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On the asymptotic behavior of solutions to a class of grand canonical master equations

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Abstract

In this article we investigate the long-time behavior of solutions to a class of infinitely many master equations defined from transition rates that are suitable for the description of a quantum system approaching thermodynamical equilibrium with a heat bath at fixed temperature and a reservoir consisting of one species of particles characterized by a fixed chemical potential. We do so by proving a result which pertains to the spectral resolution of the semigroup generated by the equations, whose infinitesimal generator is realized as a trace-class self-adjoint operator defined in a suitably weighted sequence space. This allows us to prove the existence of global solutions which all stabilize toward the grand canonical equilibrium probability distribution as the time variable becomes large, some of them doing so exponentially rapidly. When we set the chemical potential equal to zero, the stability statements continue to hold in the sense that all solutions converge toward the Gibbs probability distribution of the canonical ensemble which characterizes the equilibrium of the given system with a heat bath at fixed temperature.

Keywords:

Long Time Behavior, Master Equations

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Abbreviated Title:

Time evolution and master equations

1 Introduction and outline

It is well known that the grand canonical ensemble of statistical mechanics provides a formalism suitable for the description of the properties of classical or quantum systems in thermodynamical equilibrium with a heat bath at a fixed temperature and a reservoir of possibly different species of particles, each of which being characterized by a chemical potential (see, e.g., [1] and [10] for definitions and applications of the above notions in various concrete situations). From the microscopic properties of the systems it is then possible in principle to derive all their macroscopic thermodynamical properties by means of the so-called grand canonical partition function, which depends on the temperature and on the chemical potentials we alluded to above. In order to achieve that for systems that are not in thermodynamical equilibrium initially, an important link may be provided by the solutions to certain master equations. In the simplest setting of a system described by a Hamiltonian having a discrete point spectrum, those solutions represent time-dependent probabilities which determine the chance for jumps to occur between the various quantum states. They also play a significant role in the stochastic approach to equilibrium and non equilibrium thermodynamics of chemical reactions (see, e.g., the theory and the applications developed in [13], [14] and their numerous references, as well as in Chapter V of [15]. For the investigation of master equations in a different or more general context with many important applications we also refer the reader to [3]-[7], [9], [11] and [12]).

It is precisely the long-time behavior of solutions to a class of various initial-value problems for infinitely many master equations which is the main theme of this article. The class in question is associated with sequences of real numbers (λ_m) and of non-negative integers (N_m) indexed by $m \in \mathbb{N}^+$, where the former may be interpreted for instance as the point spectrum of some Hamiltonian and the latter as the sequence of number of particles of a single species in the corresponding quantum states. More specifically, we organize the remaining part of this article in the following way: in Section 2 we define the relevant initial value problems in which the transition rates depending on (λ_m) and (N_m) are chosen in such a way that the so-called detailed balance conditions of statistical mechanics hold with respect to the grand canonical equilibrium probability distribution. We then interpret the master equations as a dynamical system defined on a suitable infinite-dimensional weighted sequence space, which allows us to realize the infinitesimal generator of the system as a trace-class self-adjoint operator whose spectral properties we investigate in detail. In particular, we prove there a localization principle for all of its eigenvalues and note the absence of a spectral gap around the zero eigenvalue. This eventually leads us to the spectral resolution of the corresponding semigroup whose consequences we analyze in Section 3, where we show that the system of master equations we consider possesses global solutions which all stabilize toward the grand canonical equilibrium probability distribution as the time variable becomes large, some of them doing so exponentially rapidly. In the important particular case where the chemical potential is set equal to zero, the stability statements remain true in that all

solutions converge toward the Gibbs equilibrium probability distribution of the canonical ensemble, some of them again exponentially rapidly. Finally, we also consider there a concrete example involving the quantum harmonic oscillator which shows how the decay properties of the Fourier coefficients of the initial conditions can impact on the speed of convergence of the solutions, ending up with power-law and even logarithmic rates of decay.

We conclude this introduction by noting that the mere idea of making the generator of a system of master equations a formally self-adjoint operator by using the detailed balance conditions already appears as a set of remarks scattered in Chapter V of [15]. As we shall see below, the method of investigation we use in this article represents a systematic and rigorous implementation of those remarks in a very specific context.

2 On the spectral resolution of the semigroup generated by a class of master equations

As outlined in the introduction, we start out with a sequence of real numbers (λ_m) and of non-negative integers (N_m) indexed by $m \in \mathbb{N}^+$, such that the grand canonical partition function satisfies

$$\Theta_{\beta,\mu} := \sum_{m=1}^{+\infty} \exp[-\beta(\lambda_m - \mu N_m)] < +\infty \quad (1)$$

for each $\beta > 0$ and every $\mu \in \mathbb{R}$, where β may be interpreted as the inverse temperature and μ as the chemical potential. By means of (1) we then define the grand canonical equilibrium probabilities by

$$p_{\beta,\mu,m} := \Theta_{\beta,\mu}^{-1} \exp[-\beta(\lambda_m - \mu N_m)] \quad (2)$$

for each $m \in \mathbb{N}^+$, and with every such m we associate the class of initial-value problems for master equations of the form

$$\begin{aligned} \frac{dp_m(\tau)}{d\tau} &= \sum_{n=1}^{+\infty} (r_{m,n} p_n(\tau) - r_{n,m} p_m(\tau)), \quad \tau \in [0, +\infty), \\ p_m(0) &= p_m^* \end{aligned} \quad (3)$$

where (p_m^*) stands for any sequence of initial-data satisfying

$$p_m^* \geq 0, \quad \sum_{m=1}^{+\infty} p_m^* = 1. \quad (4)$$

In (3) the transition rates $r_{m,n} > 0$ from level n to level m are chosen in such a way that the so-called detailed balance conditions

$$r_{m,n} p_{\beta,\mu,n} = r_{n,m} p_{\beta,\mu,m} \quad (5)$$

are satisfied for each $\beta > 0$, every $\mu \in \mathbb{R}$ and all $m, n \in \mathbb{N}^+$. In this manner the $p_{\beta, \mu, m}$ provide a time-independent solution to (3) when we choose $p_m^* = p_{\beta, \mu, m}$ for every m , in addition to the fact that they make the corresponding entropy production as defined in [12] equal to zero (see also, e.g., Section II A in [13] for a thorough discussion of this point). Therefore, they do provide genuine equilibrium probabilities indeed. Furthermore, owing to (2) we may rewrite (5) as

$$\frac{r_{m,n}}{r_{n,m}} = \exp[-\beta(\lambda_m - \lambda_n) + \beta\mu(N_m - N_n)], \quad (6)$$

which is the starting point for the analysis of chemical reactions by means of stochastic thermodynamics put forward in [14] (see, in particular, Section III of that article). In particular we may take

$$r_{m,n} = c_{m,n} \exp\left[-\frac{\beta}{2}(\lambda_m - \lambda_n) + \frac{\beta\mu}{2}(N_m - N_n)\right] \quad (7)$$

where the prefactors stand for any choice of real coefficients satisfying the symmetry condition $c_{m,n} = c_{n,m}$ for all $m, n \in \mathbb{N}^+$. In what follows we investigate (3) as a dynamical system on a suitable weighted sequence space with rates of the form (7), which requires a specific and of course non unique choice of the $c_{m,n}$ to ensure that the dynamical system in question be well defined. In fact, in order to keep our upcoming computations as simple as possible we shall settle for

$$c_{m,n} = \exp[-\beta(\lambda_m + \lambda_n) - \beta\mu(N_m + N_n)], \quad (8)$$

which will play the role of convergence factors in Proposition 1 below as we shall soon explain. Thus, let us denote by $l_{\mathbb{C}, w_{\beta, \mu}}^2$ the set of all complex sequences $\mathbf{p} := (p_m)$ satisfying

