JOURNAL OF MATHEMATICAL PHYSICS **49**, 032106 (2008)

Spectral properties of the two-photon absorption and emission process

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(Received 22 January 2008; accepted 6 February 2008; published online 13 March 2008)

The quantum Markov semigroup of the two-photon absorption and emission process has two extremal normal invariant states. Starting from an arbitrary initial state it converges toward some convex combination of these states as time goes to infinity (approach to equilibrium). We compute the exact exponential rate of this convergence showing that it depends only on the emission rates. Moreover, we show that off-diagonal matrix elements of any initial state go to zero with an exponential rate which is smaller than the exponential rate of convergence of the diagonal part. In other words quantum features of a state survive longer than the relaxation time of its classical part. © *2008 American Institute of Physics.*
[DOI: 10.1063/1.2890700]

I. INTRODUCTION

The two-photon absorption process consists in simultaneous absorptions of pairs of two photon exciting molecules or atoms from their ground state to an excited state. Originally proposed by Göppert-Mayer[9] in 1931, it was experimentally verified in the 1960s (Kaiser and Garrett[11]) and it is now exploited to produce states with typical quantum features (e.g., squeezing and oscillation in the photon-number distribution[1,4,8,10,14] retaining substantial coherence in contrast with those of the one-photon absorption process.

The model for the two-photon absorption process, see Gilles and Knight,[8] can be obtained in the weak coupling limit of the system, a one-mode electromagnetic (EM) field, with a Bosonic Gaussian zero-temperature reservoir of two-photon absorbing atoms (see, e.g., Fagnola and Quezada[6] Sec. 8, for details). Typical quantum states appear, in this model, as a nontrivial, noncommutative, family of stationary states described by Eq. (2) here below.

While it is possible to cool reservoirs to a very low temperature, the absolute 0 may actually never be achieved and quantum features of light are very sensitive to temperature. Therefore it is interesting to investigate the positive temperature case to find out how zero-temperature phenomena survive or transform.

The evolution of observables of a one-mode EM field, weakly coupled with a Bosonic Gaussian positive temperature (gauge invariant) reservoir of two-photon absorbing atoms, is given by the quantum Markov semigroup generated by

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$$£(x) = i\kappa[a^{+2}a^2,x] - \frac{\mu^2}{2}(a^{+2}a^2x - 2a^{+2}xa^2 + xa^{+2}a^2) - \frac{\lambda^2}{2}(a^2a^{+2}x - 2a^2xa^{+2} + xa^2a^{+2}), \qquad (1)$$

where a, a^+ are the usual annihilation and creation operators, κ is a real constant, and μ^2 (λ^2) is the absorption (emission) rate. The analysis of the full (system and reservoir) model reveals that these rates are related to the inverse temperature β, up to the same positive constant, by

$$\mu^2 = \frac{e^{\beta\omega}}{e^{\beta\omega}-1}, \quad \lambda^2 = \frac{1}{e^{\beta\omega}-1},$$

where $\omega > 0$ is a characteristic constant and (consequently) $0 < \lambda^2 < \mu^2$.

This process is called the *two-photon absorption and emission process*. We refer to Ref. 6 for the construction of the quantum Markov semigroup $\mathcal{T}$ associated with the formal generator (1) by the minimal semigroup method, the characterization of invariant states and the convergence toward invariant states.

Note that, for $\beta \to +\infty$, $\lambda \to 0$ and we recover the two-photon absorption process.

The one-mode EM field Hilbert space can be realized as $\ell^2(\mathbb{N})$, the space of complex-valued square summable sequences, with canonical orthonormal basis $(e_n)_{n\geq 0}$. The annihilation and creation operators a, a^+ act as $ae_0 = 0$, $ae_n = \sqrt{n}e_{n-1}$ for $n \geq 1$, $a^+e_n = \sqrt{n+1}e_{n+1}$. It was shown in Refs. 6, 8, and 14 that invariant states of the two-photon absorption process are of the form

$$\rho = \alpha|e_0\rangle\langle e_0| + \bar{z}|e_1\rangle\langle e_0| + z|e_0\rangle\langle e_1| + (1-\alpha)|e_1\rangle\langle e_1|, \qquad (2)$$

