathcal{H}_{\beta}^{\mathrm{f}}$ cyclic for $\ell(\mathcal{P})$, and a unitary one-parameter group $\mathrm{e}^{-\mathrm{i}t\mathcal{L}_{\mathrm{f}}}$, $t \in \mathbb{R}$, such that

$$\begin{aligned}
\omega_{\beta}^{\mathrm{f}}(a) &= \langle \Omega_{\beta}^{\mathrm{f}} | \ell(a) \Omega_{\beta}^{\mathrm{f}} \rangle \\
\ell(\alpha_t(a)) &= \mathrm{e}^{\mathrm{i}t\mathcal{L}_{\mathrm{f}}} \ell(a) \mathrm{e}^{-\mathrm{i}t\mathcal{L}_{\mathrm{f}}}, \quad a \in \mathcal{P}.
\end{aligned} \qquad (18.69)$$

We follow Araki and Woods to construct, as for a bounded quantum system, an isomorphism I_T between $\mathcal{H}^{\mathrm{f}}_\beta$ and $\mathcal{F} \otimes \mathcal{F}$. On $\mathcal{F} \otimes \mathcal{F}$ we introduce the Bose fields

$$a^\sharp_\ell(f) = a^\sharp(f) \otimes 1, \quad a^\sharp_r(f) = 1 \otimes a^\sharp(\tau f). \tag{18.70}$$

Note that $a^\sharp_r$ is an antilinear representation of the CCR. The isomorphism I_T is then defined through the following relations,

$$I_T \Omega^{\mathrm{f}}_\beta = \Omega \otimes \Omega, \tag{18.71}$$

$$I_T \ell(a(f)) I_T^{-1} = a_\ell(\sqrt{1 + \rho_\beta} f) + a^*_r(\sqrt{\rho_\beta} f), \tag{18.72}$$

$$I_T r(a(f)) I_T^{-1} = a^*_\ell(\sqrt{\rho_\beta} \tau f) + a_r(\sqrt{1 + \rho_\beta} \tau f). \tag{18.73}$$

As it should be, (18.72) is linear and (18.73) is antilinear in f.

$I_T \ell(a^\sharp(f)) I_T^{-1}$ and $I_T r(a^\sharp(f)) I_T^{-1}$ satisfy the CCR and one only has to check that the two-point function is properly transported,

$$\begin{aligned}
&\langle \Omega \otimes \Omega | I_T \ell(a^*(f)) \ell(a(g)) I_T^{-1} \Omega \otimes \Omega \rangle \\
&= \langle \Omega \otimes \Omega | a_r(\sqrt{\rho_\beta} f) a^*_r(\sqrt{\rho_\beta} g) \Omega \otimes \Omega \rangle = \langle \tau f, \rho_\beta g \rangle_{\mathfrak{h}} \\
&= \omega^{\mathrm{f}}_\beta(a^*(f) a(g)) = \langle \Omega^{\mathrm{f}}_\beta | \ell(a^*(f)) \ell(a(g)) \Omega^{\mathrm{f}}_\beta \rangle
\end{aligned} \tag{18.74}$$

and likewise for the right representation. We conclude that, indeed, $I_T : \mathcal{H}^{\mathrm{f}}_\beta \to \mathcal{F} \otimes \mathcal{F}$ is an isometry.

The Liouvillean is transported as $L_{\mathrm{f}} = I_T \mathcal{L}_{\mathrm{f}} I_T^{-1}$. From the bounded systems one would expect that

$$L_{\mathrm{f}} = \int \mathrm{d}k\, \omega(k) \big(a^*_\ell(k) a_\ell(k) - a^*_r(k) a_r(k) \big). \tag{18.75}$$

Then indeed, as required,

$$\mathrm{e}^{\mathrm{i}t L_{\mathrm{f}}} a_\ell(k) \mathrm{e}^{-\mathrm{i}t L_{\mathrm{f}}} = \mathrm{e}^{-\mathrm{i}t \omega(k)} a_\ell(k), \quad \mathrm{e}^{\mathrm{i}t L_{\mathrm{f}}} a_r(k) \mathrm{e}^{-\mathrm{i}t L_{\mathrm{f}}} = \mathrm{e}^{\mathrm{i}t \omega(k)} a_r(k) \tag{18.76}$$

and

$$\mathrm{e}^{\mathrm{i}t L_{\mathrm{f}}} I_T \ell(a(k)) I_T^{-1} \mathrm{e}^{-\mathrm{i}t L_{\mathrm{f}}} = \mathrm{e}^{-\mathrm{i}t \omega(k)} I_T \ell(a(k)) I_T^{-1} = I_T \ell(\alpha_t(a(k))) I_T^{-1}; \tag{18.77}$$

similarly for the right representation.