$$\|\mathbf{p}\|_{2, w_{\beta, \mu}}^2 := \sum_{m=1}^{+\infty} w_{\beta, \mu, m} |p_m|^2 < +\infty \quad (9)$$

where $w_{\beta, \mu, m} := \exp[\beta(\lambda_m - \mu N_m)]$, which becomes a complex separable Hilbert space when endowed with the usual operations and the sesquilinear form

$$(\mathbf{p}, \mathbf{q})_{2, w_{\beta, \mu}} := \sum_{m=1}^{+\infty} w_{\beta, \mu, m} p_m \bar{q}_m \quad (10)$$

defined with respect to the weight sequence $w_{\beta, \mu} := (w_{\beta, \mu, m})$. Furthermore, let us reformulate (3) as

$$\begin{aligned} \frac{dp_m(\tau)}{d\tau} &= \sum_{n=1}^{+\infty} a_{m,n} p_n(\tau), \quad \tau \in [0, +\infty), \\ p_m(0) &= p_m^* \end{aligned} \quad (11)$$

where

$$a_{m,n} = \begin{cases} -\sum_{k=1, k \neq m}^{+\infty} r_{k,m} & \text{for } m = n, \\ r_{m,n} & \text{for } m \neq n. \end{cases} \quad (12)$$

Then the following preliminary result holds, which is interesting in its own right:

Proposition 1. *For each $\mathfrak{p} \in l_{\mathbb{C}, w_{\beta, \mu}}^2$, the expression*

$$(A\mathfrak{p})_{\mathfrak{m}} := \sum_{n=1}^{+\infty} a_{\mathfrak{m}, n} p_n \quad (13)$$

defines a linear, self-adjoint trace-class operator $A : l_{\mathbb{C}, w_{\beta, \mu}}^2 \mapsto l_{\mathbb{C}, w_{\beta, \mu}}^2$ whose trace is given by

$$\text{Tr } A = \Theta_{2\beta, -\mu} - \Theta_{\frac{\beta}{2}, -3\mu} \Theta_{\frac{3\beta}{2}, -\frac{\mu}{3}} < 0. \quad (14)$$

Proof. We begin by showing that A is a bounded operator. Rewriting (13) as

$$(A\mathfrak{p})_{\mathfrak{m}} = \sum_{n=1}^{+\infty} \left(a_{\mathfrak{m}, n} w_{\beta, \mu, n}^{-\frac{1}{2}} \right) \left(w_{\beta, \mu, n}^{\frac{1}{2}} p_n \right)$$

and using the Cauchy-Schwarz inequality we first obtain

$$\|A\mathfrak{p}\|_{2, w_{\beta, \mu}}^2 \leq \sum_{\mathfrak{m}=1}^{+\infty} w_{\beta, \mu, \mathfrak{m}} \sum_{n=1}^{+\infty} w_{\beta, \mu, n}^{-1} |a_{\mathfrak{m}, n}|^2 \times \|\mathfrak{p}\|_{2, w_{\beta, \mu}}^2. \quad (15)$$

Furthermore, using (12) we may write and estimate the right-hand side in (15) as

$$\begin{aligned} & \sum_{\mathfrak{m}=1}^{+\infty} w_{\beta, \mu, \mathfrak{m}} \sum_{n=1}^{+\infty} w_{\beta, \mu, n}^{-1} |a_{\mathfrak{m}, n}|^2 \\ &= \sum_{\mathfrak{m}=1}^{+\infty} \left(|a_{\mathfrak{m}, \mathfrak{m}}|^2 + w_{\beta, \mu, \mathfrak{m}} \sum_{n=1, n \neq \mathfrak{m}}^{+\infty} w_{\beta, \mu, n}^{-1} r_{\mathfrak{m}, n}^2 \right) \\ &\leq \sum_{\mathfrak{m}=1}^{+\infty} \left(\left(\sum_{n=1}^{+\infty} r_{\mathfrak{m}, n} \right)^2 + w_{\beta, \mu, \mathfrak{m}} \sum_{n=1}^{+\infty} w_{\beta, \mu, n}^{-1} r_{\mathfrak{m}, n}^2 \right). \end{aligned} \quad (16)$$

In addition, putting (8) into (7) gives

$$r_{\mathfrak{m}, n} = \exp \left[-\frac{\beta}{2} (3\lambda_{\mathfrak{m}} + \mu N_{\mathfrak{m}}) - \frac{\beta}{2} (\lambda_n + 3\mu N_n) \right], \quad (17)$$

so that by taking (1) and the expression for $w_{\beta, \mu, \mathfrak{m}}$ into account we obtain

$$\sum_{n=1}^{+\infty} r_{\mathfrak{m}, n} = \Theta_{\frac{3\beta}{2}, -\frac{\mu}{3}} \exp \left[-\frac{\beta}{2} (\lambda_{\mathfrak{m}} + 3\mu N_{\mathfrak{m}}) \right]$$

and

$$\sum_{n=1}^{+\infty} w_{\beta, \mu, n}^{-1} r_{\mathfrak{m}, n}^2 = \Theta_{2\beta, -\mu} \exp \left[-\beta (3\lambda_{\mathfrak{m}} + \mu N_{\mathfrak{m}}) \right].$$

The substitution of these expressions into the last line of (16) and a straight-forward computation then lead to the estimate

$$\sum_{m=1}^{+\infty} w_{\beta,\mu,m} \sum_{n=1}^{+\infty} w_{\beta,\mu,n}^{-1} |a_{m,n}|^2 \leq \Theta_{\beta,-3\mu} \Theta_{\frac{3\beta}{2},-\frac{\mu}{3}}^2 + \Theta_{2\beta,-\mu}^2 < +\infty, \quad (18)$$

which proves that A is indeed a bounded operator.

Next, we observe that the detailed balance conditions (5) may be rewritten as

$$a_{m,n} w_{\beta,\mu,m} = a_{n,m} w_{\beta,\mu,n}$$

for all $m, n \in \mathbb{N}^+$, which immediately implies the relation

$$(Ap, q)_{2, w_{\beta,\mu}} = \sum_{m,n=1}^{+\infty} w_{\beta,\mu,m} a_{m,n} p_n \bar{q}_m = \sum_{m,n=1}^{+\infty} w_{\beta,\mu,n} a_{n,m} p_n \bar{q}_m = (p, Aq)_{2, w_{\beta,\mu}}$$

so that A is self-adjoint.

In order to prove that A is trace-class let us introduce the sequence of canonical vectors (\mathbf{e}_m) given by $(\mathbf{e}_m)_n = \delta_{m,n}$ for all $m, n \in \mathbb{N}^+$, and let us consider the sequence defined by $\mathbf{f}_m = w_{\beta,\mu,m}^{-\frac{1}{2}} \mathbf{e}_m$ for each $m \in \mathbb{N}^+$. From this and (10) it follows immediately that the \mathbf{f}_m form an orthonormal system in $l_{\mathbb{C}, w_{\beta,\mu}}^2$. Moreover we have $(\mathbf{f}_m, \mathbf{q})_{2, w_{\beta,\mu}} = w_{\beta,\mu,m}^{\frac{1}{2}} \bar{q}_m$ for every $\mathbf{q} \in l_{\mathbb{C}, w_{\beta,\mu}}^2$, so that if $(\mathbf{f}_m, \mathbf{q})_{2, w_{\beta,\mu}} = 0$ for each m then $\mathbf{q} = 0$. Therefore the \mathbf{f}_m constitute an orthonormal basis in $l_{\mathbb{C}, w_{\beta,\mu}}^2$, and furthermore a direct computation shows that

$$(A\mathbf{f}_m, \mathbf{f}_n)_{2, w_{\beta,\mu}} = w_{\beta,\mu,n}^{\frac{1}{2}} a_{n,m} w_{\beta,\mu,m}^{-\frac{1}{2}} \quad (19)$$