with $\alpha \in [0,1]$ and $|z|^2 \leq \alpha(1-\alpha)$, while, at positive temperature, nonclassical (i.e., nondiagonal) stationary states disappear. Indeed, there exist infinitely many commuting invariant states ρ_α, $\alpha \in [0,1]$, which are convex combinations $\rho_\alpha = \alpha\rho_e + (1-\alpha)\rho_o$ of the even and odd extremal invariant states,

$$\rho_e = (1-\nu^2)\sum_{k\geq 0}\nu^{2k}|e_{2k}\rangle\langle e_{2k}|, \quad \rho_o = (1-\nu^2)\sum_{k\geq 0}\nu^{2k}|e_{2k+1}\rangle\langle e_{2k+1}|, \quad \nu = \lambda/\mu.$$

All these states are equilibrium (detailed balance) states and any initial state σ_0 converges to an invariant state as time goes to infinity. Thus the system exhibits approach to equilibrium and decoherence destroying quantum features of states.

We prove here, however, that the off-diagonal elements (coherences) of a state σ (in the given basis) decay with an exponential rate *smaller* than that of convergence of diagonal matrix elements. Thus coherences survive for a long time. More precisely, we show that, for every initial state σ_0 such that $\rho^{-1/4}\sigma_0\rho^{-1/4}$ is a Hilbert–Schmidt operator, the state σ_t at time t converges to an invariant state $\rho = \sigma_\infty$ and the following inequalities hold:

$$|\langle e_j, \sigma_t e_k\rangle| \leq e^{-\lambda^2 t}c_1(j,k,\sigma_0) \;\; j \neq k, \quad |\langle e_j, \sigma_t e_j\rangle - \langle e_j, \rho e_j\rangle| \leq e^{-\mathrm{g}t}c_2(j,\sigma_0), \qquad (3)$$

with

$$\lambda^2 < \mu^2 < \mu^2(1+\sqrt{1-e^{-\beta\omega}}) < g < 2\mu^2 \qquad (4)$$

and $c_1(j,k,\sigma_0), c_2(j,\sigma_0)$, two positive constants independent of t [see relations (13) and (24), and Theorem 10].

One could also say that the off-diagonal part of σ_t vanishes with an exponential rate λ^2 in the weak topology and the diagonal part converges *faster* toward an invariant state with a bigger exponential rate g [see relations (24), from which are derived].

The inequalities (3), which are optimal in some sense that we shall clarify later (remark 3 at the end of the paper), show that coherences survive for a time longer than the relaxation time of the classical part of the system: the smallest is the temperature, the longest is the survival.

The above results do not follow from (almost) explicit computations as for the zero-temperature case, where the only allowed transitions are from a level to the next lower level with

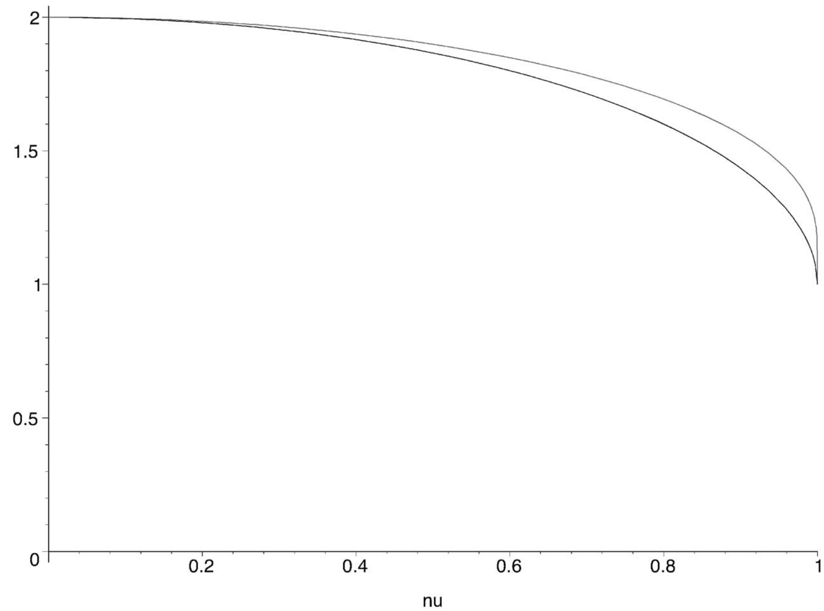

FIG. 1. Bounds for the classical spectral gap as functions of ν.

the same parity, and one can easily solve a system of *first* order difference-differential equations. In the positive temperature case, the matrix elements $\langle e_j, \sigma_t e_k \rangle$ satisfy systems of *second* order difference-differential equations.