18.5 Atom in interaction with the photon gas

The atomic Hamiltonian H_{at} has N, possibly degenerate, eigenvalues, $\varepsilon_1 \le \varepsilon_2 \le \cdots \le \varepsilon_N$, and the atomic Hilbert space is $\mathcal{H}_{\mathrm{at}} = \mathbb{C}^N$. We fix a corresponding eigenbasis, $H_{\mathrm{at}} \varphi_j = \varepsilon_j \varphi_j$, $j = 1, \ldots, N$. The algebra of observables is the $N \times N$ complex matrices $\mathcal{M}_N$ and it carries the thermal state $\omega^{\mathrm{at}}_\beta = Z^{-1} \mathrm{e}^{-\beta H_{\mathrm{at}}}$. As long

as there is no interaction we merely tensor the atom with the photon field. The algebra of observables is $\mathcal{M}_N \otimes \mathcal{P}$, the thermal state is

$$\omega_\beta^0 = \omega_\beta^{\mathrm{at}} \otimes \omega_\beta^{\mathrm{f}}, \tag{18.78}$$

and the dynamics is generated by $\alpha_t^0 = \alpha_t^{\mathrm{at}} \otimes \alpha_t^{\mathrm{f}}$. As before, the GNS construction determines a separable Hilbert space $\mathcal{H}_\beta^0$ with cyclic vector Ω_β^0 and a unitary time evolution $\mathrm{e}^{-it\mathcal{L}_0}$. With C denoting complex conjugation in the given basis of $\mathcal{H}_{\mathrm{at}}$, the map $I_0 = I_C \otimes I_T : \mathcal{H}_\beta^0 \to \mathcal{H}_{\mathrm{at}} \otimes \mathcal{H}_{\mathrm{at}} \otimes \mathcal{F} \otimes \mathcal{F} = \widehat{\mathcal{H}}_\beta$ is an isomorphism. In particular, $I_0\Omega_\beta^0 = \widehat{\Omega}_\beta^0$ with

$$\widehat{\Omega}_\beta^0 = \sum_{j=1}^N \mathrm{e}^{-\beta\varepsilon_j} \varphi_j \otimes \varphi_j \otimes \Omega \otimes \Omega. \tag{18.79}$$

The Liouvillean is mapped as

$$I_0\mathcal{L}_0 I_0^{-1} = L_0 = L_{\mathrm{at}} \otimes 1 + 1 \otimes L_{\mathrm{f}}, \quad L_{\mathrm{at}} = H_{\mathrm{at}} \otimes 1 - 1 \otimes H_{\mathrm{at}}. \tag{18.80}$$

The real task is to find out how the interaction is mapped to the Araki–Woods representation space. According to (18.1) one has

$$H_{\mathrm{int}} = Q \cdot E_\varphi = \sum_{\lambda=1,2} \int \mathrm{d}^3k \, \widehat{\varphi}(k)\sqrt{\omega/2}Q \cdot e_\lambda\big(ia(k,\lambda) - ia^*(k,\lambda)\big). \tag{18.81}$$

It is more convenient to slightly generalize from (18.81) as

$$H_{\mathrm{int}} = \int \mathrm{d}k\big(G(k) \otimes a^*(k) + G(k)^* \otimes a(k)\big), \tag{18.82}$$

where $G : \mathbb{R}^3 \times \{1, 2\} \to \mathcal{M}_N$ as a matrix-valued function, with the memo that some specific features of the coupling in (18.81) will be used in the spectral analysis below.

If $G \in \mathcal{S}_0(\mathbb{R}^3 \times \{1, 2\}, \mathcal{M}_N)$ as matrix-valued function, one has $H_{\mathrm{int}} \in \mathcal{M}_N \otimes \mathcal{P}$. Thus the Liouvillean in the GNS space necessarily takes the form

$$\mathcal{L}_\lambda = \mathcal{L}_0 + \lambda\ell(H_{\mathrm{int}}) - \lambda r(H_{\mathrm{int}}) = \mathcal{L}_0 + \lambda\mathcal{L}_{\mathrm{int}} \tag{18.83}$$

and only the transformations (18.72), (18.73) have to be applied, resulting in

$$L_{\mathrm{int}} = I_0\mathcal{L}_{\mathrm{int}}I_0^{-1} \tag{18.84}$$

$$= \int \mathrm{d}k\Big\{\big(\sqrt{1+\rho_\beta}G_\ell(k) - \sqrt{\rho_\beta}\,\overline{G}_r^*(k)\big)a_\ell^*(k)$$