for all $m, n \in \mathbb{N}^+$. For any orthonormal basis (\mathbf{g}_m) in $l_{\mathbb{C}, w_{\beta,\mu}}^2$ we now have

$$A\mathbf{g}_m = \sum_{j=1}^{+\infty} (\mathbf{g}_m, \mathbf{f}_j)_{2, w_{\beta,\mu}} A\mathbf{f}_j$$

after expanding each \mathbf{g}_m along the basis (\mathbf{f}_j) . In this manner we obtain

$$(A\mathbf{g}_m, \mathbf{g}_m)_{2, w_{\beta,\mu}} = \sum_{j,k=1}^{+\infty} w_{\beta,\mu,k}^{\frac{1}{2}} a_{k,j} w_{\beta,\mu,j}^{-\frac{1}{2}} (\mathbf{g}_m, \mathbf{f}_j)_{2, w_{\beta,\mu}} (\mathbf{f}_k, \mathbf{g}_m)_{2, w_{\beta,\mu}}$$

according to (19), so that the estimate

$$\begin{aligned} & \sum_{m=1}^{+\infty} \left| (A\mathbf{g}_m, \mathbf{g}_m)_{2, w_{\beta,\mu}} \right| \\ & \leq \frac{1}{2} \sum_{j,k=1}^{+\infty} w_{\beta,\mu,k}^{\frac{1}{2}} |a_{k,j}| w_{\beta,\mu,j}^{-\frac{1}{2}} \sum_{m=1}^{+\infty} \left(\left| (\mathbf{g}_m, \mathbf{f}_j)_{2, w_{\beta,\mu}} \right|^2 + \left| (\mathbf{g}_m, \mathbf{f}_k)_{2, w_{\beta,\mu}} \right|^2 \right) \quad (20) \\ & = \sum_{j,k=1}^{+\infty} w_{\beta,\mu,k}^{\frac{1}{2}} |a_{k,j}| w_{\beta,\mu,j}^{-\frac{1}{2}} \end{aligned}$$

holds. The last equality in (20) follows from the expansion of each f_j along the basis (\mathbf{g}_m) , which entails the relation

$$\sum_{m=1}^{+\infty} \left| (\mathbf{g}_m, f_j)_{2, w_{\beta, \mu}} \right|^2 = \|f_j\|_{2, w_{\beta, \mu}}^2 = 1$$

for every $j \in \mathbb{N}^+$. According to (12) we then have

$$\begin{aligned} & \sum_{k=1}^{+\infty} w_{\beta, \mu, k}^{\frac{1}{2}} \sum_{j=1}^{+\infty} |a_{k,j}| w_{\beta, \mu, j}^{-\frac{1}{2}} \\ &= \sum_{k=1}^{+\infty} \left(|a_{k,k}| + w_{\beta, \mu, k}^{\frac{1}{2}} \sum_{j=1, j \neq k}^{+\infty} r_{k,j} w_{\beta, \mu, j}^{-\frac{1}{2}} \right) \\ &\leq \sum_{k=1}^{+\infty} \left(\sum_{j=1}^{+\infty} r_{j,k} + w_{\beta, \mu, k}^{\frac{1}{2}} \sum_{j=1}^{+\infty} r_{k,j} w_{\beta, \mu, j}^{-\frac{1}{2}} \right) < +\infty \end{aligned}$$

for the right-hand side of the equality in (20), where we used (17) and computations similar to those leading to (18) to prove convergence. The series

$$\sum_{m=1}^{+\infty} (A\mathbf{g}_m, \mathbf{g}_m)_{2, w_{\beta, \mu}}$$

is therefore itself convergent and since the orthonormal basis (\mathbf{g}_m) was arbitrary we may conclude that A is trace-class, with

$$\mathrm{Tr} A = \sum_{m=1}^{+\infty} (Af_m, f_m)_{2, w_{\beta, \mu}} = \sum_{m=1}^{+\infty} a_{m,m} = - \sum_{m=1}^{+\infty} \sum_{n=1, n \neq m}^{+\infty} r_{n,m}$$

as a consequence of (12) and (19), which eventually leads to (14). \blacksquare

REMARK. Had we chosen (7) for the rates with $c_{m,n} = 1$ for all $m, n \in \mathbb{N}^+$ instead of (17), some of the series in the proof of Proposition 1 would have been divergent, for instance the very last series on the right-hand side of (16). That is the reason why we referred to (8) as convergence factors.

In what follows we state and prove the main result of this section, in which we investigate in detail the spectral properties of A including in particular a principle of localization of the eigenvalues, from which we obtain the spectral resolution of the semigroup generated by A . In this context the sequence (b_m) given by

$$b_m = \Theta_{\frac{3\beta}{2}, -\frac{\mu}{3}} \exp \left[-\frac{\beta}{2} (\lambda_m + 3\mu N_m) \right] \quad (21)$$

plays an important role.

Theorem 1. *Let A be the operator defined by (13). Then the spectrum of A , $\sigma(A)$, is a discrete compact set with infinitely many real elements (ν_k) indexed by $k \in \mathbb{N}^+$, which are all eigenvalues including $\nu_1 = 0$.*

Assuming in addition that

$$\lambda_{m+1} - \lambda_m > 3\mu (\mathbf{N}_m - \mathbf{N}_{m+1}) \quad (22)$$

for every $m \in \mathbb{N}^+$, the following two statements also hold:

(a) *Each eigenvalue of A is simple and the corresponding eigenspace is spanned by $\hat{\mathbf{p}}_k = (\hat{p}_{k,m})$ where*

$$\hat{p}_{k,m} = \frac{\exp\left[-\frac{\beta}{2}(3\lambda_m + \mu\mathbf{N}_m)\right]}{\nu_k + b_m}.$$

Moreover, each such an eigenvalue is implicitly characterized by the relation

$$\sum_{m=1}^{+\infty} \frac{\exp[-\beta(3\lambda_m + \mu\mathbf{N}_m)]}{\nu_k + b_m} = 1. \quad (23)$$

Furthermore, the set of normalized eigenvectors given by

$$\hat{\mathbf{q}}_k := \frac{\hat{\mathbf{p}}_k}{\|\hat{\mathbf{p}}_k\|_{2,\mathbf{w}_{\beta,\mu}}}$$

for every $k \in \mathbb{N}^+$ constitutes an orthonormal basis of $l_{\mathbb{C},\mathbf{w}_{\beta,\mu}}^2$.

(b) *If the nonzero eigenvalues of A are ordered as $\nu_k < \nu_{k+1}$ for every $k \in \{2, 3, \dots\}$, then they are localized according to*

$$\nu_k \in (-b_{k-1}, -b_k) \quad (24)$$

for every such k . In particular, all the nonzero elements of $\sigma(A)$ are negative and furthermore, for every $\mathbf{p} \in l_{\mathbb{C},\mathbf{w}_{\beta,\mu}}^2$ we have the norm-convergent spectral resolution

$$\exp[\tau A] \mathbf{p} = \sum_{k=1}^{+\infty} (\mathbf{p}, \hat{\mathbf{q}}_k)_{2,\mathbf{w}_{\beta,\mu}} \exp[\tau \nu_k] \hat{\mathbf{q}}_k \quad (25)$$

of the semigroup $\exp[\tau A]_{\tau \in [0, +\infty)}$ generated by A .

Proof. From (2) it is straightforward to check that $\mathbf{p}_{\beta,\mu} := (p_{\beta,\mu,m}) \in l_{\mathbb{C},\mathbf{w}_{\beta,\mu}}^2$. Moreover, we infer from Proposition 1 that A is a compact self-adjoint operator in $l_{\mathbb{C},\mathbf{w}_{\beta,\mu}}^2$, which implies in particular the very first statement of the theorem since we have

$$A\mathbf{p}_{\beta,\mu} = 0$$

as a consequence of (5), (12) and (13).