We overcome this difficulty investigating the spectral gap of the quantum Markov semigroup generated by (1) following the approach of Ref. 3 and the spectral gap of the classical birth-and-death generator obtained by restriction of (1) to diagonal matrices using a variational formula due to Liggett.[13] We show that the first is equal to λ^2 and we prove the estimate (4) for the second [Theorem (10)]. We do not know the exact value of the classical spectral gap g although it can be characterized by several variational formulas (see, e.g., Ref. 5). The plot in Fig. 1 shows that our estimate (4) of g is quite close the unknown value. Indeed, the graph of g as a function of ν lies between the two curves (see Sec. VI).

Surprisingly the spectral gap λ^2 of the two-photon absorption and emission process depends only on the emission rates in contrast with the one-photon absorption and emission process where it depends on both (see Ref. 2).

The paper is organized as follows. In Sec. II we define an embedding of the von Neumann algebra $\mathcal{B}(h)$ into the Hilbert space $L_2(h)$ of Hilbert–Schmidt operators on h, compute the embedded Lindblad generator and its corresponding Dirichlet form. In Sec. III we describe an orthogonal decomposition of $L^2(h)$ into a family of invariant subspaces and state our main Theorem 3, whose proof is developed in the next two sections. The minima of the Dirichlet form restricted to the off-diagonal invariant subspaces are computed in Sec. IV, and in Section V we deduce a sharp estimate of the minima of the Dirichlet form when restricted to the diagonal subspaces.

II. L^2 NORMS AND DIRICHLET FORM

Let h denote the Hilbert space $l^2(\mathbb{N})$ and $\mathcal{B}(h)$ the space of bounded operators on h.

Let $\mathcal{M}$ denote the dense linear subspace of $\mathcal{B}(h)$ whose elements x are the operators which can be expressed by $x=\sum_{j,k\geq 0} x_{j,k} |e_j\rangle\langle e_k|$ with only a finite number of summands, where $x_{j,k}$ is the (j,k) matrix element of x, i.e., $x_{j,k}=\langle e_j, x e_k\rangle$.

The Lindblad generator $\pounds$ of the model can be formally described as an operator on $\mathcal{B}(h)$, and by (1) we can write

$$£(x) = \sum_{j,k\geqslant 0} |e_j\rangle\langle e_k| \Bigg\{ \mu^2([k]_2[j]_2)^{1/2} x_{j-2,k-2} + \lambda^2([k+2]_2[j+2]_2)^{1/2} x_{j+2,k+2} - \Bigg[\frac{\mu^2}{2}([k]_2+[j]_2) + \frac{\lambda^2}{2}([j+2]_2+[k+2]_2) + i\kappa([j]_2-[k]_2) \Bigg] x_{j,k} \Bigg\} \quad (5)$$

at least for x in $\mathcal{M}$ [where we denote $[k]_2 := k(k-1)$].

Following some classical well-known techniques, it is fruitful to study the convergence of the semigroup with respect to some appropriate L^2 norms induced by an invariant faithful state. So, for each faithful invariant state $\rho_\alpha = \alpha\rho_e + (1-\alpha)\rho_o$ with $\alpha \in (0,1)$, we define the embedding of $\mathcal{B}(h)$ into $L_2(h)$, the space of Hilbert–Schmidt operators on h, by means of

$$\iota : \mathcal{B}(h) \to L_2(h), \quad \iota(x) = \rho_\alpha^{\theta/2} x \rho_\alpha^{(1-\theta)/2},$$