$$+ \big(\sqrt{1+\rho_\beta}G_\ell^*(k) - \sqrt{\rho_\beta}\,\overline{G}_r(k)\big)a_\ell(k)$$

$$+ \big(\sqrt{\rho_\beta}G_\ell^*(k) - \sqrt{1+\rho_\beta}\,\overline{G}_r(k)\big)a_r^*(k)$$

$$+ \big(\sqrt{\rho_\beta}G_\ell(k) - \sqrt{1+\rho_\beta}\,\overline{G}_r^*(k)\big)a_r(k)\Big\}.$$

Here $G_\ell^\sharp = G^\sharp \otimes 1$, $G_r^\sharp = 1 \otimes G^\sharp$, $\overline{G}^\sharp = I_C G^\sharp I_C^{-1}$. Extending the test function notation to matrix-valued test functions, L_{int} may be written more concisely as

$$L_{\text{int}} = a_\ell^*\big(\sqrt{1 + \rho_\beta}\, G_\ell - \sqrt{\rho_\beta}\, \overline{G}_r^*\big) + a_\ell\big(\sqrt{1 + \rho_\beta}\, G_\ell^* - \sqrt{\rho_\beta}\, \overline{G}_r\big)$$
$$+ a_r^*\big(\sqrt{\rho_\beta}\, G_\ell^* - \sqrt{1 + \rho_\beta}\, \overline{G}_r\big) + a_r\big(\sqrt{\rho_\beta}\, G_\ell - \sqrt{1 + \rho_\beta}\, \overline{G}_r^*\big). \quad (18.85)$$

With some effort we thus achieved our goal of writing the Liouvillean for the excitations away from equilibrium. Note that through ρ_β the interaction is temperature-dependent and becomes singular as $\beta \to \infty$, which only reflects the fact that the ground state does not fall into the scheme explained before.

Two problems remain to be sorted out. First, $L_\lambda = L_0 + \lambda L_{\text{int}}$ must generate a unitary time evolution on $\widehat{\mathcal{H}}_\beta$. If

$$\int \mathrm{d}k\big(\omega(k) + \omega(k)^{-3}\big)\|G(k)\|^2 < \infty, \quad (18.86)$$

then the self-adjointness of L_λ follows from the Nelson commutator theorem. Note that for the physical case (18.81) the condition (18.86) translates to $\int \mathrm{d}^3 k |\widehat{\varphi}|^2 (\omega^2 + \omega^{-2}) < \infty$, which is satisfied.

Secondly, the equilibrium state of the interacting system must be represented by a vector in $\widehat{\mathcal{H}}_\beta$. The thermal perturbation theory of section 18.2 tells us that this new vector is formally given by

$$\widehat{\Omega}_\beta^\lambda = (Z_\beta)^{-1/2} \mathrm{e}^{-\beta L_\ell/2} \widehat{\Omega}_\beta^0 = (Z_\beta)^{-1/2} \mathrm{e}^{\beta L_r/2} \widehat{\Omega}_\beta^0, \quad (18.87)$$

where, according to (18.33), (18.85)

$$L_\ell = L_0 + \lambda L_{\text{int}\ell}, \quad L_r = L_0 - \lambda L_{\text{int}r} \quad (18.88)$$

and

$$L_{\text{int}\ell} = a_\ell^*(\sqrt{1 + \rho_\beta}\, G_\ell) + a_\ell(\sqrt{1 + \rho_\beta}\, G_\ell^*) + a_r^*(\sqrt{\rho_\beta}\, G_\ell^*) + a_r(\sqrt{\rho_\beta}\, G_\ell),$$
$$L_{\text{int}r} = a_\ell^*(\sqrt{\rho_\beta}\, \overline{G}_r^*) + a_\ell(\sqrt{\rho_\beta}\, \overline{G}_r) + a_r^*(\sqrt{1 + \rho_\beta}\, \overline{G}_r) + a_r(\sqrt{1 + \rho_\beta}\, \overline{G}_r^*).$$
$$(18.89)$$

$(Z_\beta)^{-1/2}$ normalizes the vector to one. It can be shown that $Z_\beta < \infty$ provided

$$\int \mathrm{d}k(1 + \omega^{-1})\|G(k)\|^2 < \infty. \quad (18.90)$$

Therefore under the condition (18.86), $\widehat{\Omega}_\beta^\lambda \in \widehat{\mathcal{H}}_\beta$.