As for the proof of Statement (a), we first note that the eigenvalue equation

$$A\mathbf{p} = \nu_k \mathbf{p}$$

is equivalent to having the relation

$$\sum_{n=1}^{+\infty} r_{m,n} p_n = \left(\nu_k + \sum_{n=1}^{+\infty} r_{n,m} \right) p_m \quad (26)$$

satisfied for all $m, k \in \mathbb{N}^+$. We then use (17) in (26) to get

$$c_{\mathbf{p},\beta,\mu} \exp \left[-\frac{\beta}{2} (3\lambda_m + \mu N_m) \right] = (\nu_k + b_m) p_m \quad (27)$$

where we took (21) into account and defined

$$c_{\mathbf{p},\beta,\mu} := \sum_{n=1}^{+\infty} \exp \left[-\frac{\beta}{2} (3\lambda_n + \mu N_n) \right] p_n. \quad (28)$$

Now for any $\mathbf{p} \in l_{\mathbb{C},w_{\beta,\mu}}^2$ we evidently have either $c_{\mathbf{p},\beta,\mu} \neq 0$ or $c_{\mathbf{p},\beta,\mu} = 0$. In the first case Relation (27) implies that $(\nu_k + b_m) p_m \neq 0$ for each $m \in \mathbb{N}^+$, so that we may solve for p_m and get

$$p_{k,m} = c_{\mathbf{p}_{k,\beta,\mu}} \hat{p}_{k,m} \quad (29)$$

where

$$\hat{p}_{k,m} := \frac{\exp \left[-\frac{\beta}{2} (3\lambda_m + \mu N_m) \right]}{\nu_k + b_m}. \quad (30)$$

Moreover, with the $\hat{p}_{k,m}$ given by (30) we claim that $\hat{\mathbf{p}}_k := (\hat{p}_{k,m}) \in l_{\mathbb{C},w_{\beta,\mu}}^2$. On the one hand, this is clear if $\nu_k = 0$ for then (30) reduces to $\mathbf{p}_{\beta,\mu}$ up to a trivial multiplicative constant. On the other hand, if $\nu_k \neq 0$ we have

$$\begin{aligned} & \sum_{m=1}^{+\infty} w_{\beta,\mu,m} |\nu_k + b_m|^2 |\hat{p}_{k,m}|^2 \\ &= \sum_{m=1}^{+\infty} \exp [-2\beta (\lambda_m + \mu N_m)] = \Theta_{2\beta,-\mu} < +\infty \end{aligned} \quad (31)$$

from (30) and (1), the latter also implying that $\lim_{m \rightarrow +\infty} b_m = 0$. Therefore we have

$$\lim_{m \rightarrow +\infty} |\nu_k + b_m| = |\nu_k| \neq 0$$

so that (31) implies

$$\sum_{m=1}^{+\infty} w_{\beta,\mu,m} |\hat{p}_{k,m}|^2 < +\infty$$

by asymptotic comparison, as desired. In this manner the $\hat{\mathbf{p}}_k$ provide a set of eigenvectors of A associated with the ν_k , and we now prove that there are no others. Indeed, in the second case we alluded to above where $c_{\mathbf{p},\beta,\mu} = 0$, we

have $(\nu_k + b_m)p_m = 0$ for each $m \in \mathbb{N}^+$ and therefore there exists an $m^* \in \mathbb{N}^+$ such that $\nu_k + b_{m^*} = 0$ since $\mathbf{p} = 0$ is not an eigenvector. But the spectral condition (22) is equivalent to having $b_{m+1} < b_m$ for each $m \in \mathbb{N}^+$, so that the m^* in question is unique. Consequently we necessarily have $p_m = 0$ for every $m \neq m^*$ and $p_{m^*} \neq 0$, which implies the relation

$$c_{\mathbf{p}, \beta, \mu} = \exp \left[-\frac{\beta}{2} (3\lambda_{m^*} + \mu N_{m^*}) \right] p_{m^*} \neq 0,$$

a contradiction. Finally, the characterization (23) of the eigenvalues is a direct consequence of the substitution of (29) into (28). The preceding considerations thus prove the first part of Statement (a), while the second part follows immediately from the fact that A is a compact self-adjoint operator.

Let us now prove Statement (b) by first ordering the non-zero eigenvalues of A as $\nu_k < \nu_{k+1}$ for every $k \in \{2, 3, \dots\}$. To this end we consider the auxiliary function $\mathbf{a} : (-\infty, 0) \setminus \{-b_m, m \in \mathbb{N}^+\}$ defined by

$$\mathbf{a}(\nu) := \sum_{m=1}^{+\infty} \frac{\exp[-\beta(3\lambda_m + \mu N_m)]}{\nu + b_m},$$

and remark that this series is absolutely convergent by virtue of (1) and the fact that $b_m \rightarrow 0$ as $m \rightarrow +\infty$. Furthermore, it is easily verified that

$$\begin{aligned} \lim_{\nu \searrow -b_{k-1}} \mathbf{a}(\nu) &= +\infty, \\ \lim_{\nu \nearrow -b_k} \mathbf{a}(\nu) &= -\infty, \end{aligned}$$

and that $\mathbf{a}'(\nu) < 0$ for every $\nu \in (-b_{k-1}, -b_k)$, which implies the existence of a unique $\nu_k^* \in (-b_{k-1}, -b_k)$ satisfying $\mathbf{a}(\nu_k^*) = 1$. Therefore, from the characterization (23) of the eigenvalues we necessarily have $\nu_k^* = \nu_k$ for every $k \in \{2, 3, \dots\}$, thereby proving the first part of Statement (b). Finally, for every $\mathbf{p} \in l_{\mathbb{C}, \mathbf{w}_{\beta, \mu}}^2$ we have the norm-convergent expansion

$$\mathbf{p} = \sum_{k=1}^{+\infty} (\mathbf{p}, \hat{\mathbf{q}}_k)_{2, \mathbf{w}_{\beta, \mu}} \hat{\mathbf{q}}_k$$

from the last part of Statement (a), which implies (25) at once. \blacksquare

REMARK. Since A is trace-class, it follows from Lidskii's theorem (see, e.g., Theorem 8.4 in Chapter III of [8]) that the so-called matrix trace (14) coincides with the spectral trace, to wit,

$$\sum_{k=1}^{+\infty} \nu_k = \Theta_{2\beta, -\mu} - \Theta_{\frac{\beta}{2}, -3\mu} \Theta_{\frac{3\beta}{2}, -\frac{\mu}{3}},$$

which implies that $\lim_{k \rightarrow +\infty} \nu_k = 0 = \nu_1$. Therefore, there is no spectral gap around the zero eigenvalue of A whose eigenspace is generated by $\mathbf{p}_{\beta, \mu}$. In the next section we investigate some consequences of this fact.

3 On the eigenspace associated with the zero eigenvalue of A as a global attractor

Since $\nu_1 = 0$ is an accumulation point of $\sigma(A)$, we might want to truncate expansion (25) in order to get an exponential decay of some sort for the solutions to (3), or else proceed more generally to obtain convergence statements without error bounds, or more specifically with bounds that may be slower than exponential. We first make the idea of truncation precise by writing $\bigvee_{k=1}^N E_{\nu_k}(A)$ for the closed linear hull of $\bigcup_{k=1}^N E_{\nu_k}(A)$ in $l_{\mathbb{C}, w_{\beta, \mu}}^2$ for any $N \in \mathbb{N}^+$, where $E_{\nu_k}(A)$ stands for the eigenspace of A associated with the eigenvalue ν_k . Then we have:

Theorem 2. *Let A be the operator defined by (13), and let $\mathbf{p}^* \in l_{\mathbb{C}, w_{\beta, \mu}}^2$ be any initial condition satisfying (4). Then*

$$(\exp[\tau A] \mathbf{p}^*)_{\mathbf{m}} \geq 0, \quad \sum_{\mathbf{m}=1}^{+\infty} (\exp[\tau A] \mathbf{p}^*)_{\mathbf{m}} = 1 \quad (32)$$

for every $\tau \in [0, +\infty)$.