for some fixed $\theta \in [0,1]$ [we remember $L^2(h)$ is a Hilbert space with scalar product induced by the trace]. The map ι is an injective contraction with a dense range and it is a completely positive map for $\theta = 1/2$. We call $\mathcal{T}$ the semigroup generated by £ and define $T_t^\alpha(\iota(x)) = \iota(\mathcal{T}_t(x))$ for every $t \geqslant 0$ and $x \in \mathcal{B}(h)$. The operators T_t^α can be extended to the whole $L_2(h)$ and they define a unique strongly continuous contraction semigroup $T^\alpha = (T_t^\alpha)_{t\geqslant 0}$ on $L_2(h)$ (see Ref. 3). Moreover, if L^α is the infinitesimal generator of T^α and $D(£)$ is the domain of £, then $\iota(D(£))$ is contained in the domain of L^α and

$$L^\alpha(\rho_\alpha^{\theta/2} x \rho_\alpha^{(1-\theta)/2}) = \rho_\alpha^{\theta/2}\, £\,(x) \rho_\alpha^{(1-\theta)/2}, \quad \text{for } x \in D(£). \quad (6)$$

Notice that we can define the map ι also for $\alpha = 0,1$, but it will not be injective in these cases, so it will not define an embedding of the semigroup because the information about a part of the semigroup will be erased.

We should remember also the dependence of T on θ in the notations, but we will see in a while that it is not necessary because the generator L does not really depend on α and θ.

For x in $\mathcal{M}$, we can easily compute, remembering the exponential form of the invariant state ρ_α,

$$\begin{aligned} L^\alpha(x) &= \rho_\alpha^{\theta/2}\, £\,(\rho_\alpha^{-\theta/2} x \rho_\alpha^{-(1-\theta)/2}) \rho_\alpha^{(1-\theta)/2} \\ &= \sum_{j,k\geqslant 0} |e_j\rangle\langle e_k| \Bigg\{ \lambda\mu([k]_2[j]_2)^{1/2} x_{j-2,k-2} + \lambda\mu([k+2]_2[j+2]_2)^{1/2} x_{j+2,k+2} \\ &\quad - \Bigg[\frac{\mu^2}{2}([k]_2+[j]_2) + \frac{\lambda^2}{2}([j+2]_2+[k+2]_2) + i\kappa([j]_2-[k]_2) \Bigg] x_{j,k} \Bigg\}. \end{aligned} \quad (7)$$

So the expression of the generators L^α is the same on $\mathcal{M}$ and also the domain is the same, since $\mathcal{M}$ is a core for L^α by Proposition 5.1 in Ref. 6.

Hence we can drop the α in the notation since it is clear that the embedded generator L does not depend on the choice of α and θ.

Remark: We underline that embedding the minimal semigroup in $L^2(h)$ is completely equivalent to considering the norms of the original semigroup in the space $L^2(h,\rho)$, where we define as usual $\|x\|_{L^2(h,\rho)} = \mathrm{tr}(\iota(x^*)\iota(x))$.

The *Dirichlet form*, defined for $\xi \in D(L)$, is the quadratic form $\mathcal{E}$

$$\mathcal{E}(\xi) = -\mathrm{Re}\langle \xi, L(\xi) \rangle.$$

Obviously, also the Dirichlet form will not depend on α and θ and we find the exlicit expression in the following.

Lemma 1: Let $\alpha \in (0,1)$, $\theta \in [0,1]$, $\xi \in D(L)$, with $\xi = \sum_{j,k} \xi_{j,k} |e_j\rangle\langle e_k|$, then

$$\mathcal{E}(\xi)=\tfrac{1}{2}\sum_{k\geq 0}\mu^2(k+1)(k+2)(|\xi_{0,k+2}|^2+|\xi_{1,k+2}|^2+|\xi_{k+2,0}|^2+|\xi_{k+2,1}|^2)$$
$$+\tfrac{1}{2}\sum_{j,k\geq 0}|\mu\sqrt{(k+1)(k+2)}\xi_{j+2,k+2}-\lambda\sqrt{(j+1)(j+2)}\xi_{j,k}|^2+\tfrac{1}{2}\sum_{j,k\geq 0}|\mu\sqrt{(j+1)(j+2)}\xi_{j+2,k+2}$$
$$-\lambda\sqrt{(k+1)(k+2)}\xi_{j,k}|^2. \tag{8}$$

In particular, $\mathcal{E}(\xi)=\mathcal{E}(\xi^*)$, *where* ξ^* *is the adjoint operator of* ξ.