By construction $L_\lambda \widehat{\Omega}_\beta^\lambda = 0$. Thus L_λ has a zero eigenvector, which does not change under the dynamics and represents the state of global equilibrium. According to Proposition 18.1, we have to make sure that $\widehat{\Omega}_\beta^\lambda$ is the only eigenvector

of L_λ and that apart from the zero eigenvalue, the spectrum is purely absolutely continuous.

18.6 Complex translations

L_f has the full real line as spectrum. Its structure is more easily investigated by switching to spherical coordinates in momentum space and to the corresponding Bose field denoted here by $b(\omega, \widehat{k})$. We set

$$(k, \lambda) = (\omega, \widehat{k}), \quad dk = \omega^2 d\omega d\widehat{k}, \tag{18.91}$$

where $\widehat{k} = (k/|k|, \lambda)$. The right representation in L_f has negative excitation energies, which we associate with $\omega < 0$. Thus the Bose field $b^\sharp(\omega, \widehat{k})$ lives on $\mathbb{R} \times S^2 \times \{1, 2\}$ and is defined by

$$b^\sharp(\omega, \widehat{k}) = \begin{cases} \omega a_\ell^\sharp(k) & \text{for} \quad \omega = |k|, \\ \omega a_r^\sharp(k) & \text{for} \quad \omega = -|k|. \end{cases} \tag{18.92}$$

From the definition of $a_\ell^\sharp$, $a_r^\sharp$ one confirms that b, $b^\sharp$ satisfy the CCR as

$$[b(\omega, \widehat{k}), b(\omega', \widehat{k}')] = 0 = [b^*(\omega, \widehat{k}), b^*(\omega', \widehat{k}')] \tag{18.93}$$

and

$$[b(\omega, \widehat{k}), b^*(\omega', \widehat{k}')] = \delta(\omega - \omega')\delta(\widehat{k} - \widehat{k}'). \tag{18.94}$$

In the new coordinates the Liouvillean becomes

$$L_f = \int_\mathbb{R} d\omega \int_{S^2 \times \{1,2\}} d\widehat{k}\, \omega b^*(\omega, \widehat{k}) b(\omega, \widehat{k}). \tag{18.95}$$

We rewrite the interaction. Let us define the matrix-valued functions

$$F_\ell(\omega, \widehat{k}) = \begin{cases} \omega^{-1/2} G_\ell(k) & \text{for} \quad \omega = |k|, \\ -(-\omega)^{-1/2} G_\ell^*(k) & \text{for} \quad \omega = -|k|, \end{cases} \tag{18.96}$$

$$F_r(\omega, \widehat{k}) = \begin{cases} \omega^{1/2} C G_r^*(k) C & \text{for} \quad \omega = |k|, \\ -(-\omega)^{-1/2} C G_r(k) C & \text{for} \quad \omega = -|k|, \end{cases} \tag{18.97}$$

$$F_\ell^{(\beta)}(\omega, \widehat{k}) = \left(\omega(1 - e^{-\beta\omega})^{-1}\right)^{1/2} F_\ell(\omega, \widehat{k}),$$
$$F_r^{(\beta)}(\omega, \widehat{k}) = \left(-\omega(1 - e^{\beta\omega})^{-1}\right)^{1/2} F_r(\omega, \widehat{k}). \tag{18.98}$$

Then

$$L_{\text{int}} = L_{\text{int}\ell} - L_{\text{int}r} \tag{18.99}$$

with

$$L_{\text{int}\sharp} = \int_{\mathbb{R}} d\omega \int_{S^2 \times \{1,2\}} d\widehat{k} \big(F_\sharp^{(\beta)}(\omega, \widehat{k}) b^*(\omega, \widehat{k}) + F_\sharp^{(\beta)}(\omega, \widehat{k})^* b(\omega, \widehat{k}) \big). \tag{18.100}$$

With (18.95) and the definitions (18.99), (18.100) one concludes

$$L_\lambda = L_{\text{at}} + L_{\text{f}} + \lambda L_{\text{int}} = L_0 + \lambda L_{\text{int}}. \tag{18.101}$$

Since L_{f} has the real line for its continuous spectrum, it is natural to try to move it through a downward translation. The generator T of translations along the ω-axis is given by

$$T = \int d\omega \int d\widehat{k} b^*(\omega, \widehat{k})(-i\partial_\omega) b(\omega, \widehat{k}). \tag{18.102}$$