Assuming moreover that (22) holds, and that the ordering $\nu_k < \nu_{k+1}$ for every $k \in \{2, 3, \dots\}$ is still valid, then for each $N \in \mathbb{N}^+$ with $N \geq 2$ and $\mathbf{p}^* \in \bigvee_{k=1}^N E_{\nu_k}(A)$ satisfying (4) we have the exponential decay estimate

$$\|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_{\beta, \mu}\|_{2, w_{\beta, \mu}} \leq \exp[-\tau |\nu_N|] \|\mathbf{p}^*\|_{2, w_{\beta, \mu}} \quad (33)$$

for every $\tau \in [0, +\infty)$, where $\mathbf{p}_{\beta, \mu}$ is given by (2).

Proof. Relations (32) are an immediate consequence of some continuity arguments and of the summation of (3) over $\mathbf{m} \in \mathbb{N}^+$.

As for the proof of (33), we start out from (25) to get

$$\exp[\tau A] \mathbf{p}^* - (\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2, w_{\beta, \mu}} \hat{\mathbf{q}}_1 = \sum_{k=2}^N (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2, w_{\beta, \mu}} \exp[\tau \nu_k] \hat{\mathbf{q}}_k$$

since \mathbf{p}^* is orthogonal to $\hat{\mathbf{q}}_k$ in $l_{\mathbb{C}, w_{\beta, \mu}}^2$ for each $k \geq N+1$, so that from Parseval's relation we obtain

$$\left\| \exp[\tau A] \mathbf{p}^* - (\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2, w_{\beta, \mu}} \hat{\mathbf{q}}_1 \right\|_{2, w_{\beta, \mu}}^2 \leq \exp[-2\tau |\nu_N|] \|\mathbf{p}^*\|_{2, w_{\beta, \mu}}^2 \quad (34)$$

for every $\tau \in [0, +\infty)$. It remains to show that

$$(\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2, w_{\beta, \mu}} \hat{\mathbf{q}}_1 = \mathbf{p}_{\beta, \mu}. \quad (35)$$

From (2) and (9) we first have

$$\|\mathbf{p}_{\beta, \mu}\|_{2, w_{\beta, \mu}}^2 = \Theta_{\beta, \mu}^{-2} \sum_{\mathbf{m}=1}^{+\infty} \exp[-\beta(\lambda_{\mathbf{m}} - \mu N_{\mathbf{m}})] = \Theta_{\beta, \mu}^{-1}$$

as a consequence of (1), so that we may choose $\hat{\mathbf{q}}_1 = \Theta_{\beta, \mu}^{\frac{1}{2}} \mathbf{p}_{\beta, \mu}$ as one of the unit eigenvectors associated with $\nu_1 = 0$. Moreover, using (9) on the left-hand side of (34) we eventually get

$$\left| (\exp[\tau A] \mathbf{p}^*)_m - (\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2, \mathbf{w}_{\beta, \mu}} \hat{\mathbf{q}}_{1, m} \right| \leq \exp \left[-\frac{\beta}{2} (\lambda_m - \mu N_m) \right] \exp[-\tau |\nu_N|] \|\mathbf{p}^*\|_{2, \mathbf{w}_{\beta, \mu}}$$

for every m . Therefore, the summation of both sides of this expression over $m \in \mathbb{N}^+$ leads to

$$\left| 1 - (\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2, \mathbf{w}_{\beta, \mu}} \sum_{m=1}^{+\infty} \hat{\mathbf{q}}_{1, m} \right| \leq \Theta_{\frac{\beta}{2}, \mu} \exp[-\tau |\nu_N|] \|\mathbf{p}^*\|_{2, \mathbf{w}_{\beta, \mu}}$$

where we have used (1) and the normalization condition in (32), so that letting $\tau \rightarrow +\infty$ in the preceding relation necessarily gives

$$(\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2, \mathbf{w}_{\beta, \mu}} \sum_{m=1}^{+\infty} \hat{\mathbf{q}}_{1, m} = 1. \quad (36)$$

But from our choice of $\hat{\mathbf{q}}_1$ we have

$$\sum_{m=1}^{+\infty} \hat{\mathbf{q}}_{1, m} = \Theta_{\beta, \mu}^{\frac{1}{2}} \sum_{m=1}^{+\infty} \mathbf{p}_{\beta, \mu, m} = \Theta_{\beta, \mu}^{\frac{1}{2}}$$

and thereby

$$(\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2, \mathbf{w}_{\beta, \mu}} = \Theta_{\beta, \mu}^{-\frac{1}{2}}$$

independently of \mathbf{p}^* . Consequently we end up with

$$(\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2, \mathbf{w}_{\beta, \mu}} \hat{\mathbf{q}}_1 = \Theta_{\beta, \mu}^{-\frac{1}{2}} \hat{\mathbf{q}}_1 = \mathbf{p}_{\beta, \mu},$$

as desired. ■

REMARK. All the $\mathbf{p}^* \in \vee_{k=1}^N E_{\nu_k}(A)$ satisfying (4) provide a large supply of initial data for which estimate (33) holds, which obviously grows with N . But this is at the expense of having a smaller exponential rate of decay whenever N becomes large since $|\nu_N| > |\nu_{N+1}|$ and $\lim_{N \rightarrow +\infty} \exp[-\tau |\nu_N|] = 1$.

We can avoid the truncation method and yet obtain convergence results for the solutions to (3) by modifying the basic argument, but that is at the expense of having no error bounds in general unless we impose additional conditions regarding the Fourier coefficients of the initial data, as in Corollary 2 below. We begin with the crucial observation that (35) still holds for an arbitrary initial condition $\mathbf{p}^* \in l_{\mathbb{C}, \mathbf{w}_{\beta, \mu}}^2$ satisfying (4). More precisely we have:

Lemma 1. *Let $\mathbf{p}^* \in l_{\mathbb{C}, \mathbf{w}_{\beta, \mu}}^2$ satisfy the second relation in (4). Then we have*

$$(\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2, \mathbf{w}_{\beta, \mu}} \hat{\mathbf{q}}_1 = \mathbf{p}_{\beta, \mu}.$$

Proof. From (2) and the definition of the weights $w_{\beta,\mu,m}$ we have

$$(\mathbf{p}_{\beta,\mu}, \hat{\mathbf{q}}_k)_{2,w_{\beta,\mu}} = \Theta_{\beta,\mu}^{-1} \sum_{m=1}^{+\infty} \hat{\mathbf{q}}_{k,m} = 0$$

for each $k \in \{2, 3, \dots\}$ by virtue of the orthogonality of the eigenvectors of A , so that

$$\sum_{m=1}^{+\infty} \hat{\mathbf{q}}_{k,m} = 0 \quad (37)$$

for every such k . Furthermore, for $\mathbf{p}^* \in l_{\mathbb{C},w_{\beta,\mu}}^2$ we have the norm-convergent series expansion

$$\mathbf{p}^* = (\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2,w_{\beta,\mu}} \hat{\mathbf{q}}_1 + \sum_{k=2}^{+\infty} (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2,w_{\beta,\mu}} \hat{\mathbf{q}}_k$$

and therefore

$$\sum_{m=1}^{+\infty} \mathbf{p}_m^* = (\mathbf{p}^*, \hat{\mathbf{q}}_1)_{2,w_{\beta,\mu}} \sum_{m=1}^{+\infty} \hat{\mathbf{q}}_{1,m} = 1$$

as a consequence of (37) and the second relation in (4). In this way (36) holds again, so that we may conclude as in the proof of Theorem 2. ■