Proof: Relation (7), for ξ in $\mathcal{M}$, leads to

$$\mathcal{E}(\xi)=-\operatorname{Re}\langle\xi,L(\xi)\rangle=-\operatorname{Re}\{\operatorname{tr}(\xi^*L(\xi))\}$$
$$=-\lambda\mu\sum_{j,k}(k(k-1)j(j-1))^{1/2}\operatorname{Re}\bar{\xi}_{j,k}\xi_{j-2,k-2}$$
$$-\lambda\mu\sum_{j,k}((k+1)(k+2)(j+1)(j+2))^{1/2}\operatorname{Re}\bar{\xi}_{j,k}\xi_{j+2,k+2}$$
$$+\sum_{j,k}\left\{\frac{\mu^2}{2}(k(k-1)+j(j-1))+\frac{\lambda^2}{2}((j+1)(j+2)+(k+1)(k+2))\right\}|\xi_{j,k}|^2,$$

and expression (8) immediately follows from a rearrangement of these terms.

Now, for $\xi=\sum_{i,j}\xi_{ij}|e_i\rangle\langle e_j|\in D(L)$, $\xi\notin\mathcal{M}$, it is sufficient to consider the sequence of truncated elements ξ^n,

$$\xi^n=\sum_{i,j\leq n}\xi_{ij}|e_i\rangle\langle e_j|\in\mathcal{M},\quad \xi^n\to\xi \text{ in } L^2(h).$$

Then, since L is a closed operator and $\mathcal{M}$ is a core for L, $L(\xi^n)\to L(\xi)$ in $L^2(h)$ and

$$|\mathcal{E}(\xi^n)-\mathcal{E}(\xi)|\leq|\langle\xi^n,L(\xi^n)\rangle-\langle\xi,L(\xi)\rangle|\leq|\langle\xi^n-\xi,L(\xi)\rangle-\langle\xi,L(\xi)-L(\xi^n)\rangle|$$
$$\leq\|\xi^n-\xi\|\|L(\xi)\|+\|\xi\|\|L(\xi)-L(\xi^n)\|\to 0.$$

So the series in (8) converges and its limit is $\mathcal{E}(\xi)$. The second part of the thesis easily follows from (8), but it can also be deduced independently since we can notice that $L(x)^*=L(x^*)$ for all x in $\mathcal{M}$. □

The following proposition characterizes the kernel of the generator L of the embedded semigroup.

Proposition 2: If $W=\{\xi\in D(L):\mathcal{E}(\xi)=0\}$ *then*

$$\operatorname{span}\{\rho_e^{1/2},\rho_o^{1/2}\}=\iota(\operatorname{Ker}\pounds)=\operatorname{Ker}LW.$$

Proof: Let p_e and p_o be the support projections of the invariant states ρ_e and ρ_o, respectively, i.e.,

$$p_e=\sum_{k\geq 0}|e_{2k}\rangle\langle e_{2k}|,\quad p_o=\sum_{k\geq 0}|e_{2k+1}\rangle\langle e_{2k+1}|.$$

Let us notice that $\iota(p_e)=\sqrt{\alpha}\rho_e^{1/2}$ and $\iota(p_o)=\sqrt{1-\alpha}\rho_o^{1/2}$.

By Theorem 4.5 in Ref. 6, we have that p_e and p_o are invariant for the semigroup generated by £, hence $\iota(p_e)$ and $\iota(p_o)$ are T_t-invariant. Therefore any linear combination of $\rho_e^{1/2}$ and $\rho_o^{1/2}$ belongs to $\iota(\operatorname{Ker}\pounds)$ which, clearly, is a subspace of $\operatorname{Ker}L$ since $\iota(D(\pounds))\subset D(L)$ and (6). By the definition of the Dirichlet form, it is also clear that $\operatorname{Ker}L\subset W$. So, it suffices to show that each $\xi\in W$ is a linear combination of $\rho_e^{1/2}$ and $\rho_o^{1/2}$.