Let $\theta \in \mathbb{C}$. Then

$$L_0(\theta) = e^{-i\theta T} L_0 e^{i\theta T} = L_{\text{at}} + L_{\text{f}} - \theta N_{\text{f}} \tag{18.103}$$

with the number operator

$$N_{\text{f}} = \int d\omega \int d\widehat{k} b^*(\omega, \widehat{k}) b(\omega, \widehat{k}). \tag{18.104}$$

We set $\theta = i\vartheta$, $\vartheta > 0$. Then $L_0(\theta)$ has $\mathbb{R} - i\vartheta$ as continuous spectrum and the isolated eigenvalues $\{\varepsilon_i - \varepsilon_j \,|\, i, j = 1, \ldots, N\}$ on the real axis.

To be able to apply the theory of complex deformations $\theta \mapsto e^{-i\theta T} L_{\text{int}} e^{i\theta T} = L_{\text{int}}(\theta)$ has to be analytic in a strip around the real axis. $L_{\text{int}}(\theta)$ is obtained by shifting $F_\sharp^{(\beta)}(\omega, \widehat{k})$ in (18.100) to $F_\sharp^{(\beta)}(\omega + \theta, \widehat{k})$. Thus the issue is whether $F_\sharp^{(\beta)}(\omega, \widehat{k})$ extends to an analytic function near the real axis. For the physical coupling

$$G(k, \lambda) = -iQ \cdot e_\lambda \sqrt{\omega/2} \widehat{\varphi}(k). \tag{18.105}$$

By assumption φ is radial and has compact support in position space. Thus $\widehat{\varphi}_{\text{r}}$ is an analytic function on $\mathbb{C}$. Therefore F_ℓ, F_r of (18.96), (18.97) are analytic in ω. The prefactors in (18.98) have simple poles at $\pm 2\pi i\beta n$, $n = 1, 2, \ldots$. We conclude that $F_\sharp^{(\beta)}(\omega, \widehat{k})$ are analytic in ω in the strip $\mathcal{S}_{2\pi/\beta} = \{\theta \,|\, |\text{Im}\,\theta| < 2\pi/\beta\}$. $L_\lambda(\theta) = L_0(\theta) + \lambda L_{\text{int}}(\theta)$ is jointly analytic in λ and $\theta \in \mathcal{S}_{2\pi/\beta}$. To derive this result we used the assumption that the photons have zero mass. Otherwise L_{f} would have a spectral gap and complex translations could not be implemented. We also assumed that there is a $\sqrt{\omega}$ prefactor in the physical coupling. Both assumptions could be
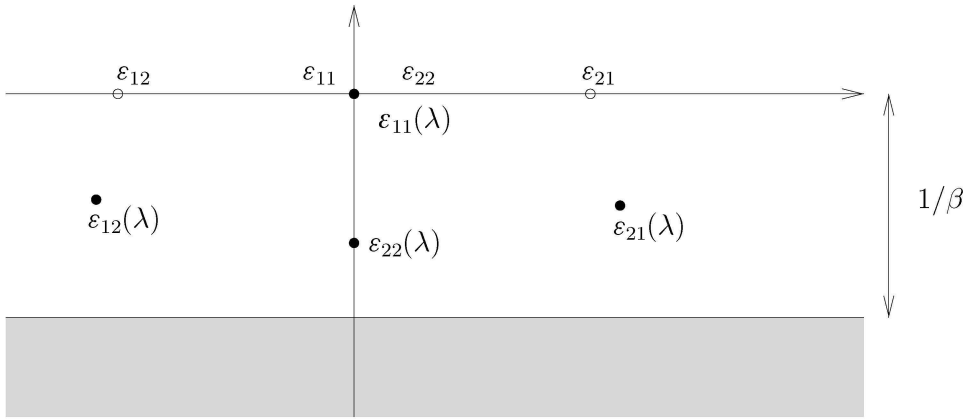
Figure 18.1: Spectrum of the complex translated Liouvillean in the case of a two-level atom for zero and nonzero coupling.

avoided at the expense of a considerably more involved analysis. Note that the width of the strip of analyticity decreases as $1/\beta$ which indicates that our estimates worsen as zero temperature is approached.