Lemma 1 now allows us to get the following generalization of the preceding theorem:

Theorem 3. *Let A be the operator defined by (13), and let $\mathbf{p}^* \in l_{\mathbb{C},w_{\beta,\mu}}^2$ be any initial condition satisfying (4). Assuming moreover that (22) holds, and that the ordering $\nu_k < \nu_{k+1}$ for every $k \in \{2, 3, \dots\}$ is still valid, we have*

$$\lim_{\tau \rightarrow +\infty} \|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_{\beta,\mu}\|_{2,w_{\beta,\mu}} = 0.$$

Proof. From the preceding lemma and its proof we may write

$$\mathbf{p}^* = \mathbf{p}_{\beta,\mu} + \sum_{k=2}^{+\infty} (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2,w_{\beta,\mu}} \hat{\mathbf{q}}_k$$

and therefore

$$\|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_{\beta,\mu}\|_{2,w_{\beta,\mu}}^2 = \sum_{k=2}^{+\infty} \left| (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2,w_{\beta,\mu}} \right|^2 \exp[2\tau\nu_k] < +\infty \quad (38)$$

for every $\tau \in [0, +\infty]$, without truncation. Now for every fixed $k \in \{2, 3, \dots\}$ we have

$$\lim_{\tau \rightarrow +\infty} \left| (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2,w_{\beta,\mu}} \right|^2 \exp[2\tau\nu_k] = 0$$

since $\nu_k < 0$, and moreover

$$\left| (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2, \mathbf{w}_{\beta, \mu}} \right|^2 \exp [2\tau \nu_k] \leq \left| (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2, \mathbf{w}_{\beta, \mu}} \right|^2$$

for every k uniformly in $\tau \in [0, +\infty]$, with

$$\sum_{k=2}^{+\infty} \left| (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2, \mathbf{w}_{\beta, \mu}} \right|^2 \leq \|\mathbf{p}^*\|_{2, \mathbf{w}_{\beta, \mu}}^2 < +\infty.$$

The result then follows from dominated convergence. ■

All the preceding results remain valid when $\mu = 0$, which corresponds to the description of a quantum system in thermodynamical equilibrium with a heat bath at inverse temperature $\beta > 0$, and to transition rates in (3) of the form

$$r_{m,n} = \exp \left[-\frac{\beta}{2} (3\lambda_m + \lambda_n) \right] \quad (39)$$

according to (17). Furthermore, in this case the components (30) of the eigenvectors of A reduce to

$$\hat{p}_{k,m} = \frac{\exp \left[-\frac{3\beta}{2} \lambda_m \right]}{\nu_k + b_m} \quad (40)$$

where

$$b_m = Z_{\frac{3\beta}{2}} \exp \left[-\frac{\beta}{2} \lambda_m \right]. \quad (41)$$

In the preceding expression we have defined

$$Z_\beta := \Theta_{\beta,0} = \sum_{m=1}^{+\infty} \exp [-\beta \lambda_m] < +\infty$$

for every $\beta > 0$, which stands for the usual partition function of the canonical ensemble. Eigenvectors (40) then constitute an orthonormal basis of $l_{\mathbb{C}, \mathbf{w}_\beta}^2$ where $\mathbf{w}_\beta := \mathbf{w}_{\beta, \mu=0} = (w_{\beta, \mu=0, m}) = (\exp [\beta \lambda_m])$, and moreover the grand canonical equilibrium distribution $\mathbf{p}_{\beta, \mu}$ reduces to $\mathbf{p}_\beta := \mathbf{p}_{\beta, \mu=0}$ whose components are given by

$$p_{\beta, m} = Z_\beta^{-1} \exp [-\beta \lambda_m] \quad (42)$$

for every $m \in \mathbb{N}^+$. In the next result we state two consequences of the above theorems:

Corollary 1. *Let A be the operator defined by (13), with the $a_{m,n}$ given by (12) and (39). Then $A : l_{\mathbb{C}, \mathbf{w}_\beta}^2 \mapsto l_{\mathbb{C}, \mathbf{w}_\beta}^2$ is a linear, self-adjoint trace-class operator whose trace is given by*

$$\text{Tr } A = Z_{2\beta} - Z_{\frac{\beta}{2}} Z_{\frac{3\beta}{2}} < 0.$$

Moreover, let us assume in addition that

$$\lambda_{m+1} - \lambda_m > 0 \quad (43)$$

for every $m \in \mathbb{N}^+$, and that the ordering $\nu_k < \nu_{k+1}$ of the eigenvalues still holds for every $k \in \{2, 3, \dots\}$. Then the following statements are valid:

(a) For each $N \in \mathbb{N}^+$ with $N \geq 2$ and $\mathbf{p}^* \in \bigvee_{k=1}^N E_{\nu_k}(A)$ satisfying (4) we have the exponential decay estimate

$$\|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_\beta\|_{2, \mathbf{w}_\beta} \leq \exp[-\tau |\nu_N|] \|\mathbf{p}^*\|_{2, \mathbf{w}_\beta}$$

for every $\tau \in [0, +\infty)$, where \mathbf{p}_β is given by (42).

(b) Let $\mathbf{p}^* \in l_{\mathbb{C}, \mathbf{w}_\beta}^2$ be any initial condition satisfying (4). Then we have

$$\lim_{\tau \rightarrow +\infty} \|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_\beta\|_{2, \mathbf{w}_\beta} = 0.$$

REMARK. The operator A of the preceding corollary may also be realized as a non normal and non dissipative trace-class operator in the usual unweighted Hilbert space $l_{\mathbb{C}}^2$ consisting of all square summable complex sequences. This approach was implemented in [2], with the goal of putting the analysis of A into the perspective of the spectral theory of linear non self-adjoint operators as developed in [8]. However, this was at the expense of having to deal with a host of more complicated technical issues while imposing a more restrictive condition on the spectral condition (43), namely,

$$\lambda_{m+1} - \lambda_m > c \exp[-\theta \lambda_m]$$

for every $m \in \mathbb{N}^+$, with both $c > 0, \theta > 0$ independent of m .

We complete this section by analyzing a concrete example which illustrates the direct impact of the decay properties of the initial data in (3) on the speed of convergence of the corresponding solutions. The example involves the quantum harmonic oscillator whose spectrum we rescaled and shifted by irrelevant constants. We assume throughout that $\mu = 0$:

Corollary 2. *Let us consider the initial-value problem (3)-(4) where the transition rates are given by (39) and $\lambda_m = m \in \mathbb{N}^+$. Moreover, let us assume that the ordering $\nu_k < \nu_{k+1}$ of the eigenvalues of the operator A still holds for every $k \in \{2, 3, \dots\}$. Then the following statements are valid:*

(a) *If the Fourier coefficients of $\mathbf{p}^* \in l_{\mathbb{C}, \mathbf{w}_\beta}^2$ along the orthonormal basis $(\hat{\mathbf{q}}_k)_{k \in \mathbb{N}^+}$ of $l_{\mathbb{C}, \mathbf{w}_\beta}^2$ satisfy*

$$\left| (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2, \mathbf{w}_\beta} \right|^2 \leq \kappa \exp[-\delta k] \quad (44)$$

for every $k \in \{2, 3, \dots\}$ and some $\kappa, \delta > 0$, then we have

$$\|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_\beta\|_{2, \mathbf{w}_\beta} \leq c_{\beta, \kappa, \delta} \tau^{-\frac{\delta}{\beta}} \quad (45)$$

for all sufficiently large τ and for some $c_{\beta,\kappa,\delta} > 0$ depending solely on β, κ and δ .