We are now in a position to use the considerations from section 17.3 and choose $\theta = i\vartheta$ with ϑ close to the optimal value $2\pi/\beta$. For zero coupling the eigenvalues of $L_0(\theta)$ are $\varepsilon_{ij} = \varepsilon_i - \varepsilon_j$, $i, j = 1, \ldots, N$, see figure 18.1. The zero eigenvalue is at least N-fold degenerate. As the coupling is turned on, $\lambda \neq 0$, the eigenvalues $\varepsilon_{ij}(\lambda)$ move. From the general theory, there is a dense set of vectors, $\mathcal{E} \subset \widehat{\mathcal{H}}_\beta$, such that for $\psi, \varphi \in \mathcal{E}$ the resolvent $\langle \psi | (z - L_\lambda)^{-1} \varphi \rangle$ can be continued analytically from the upper complex plane to $\{z \mid \text{Im} z > -\vartheta\}$. In this domain $\langle \psi | (z - L_\lambda)^{-1} \varphi \rangle$ is analytic except for poles at $z = \varepsilon_{ij}(\lambda)$. Thus $\varepsilon_{ij}(\lambda)$ are the resonance poles of the resolvent. These assertions remain valid up to the first λ when a resonance hits the line $\{z = -i\vartheta\}$. Thereby the theory is restricted up to some maximal coupling λ_0, $|\lambda| < \lambda_0$.

In our convention $\text{Im}\,\varepsilon_{ij}(\lambda) < 0$ corresponds to exponential decay. Thus, since expectation values remain bounded in t, the resonances cannot move in the upper half complex plane. From the thermal perturbation theory we know that at least one eigenvalue remains at 0. Somewhat arbitrarily we label this eigenvalue by $\varepsilon_{11}(\lambda)$. To prove relaxation to equilibrium, according to Proposition 18.1, it must be ensured that all other resonances acquire a strictly negative imaginary part for $\lambda \neq 0$. At this point, second-order perturbation theory comes in handy. We require that the dissipative part $K^\natural$ in (17.32) has a nondegenerate eigenvalue 0. Then $\text{Im}\,\varepsilon_{ij}(\lambda) = \mathcal{O}(\lambda^2)$ and, possibly further reducing λ_0, the second order controls the higher orders, which implies $\text{Im}\,\varepsilon_{ij} < 0$ for $|\lambda| < \lambda_0$, except for $\varepsilon_{11}(\lambda)$.

Theorem 18.2 (Absolute continuity of the spectrum of the Liouvillean). *If $K^{\natural}$ has a simple eigenvalue 0 and if $|\lambda| < \lambda_0$ for sufficiently small λ_0, then L_λ has 0 as a simple eigenvalue. The remainder of the spectrum is absolutely continuous and covers the real line.*

From Theorem 18.2 in conjunction with Proposition 18.1 we conclude that an N-level atom coupled to the photon field relaxes to thermal equilibrium in the long-time limit.

For $|\lambda| < \lambda_0$, the discrete part of $L_\lambda(\theta)$ is cut out through the contour integral

$$\Sigma_\lambda = \oint_\gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} z(z - L_\lambda(\theta))^{-1}, \tag{18.106}$$

where γ is a contour in the complex plane which encircles all eigenvalues $\varepsilon_{ij}(\lambda)$ and stays away from the half-space $\{z \mid \mathrm{Im} z \leq -\vartheta\}$. Σ_λ remains unchanged under small shifts of ϑ. By the same token one can construct two maps $W_\lambda^{\pm}\mathcal{E} \to \mathcal{M}_N$ such that

$$\langle \phi | \mathrm{e}^{-\mathrm{i}t L_\lambda} \psi \rangle = \langle W_\lambda^- \phi | \mathrm{e}^{-\mathrm{i}t \Sigma_\lambda} W_\lambda^+ \psi \rangle + \mathcal{O}(\mathrm{e}^{-\vartheta t}) \tag{18.107}$$

for $t \geq 0$. Equation (18.107) defines the level shift operator Σ_λ. Its eigenvalues are $\varepsilon_{ij}(\lambda)$, $i, j = 1, \ldots, N$. Thus (18.107) establishes *exponentially fast* relaxation to equilibrium for a large class of initial states and of observables.

Our scheme leaves somewhat open how rapidly specific expectation values decay. For example one could prepare the atom in the n-th level and ask how the probability of survival decays as $t \to \infty$. If P_n denotes the projection on the n-th eigenstate φ_n, then the observable under consideration is $P_n \otimes 1$. As initial state one could take the uncorrelated state $P_n \otimes \omega_\beta^{\mathrm{f}}$. A physically more realistic choice would be the state $\omega^{(n)}(a) = \omega_\beta(P_n \otimes 1 a P_n \otimes 1)/\omega_\beta(P_n \otimes 1)$ with ω_β the equilibrium state of the coupled system. The issue is to compute the decay of $\omega^{(n)}(\alpha_t(P_n \otimes 1))$. Equation (18.107) suggests that $\omega^{(n)}(\alpha_t(P_n \otimes 1)) - \omega_\beta(P_n \otimes 1)$ decays exponentially to zero. To verify this one has to find the representation vectors and determine their analytic continuation in θ. In our example the observables do not depend on the field and therefore the representation vectors are in $\mathcal{E}$, which ensures exponential decay.