(b) If the Fourier coefficients of $\mathbf{p}^* \in l_{\mathbb{C},\mathbf{w}_\beta}^2$ along the orthonormal basis $(\hat{\mathbf{q}}_k)_{k \in \mathbb{N}^+}$ of $l_{\mathbb{C},\mathbf{w}_\beta}^2$ satisfy

$$\left| (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2,\mathbf{w}_\beta} \right|^2 \leq \kappa k^{-\delta} \quad (46)$$

for every $k \in \{2, 3, \dots\}$ and some $\kappa > 0, \delta > 1$, then we have

$$\|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_\beta\|_{2,\mathbf{w}_\beta} \leq c_{\beta,\kappa,\delta} (\ln \tau)^{-\frac{\delta-1}{2}} \quad (47)$$

for all sufficiently large τ and for some $c_{\beta,\kappa,\delta} > 0$ depending solely on β, κ and δ .

Proof. The starting point is the relation

$$\|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_\beta\|_{2,\mathbf{w}_\beta}^2 = \sum_{k=2}^{+\infty} \left| (\mathbf{p}^*, \hat{\mathbf{q}}_k)_{2,\mathbf{w}_\beta} \right|^2 \exp[2\tau \nu_k]$$

which is (38) with $\mu = 0$, where we assume that $\tau > 0$. Using (44) along with $\nu_k < -b_k$, the latter being a consequence of (24), we first obtain

$$\begin{aligned} & \|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_\beta\|_{2,\mathbf{w}_\beta}^2 \\ & \leq \kappa \sum_{k=2}^{+\infty} \exp \left[-\delta k - 2\tau Z_{\frac{3\beta}{2}} \exp \left[-\frac{\beta}{2} k \right] \right] \end{aligned} \quad (48)$$

by using (41). In order to extract an explicit dependence in τ from the preceding expression let us now consider the function $f(\cdot, \tau) : (0, +\infty) \mapsto \mathbb{R}^+$ given by

$$f(x, \tau) := \exp \left[-\delta x - 2\tau Z_{\frac{3\beta}{2}} \exp \left[-\frac{\beta}{2} x \right] \right]. \quad (49)$$

We remark that $f(\cdot, \tau)$ possesses a unique critical point at

$$x_c(\tau) = \ln \left(\frac{c_\beta \tau}{\delta} \right)^{\frac{2}{\beta}} \quad (50)$$

where $c_\beta = \beta Z_{\frac{3\beta}{2}}$. Furthermore we choose τ sufficiently large so that the integer part of (50) satisfies $[x_c(\tau)] \geq 3$, with $f(\cdot, \tau)$ monotone increasing for $x \in (0, x_c(\tau))$ and monotone decreasing for $x \in (x_c(\tau), +\infty)$. For the right-hand

side of (48) we then obtain the estimate

$$\begin{aligned}
& \sum_{k=2}^{+\infty} f(k, \tau) \\
= & \sum_{k=2}^{[x_c(\tau)]-1} f(k, \tau) + \sum_{k=[x_c(\tau)]-1}^{+\infty} f(k+1, \tau) \\
\leq & \int_2^{[x_c(\tau)]} dx f(x, \tau) + f([x_c(\tau)], \tau) + f([x_c(\tau)]+1, \tau) + \int_{[x_c(\tau)]+1}^{+\infty} dx f(x, \tau) \\
\leq & \int_2^{+\infty} dx f(x, \tau) + f([x_c(\tau)], \tau) + f([x_c(\tau)]+1, \tau).
\end{aligned} \tag{51}$$

It is now easy to extract the desired dependence in τ for each term in the preceding expression. For the integral this follows from the change of variables $x \rightarrow y = \tau \exp\left[-\frac{\beta}{2}x\right]$, which leads to the estimate

$$\begin{aligned}
& \int_2^{+\infty} dx \exp\left[-\delta x - 2\tau Z_{\frac{3\beta}{2}} \exp\left[-\frac{\beta}{2}x\right]\right] \\
= & \frac{2}{\beta} \left(\int_0^{\tau \exp[-\beta]} dy y^{\frac{2\delta}{\beta}-1} \exp\left[-2Z_{\frac{3\beta}{2}} y\right] \right) \tau^{-\frac{2\delta}{\beta}} \\
\leq & \frac{2}{\beta} \left(\int_0^{+\infty} dy y^{\frac{2\delta}{\beta}-1} \exp\left[-2Z_{\frac{3\beta}{2}} y\right] \right) \tau^{-\frac{2\delta}{\beta}} \\
= & c_{\beta, \delta} \Gamma\left(\frac{2\delta}{\beta}\right) \tau^{-\frac{2\delta}{\beta}}
\end{aligned} \tag{52}$$

for some $c_{\beta, \delta} > 0$ depending only on β and δ , where Γ stands for Euler's Gamma function.

As for the second and third terms on the right-hand side of (51), we first note that the direct substitution of (50) into (49) gives

$$f(x_c(\tau), \tau) = \hat{c}_{\beta, \delta} \tau^{-\frac{2\delta}{\beta}}$$

where $\hat{c}_{\beta, \delta} > 0$, and therefore we get

$$f([x_c(\tau)], \tau) \leq \hat{c}_{\beta, \delta} \tau^{-\frac{2\delta}{\beta}}$$

since $[x_c(\tau)] \leq x_c(\tau)$ and since $f(\cdot, \tau)$ is monotone increasing there. An identical estimate holds for $f([x_c(\tau)]+1, \tau)$ since $x_c(\tau) < [x_c(\tau)]+1$ with $f(\cdot, \tau)$ monotone decreasing there. The substitution of all the gathered information into (51) and the use of (48) then lead to (45).

The proof of (47) follows a similar pattern but is a little bit trickier. We start with

$$\begin{aligned}
& \|\exp[\tau A] \mathbf{p}^* - \mathbf{p}_\beta\|_{2, \mathbf{w}_\beta}^2 \\
\leq & \kappa \sum_{k=2}^{+\infty} k^{-\delta} \exp\left[-2\tau Z_{\frac{3\beta}{2}} \exp\left[-\frac{\beta}{2}k\right]\right]
\end{aligned} \tag{53}$$

and

$$f(x, \tau) := x^{-\delta} \exp \left[-2\tau Z_{\frac{3\beta}{2}} \exp \left[-\frac{\beta}{2}x \right] \right]. \quad (54)$$

It is easily seen that the possible critical points of (54) are solutions to the equation

$$\frac{\exp \left[\frac{\beta}{2}x \right]}{x} = \frac{c_\beta \tau}{\delta} \quad (55)$$

where c_β is as in (50), and that the function on the left-hand side of (55) is convex, possesses an absolute minimum at $x^* = \frac{2}{\beta}$ and is strictly increasing for $x \in (x^*, +\infty)$. Then for every sufficiently large τ there exists a unique critical point $x_c(\tau) \in (x^*, +\infty)$ of $f(\cdot, \tau)$, this function being monotone increasing for $x \in (x^*, x_c(\tau))$ and monotone decreasing for $x \in (x_c(\tau), +\infty)$. Moreover, writing $[x^*]$ for the integral part of x^* , we may break up the right-hand side of (53) as

$$\begin{aligned} & \sum_{k=2}^{+\infty} f(k, \tau) \\ = & \sum_{k=2}^{[x^*]+2} f(k, \tau) + \sum_{k=[x^*]+3}^{[x_c(\tau)]-1} f(k, \tau) + \sum_{k=[x_c(\tau)]-1}^{+\infty} f(k+1, \tau) \\ \leq & \sum_{k=2}^{[x^*]+2} f(k, \tau) + \int_{[x^*]+3}^{+\infty} dx f(x, \tau) + f([x_c(\tau)], \tau) + f([x_c(\tau)+1], \tau). \end{aligned} \quad (56)$$

We now claim that the first term on the right-hand side of the preceding inequality satisfies the exponential decay estimate

$$\sum_{k=2}^{[x^*]+2} f(k, \tau) \leq c_{\beta, \delta} \exp[-c_\beta \tau] \quad (57)$$

for some $c_{\beta, \delta}, c_\beta > 0$. Indeed we have

$$\begin{aligned} & \sum_{k=2}^{[x^*]+2} k^{-\delta} \exp \left[-2\tau Z_{\frac{3\beta}{2}} \exp \left[-\frac{\beta}{2}k \right] \right] \\ \leq & 2^{-\delta} ([x^*] + 1) \exp \left[-2\tau Z_{\frac{3\beta}{2}} \exp \left[-\frac{\beta}{2}([x^*] + 2) \right] \right] \end{aligned}$$

since $2 \leq k \leq [x^*] + 2$, which is (57) with an obvious choice for $c_{\beta, \delta}$ and c_β as $[x^*]$ depends only on β .