In specific systems, say only two levels, also the order λ^4 could be computed. Up to errors from $\mathcal{O}(\mathrm{e}^{-\vartheta t})$ the line shape is still a Lorentzian, whose location and width are given with a precision superior to the weak coupling theory.

18.7 Comparison with the weak coupling theory

The weak coupling theory of section 17.2 predicts the decay of atomic expectations in the form

$$\text{tr}[A e^{-\mathrm{i} L_{\mathrm{D}} t}(B \rho_\beta B^*)], \tag{18.108}$$

which is written somewhat differently than before to ease comparison. The trace is over $\mathbb{C}^N$, $A = A^*$ is some atomic observable, $\rho_\beta = Z^{-1} \mathrm{e}^{-\beta H_{\mathrm{at}}}$, $B \rho_\beta B^*$ is the initial density matrix of the atom normalized as $\text{tr}[\rho_\beta B^* B] = 1$, and L_{D} is the Davies generator of (17.68). We assume $\{H, Q_\alpha, \alpha = 1, 2, 3\}' = \mathbb{C}1$ and the Wiener condition $\Gamma(\omega) > 0$ for all ω. Then (18.108) converges exponentially fast to the thermal equilibrium expectation of A, $\text{tr}[\rho_\beta A]$, independently of the choice of B.

In the full microscopic theory the expectation in spirit closest to (18.108) is given by

$$\omega_\beta(B^* \otimes 1 \alpha_t^\lambda (A \otimes 1) B \otimes 1), \tag{18.109}$$

where, as before, ω_β is the thermal state of the coupled system and α_t^λ is the time evolution with Liouvillean (18.83). From the thermal perturbation theory one concludes that there exists a local operator c such that $\omega_\beta(B^* \otimes 1 a B \otimes 1) = \omega_\beta(ca)$ for all $a \in \mathcal{M}_N \otimes \mathcal{A}$. Thus

$$\omega_\beta(B^* \otimes 1 \alpha_t^\lambda (A \otimes 1) B \otimes 1) = \omega_\beta(c \alpha_t^\lambda (A \otimes 1)). \tag{18.110}$$

Since $B \otimes 1$, $A \otimes 1$ are atomic observables, in the GNS representation c and $A \otimes 1$ become vectors in $\mathcal{E}$. Therefore the long-time behavior of the expectation in (18.109) is determined by the resonances $\varepsilon_{ij}(\lambda)$. If $|\lambda| < \lambda_0$, then $\text{Im}\,\varepsilon_{ij}(\lambda) < 0$ except for $ij = 11$ when $\varepsilon_{11}(\lambda) = 0$. Thus also the expectation value in (18.109) decays exponentially fast to its equilibrium value $\omega_\beta(A \otimes 1)$.

Optimally, one would like to compare (18.108) and (18.109) for small λ. The form (18.108) is a sum of N^2 exponentials, decaying except for one constant term. Likewise, (18.109) is a sum of N^2 exponentials plus an error which has an even faster exponential decay independent of λ and can be neglected for small λ. Most naturally, amplitudes and decay rates are compared. The amplitudes differ by order λ^2, since from the thermal perturbation theory $\omega_\beta(A \otimes 1) = \text{tr}[\rho_\beta A] + \mathcal{O}(\lambda^2)$ using that $\omega_\beta^{\mathrm{f}}(E) = 0$.

The decay rates for (18.108) are the eigenvalues of L_{D}. The eigenvalues of $L_{\mathrm{at}} = [H_{\mathrm{at}}, \cdot]$ are $\varepsilon_i - \varepsilon_j = \varepsilon_{ij}$, $i, j = 1, \ldots, N$. Since L_{at} and $\mathrm{i} K^\natural$ commute, L_{D} is block diagonal with respect to the eigenvalues of L_{at}. The eigenvalues $\varepsilon_{ij}^{\mathrm{D}}$ of L_{D}

are then necessarily of the form

$$\varepsilon_{ij}^{\mathrm{D}} = \varepsilon_{ij} + \lambda^2 \varepsilon_{ij}^{\natural} \tag{18.111}$$