As for the integral we have

$$\begin{aligned} & \int_{[x^*]+3}^{+\infty} dx x^{-\delta} \exp \left[-2\tau Z_{\frac{3\beta}{2}} \exp \left[-\frac{\beta}{2}x \right] \right] \\ = & c_{\beta, \delta} \int_0^\tau \exp \left[-\frac{\beta}{2}([x^*]+3)y \right] \frac{dy}{y} \left(\ln \frac{\tau}{y} \right)^{-\delta} \exp \left[-2Z_{\frac{3\beta}{2}} y \right] \end{aligned}$$

following the same change of variables as in (52), for some $c_{\beta,\delta} > 0$. Therefore, integrating by parts and using the fact that $\delta > 1$ to control the completely integrated term we obtain, changing the value of $c_{\beta,\delta}$ if necessary,

$$\begin{aligned} & \int_{[x^*]+3}^{+\infty} dx f(x, \tau) \\ &= c_{\beta,\delta} \exp[-c_{\beta}\tau] + \hat{c}_{\beta,\delta} \int_0^{\tau \exp[-\frac{\beta}{2}([x^*]+3)]} dy \left(\ln \frac{\tau}{y} \right)^{1-\delta} \exp\left[-2Z_{\frac{3\beta}{2}} y\right] \end{aligned} \quad (58)$$

for some $c_{\beta}, \hat{c}_{\beta,\delta} > 0$, thereby exhibiting the exponential decay of the first term on the right-hand side. In order to extract the dependence in τ of the second term we start with

$$\begin{aligned} & \int_0^{\tau \exp[-\frac{\beta}{2}([x^*]+3)]} dy \left(\ln \frac{\tau}{y} \right)^{1-\delta} \exp\left[-2Z_{\frac{3\beta}{2}} y\right] \\ &= \int_0^{\sqrt{\tau}} dy \left(\ln \frac{\tau}{y} \right)^{1-\delta} \exp\left[-2Z_{\frac{3\beta}{2}} y\right] \\ & \quad + \int_{\sqrt{\tau}}^{\tau \exp[-\frac{\beta}{2}([x^*]+3)]} dy \left(\ln \frac{\tau}{y} \right)^{1-\delta} \exp\left[-2Z_{\frac{3\beta}{2}} y\right], \end{aligned}$$

which leads to the estimate

$$\begin{aligned} & \int_0^{\sqrt{\tau}} dy \left(\ln \frac{\tau}{y} \right)^{1-\delta} \exp\left[-2Z_{\frac{3\beta}{2}} y\right] \\ & \leq c_{\delta} \left(\int_0^{+\infty} dy \exp\left[-2Z_{\frac{3\beta}{2}} y\right] \right) (\ln \tau)^{1-\delta} = c_{\beta,\delta} (\ln \tau)^{1-\delta} \end{aligned} \quad (59)$$

for the first term on the right-hand side where $c_{\delta}, c_{\beta,\delta} > 0$. As for the second term we get

$$\begin{aligned} & \int_{\sqrt{\tau}}^{\tau \exp[-\frac{\beta}{2}([x^*]+3)]} dy \left(\ln \frac{\tau}{y} \right)^{1-\delta} \exp\left[-2Z_{\frac{3\beta}{2}} y\right] \\ & \leq \left(\int_{\sqrt{\tau}}^{\tau \exp[-\frac{\beta}{2}([x^*]+3)]} dy \left(\ln \frac{\tau}{y} \right)^{1-\delta} \right) \exp\left[-2Z_{\frac{3\beta}{2}} \sqrt{\tau}\right] \\ & = \left(\int_{\frac{1}{\sqrt{\tau}}}^{\exp[-\frac{\beta}{2}([x^*]+3)]} dy \left(\ln \frac{1}{y} \right)^{1-\delta} \right) \tau \exp\left[-2Z_{\frac{3\beta}{2}} \sqrt{\tau}\right] \\ & \leq \left(\int_0^{\exp[-\frac{\beta}{2}([x^*]+3)]} dy \left(\ln \frac{1}{y} \right)^{1-\delta} \right) \tau \exp\left[-2Z_{\frac{3\beta}{2}} \sqrt{\tau}\right] \\ & = \hat{c}_{\beta,\delta} \tau \exp\left[-2Z_{\frac{3\beta}{2}} \sqrt{\tau}\right] \end{aligned} \quad (60)$$

for some $\hat{c}_{\beta,\delta} > 0$, the last improper integral being convergent. The combination

of (58)-(60) thus leads to

$$\int_{[x^*]+3}^{+\infty} dx f(x, \tau) \leq c_{\beta, \delta} (\ln \tau)^{1-\delta} \quad (61)$$

for some appropriate $c_{\beta, \delta} > 0$.

It remains to estimate the last two terms on the right-hand side of inequality (56). We begin by observing that (54) implies

$$f(x_c(\tau), \tau) \leq x_c^{-\delta}(\tau) \quad (62)$$

for every $\tau \in (0, +\infty)$, while (55) and the fact that $x_c(\tau) > x^*$ for τ sufficiently large lead to

$$\exp\left[\frac{\beta}{2}x_c(\tau)\right] = x_c(\tau)\frac{c_{\beta}\tau}{\delta} \geq x^*\frac{c_{\beta}\tau}{\delta}.$$

Since $x^* = \frac{2}{\beta}$, we may therefore change the value of c_{β} if necessary and thus obtain the lower bounds

$$x_c(\tau) \geq \frac{2}{\beta} \ln \frac{c_{\beta}\tau}{\delta} \geq \frac{1}{\beta} \ln \tau \quad (63)$$

for the critical point, where the second inequality follows from the fact that we may take $\frac{c_{\beta}\tau}{\delta} > \sqrt{\tau}$ for τ sufficiently large since $\frac{c_{\beta}}{\delta} > 0$. From (62) and (63) we then get

$$f(x_c(\tau), \tau) \leq c_{\beta, \delta} (\ln \tau)^{-\delta}$$

for some suitably chosen $c_{\beta, \delta} > 0$, so that arguing as in the proof of Statement (a) we end up with

$$f([x_c(\tau)], \tau) \leq c_{\beta, \delta} (\ln \tau)^{-\delta}$$

and with an identical bound for $f([x_c(\tau)] + 1, \tau)$. The substitution of this information along with (57) and (61) into (56) then leads (47). ■

REMARK. Throughout this article we carried out our computations with transition rates given by (7) and (8) mainly for the sake of clarity and simplicity. However, there are plenty of other choices for them that lead to similar results, as long as they satisfy the detailed balance conditions (6). Furthermore, as an illustration of our considerations we showed in Corollary 2 that even if the quantum harmonic oscillator is initially steered away from thermodynamic equilibrium due to its interaction with a heat bath at inverse temperature $\beta > 0$, it will eventually return there at a rate which strongly depends on the decay properties of the initial conditions (4), a result that is complementary to those in Section 3 of [4].

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