with $\varepsilon_{ij}^{\natural}$ the eigenvalues of $\mathrm{i}K^{\natural}$ and they cluster at the eigenvalues of L_{at}. $\mathrm{i}K^{\natural}$ decomposes as

$$\mathrm{i}K^{\natural}\rho = [H_{\Delta}, \rho] + \mathrm{i}K_{\mathrm{d}}^{\natural}\rho \tag{18.112}$$

with H_{Δ} given by (17.69). $[H_{\Delta}, H_{\mathrm{at}}] = 0$ by construction. H_{Δ} shifts the atomic levels and lifts possible degeneracies of H_{at}. $K_{\mathrm{d}}^{\natural}$ and L_{at} also commute. By detailed balance $K_{\mathrm{d}}^{\natural}$ is symmetric with respect to the weighted inner product $\mathrm{tr}[\rho_{\beta} A^* B]$. Thus the eigenvalues of $K_{\mathrm{d}}^{\natural}$ are negative, real, and with a nondegenerate eigenvalue at 0. In general, $[H_{\Delta}, \cdot]$ and $\mathrm{i}K_{\mathrm{d}}^{\natural}$ do not commute. If, however, the eigenvalues of H_{at} are nondegenerate, then they do and the eigenvalues of $[H_{\Delta}, \cdot]$ and $\mathrm{i}K_{\mathrm{d}}^{\natural}$ can simply be added.

As explained the decay rates for (18.109) are determined by the resonances $\varepsilon_{ij}(\lambda)$. As a basic result one obtains that

$$|\varepsilon_{ij}(\lambda) - \varepsilon_{ij}^{\mathrm{D}}| = \mathcal{O}(\lambda^3), \tag{18.113}$$

where the naive error $\mathcal{O}(\lambda^4)$ is reduced because of possible crossings of eigenvalues. In the weak coupling theory there is some freedom in choosing the generator. For example, K and $K^{\natural}$ cannot be distinguished, see (17.28), (17.31). The nonperturbative theory of resonances identifies $K^{\natural}$ as the optimal small-λ limit. Any other version, like K, would have eigenvalues in general different from $K^{\natural}$, and its eigenvalues could thus not satisfy the bound (18.113).

Notes and references

Sections 18.1–18.6

These sections are based on the first part of Bach, Fröhlich and Sigal (2000). Jakšić and Pillet (1995, 1996a, 1996b, 1997) establish the relaxation to thermal equilibrium with the help of complex translations of the Liouvillean. Their method can be extended to the case when the small system is coupled to several reservoirs at distinct temperatures (Jakšić and Pillet 2002). By more sophisticated techniques one can control the analytic continuation of the resolvent uniformly in β (Bach, Fröhlich and Sigal 2000). Dereziński and Jakšić (2003a) use an infinitesimal version based on Mourre-type estimates. Such a technique has been used before in the simplification of the spin-boson Hamiltonian (Hübner and Spohn 1995b). Positive

commutator techniques are employed by Merkli (2001). Dereziński, Jakšić and Pillet (2003) systematically develop the W^*-algebraic approach.

The standard reference on the algebraic formulation of quantum statistical mechanics is Bratteli and Robinson (1987, 1997); see also Sewell (1986) for a more gentle introduction. The representation theory for the free Bose gas is due to Araki and Woods (1963). A very readable introduction to free quantum gases in the frame of the algebraic approach is Dubin (1974).

Within the thermal context also the translation-invariant model (15.15) is of considerable interest. The initial state can be taken to be factorized as $\rho \otimes \omega_\beta^f$, with ρ some density matrix of the electron. For small coupling, the electron has a rate proportional to λ^2 to be scattered by the photons. The collisions are approximately independent and result in a finite energy and momentum transfer. Between consecutive collisions the electron travels freely. Such a situation is well approximated by a classical linear Boltzmann equation. Only the jump rates know about the quantum nature of the electron. We refer to Spohn (1978), Erdös and Yau (1998, 2000), and Erdös (2002). Transport of independent electrons by scattering either through phonons or through impurities is discussed in Fujita (1966) and Vollhardt and Wölfle (1980).

Section 18.7

Jakšić and Pillet (1997) and Dereziński and Jakšić (2003a) introduce the level shift operator Σ_λ. Dereziński and Jakšić (2003b) discuss in more detail the relation to the weak coupling theory. If one defines $\tilde{L}_D A = (\rho_\beta)^{-1/2} L_D^*((\rho_\beta)^{1/2}A)$, then they establish that $\|\Sigma_\lambda - \tilde{L}_D\| = \mathcal{O}(\lambda^3)$.