Straightforward computations show that, for $\xi\in W$, $\xi=\sum_{j,k}\xi_{jk}|e_j\rangle\langle e_k|$, each summand in (8) vanishes. Therefore, for all $j,k\geq 0$,

$$\xi_{j+2,k+2} = \nu\sqrt{\frac{(j+1)(j+2)}{(k+1)(k+2)}}\xi_{jk}\nu\sqrt{\frac{(k+1)(k+2)}{(j+1)(j+2)}}\xi_{jk}, \tag{8'}$$

where $\nu=\lambda/\mu$ and

$$\xi_{0k} = \xi_{1k} = \xi_{k0} = \xi_{k1} = 0, \quad \text{for } k \geq 2.$$

This implies that, for all $j,k \geq 0$,

$$\xi_{j,k} = 0 \text{ or } j = k.$$

Thus, ξ is diagonal and, by (8′), $\xi_{k+2,k+2}=\nu\xi_{kk}$. Hence, for all $k\geq 0$, $\xi_{2k,2k}=\nu^k\xi_{00}$, and $\xi_{2k+1,2k+1}=\nu^k\xi_{11}$.

In other words, each ξ in W can be written

$$\xi = \xi_{00}\sum_{k\geq 0}\nu^k|e_{2k}\rangle\langle e_{2k}| + \xi_{11}\sum_{k\geq 0}\nu^k|e_{2k+1}\rangle\langle e_{2k+1}| = (1-\nu^2)^{-1/2}(\xi_{00}\rho_e^{1/2} + \xi_{11}\rho_o^{1/2}).$$

This finishes the proof. □

III. THE SPECTRAL GAP

We now concentrate on the spectral gap. We first remember the definition: the spectral gap of the operator L is the non-negative real number,

$$\text{gap } L = \inf\{\mathcal{E}(\xi): \|\xi\| = 1, \ \xi \in (\text{Ker } L)^{\perp}\}.$$

When gap L is positive, it represents the rate of uniform exponential convergence to the invariant vectors of the generated semigroup. Indeed, if we denote by P the projection on Ker L, $Px=\langle\rho_o^{1/2},x\rangle\rho_o^{1/2}+\langle\rho_e^{1/2},x\rangle\rho_e^{1/2}$, for x in $L^2(h)$, gap L is the best constant c verifying

$$\|T_t(\xi - P\xi)\| \leq e^{-ct}\|\xi - P\xi\| \quad \text{for all } \xi,t, \tag{9}$$

see, Ref. 13 or Ref. 3 for the noncommutative extension.

The particular structure of the two-photon absorption and emission semigroup allows us to use a particular orthogonal decomposition of the domain in invariant subspaces. This technique is similar to the one used in Ref. 3, but this semigroup has some distinguishing features which make it different from the class of semigroups studied in Ref. 3: for instance, the invariant state is not unique here and the diagonal restriction is the semigroup of a stochastic process which can be seen as two "orthogonal" birth and death semigroups with quadratic rates.

Our procedure will take to the following conclusion.

Theorem 3: Gap $L=\lambda^2$ *for any value of the parameters* $0<\lambda\leq\mu$.

The proof of this result will follow in this and in the next two sections.

An orthogonal decomposition. Let $m\in\mathbb{Z}$ and define the sets [closures will be taken with respect to the $L^2(h)$ norm],

$$\mathcal{G}_m^e = \overline{\text{span}\{|e_k\rangle\langle e_{k+m}|: k \text{ even}, k \geq \max\{0,-m\}\}},$$

$$\mathcal{G}_m^o = \overline{\text{span}\{|e_k\rangle\langle e_{k+m}|: k \text{ odd}, k \geq \max\{1,-m\}\}}.$$

If we identify an element x in $L^2(h)$ with its matrix representation, $\mathcal{G}_m^e$ ($\mathcal{G}_m^o$) is the space of matrices whose elements are zero except for the components on the mth diagonal with even (odd) first index.

Some properties, all trivial to verify the following.

(1) $\xi\in\mathcal{G}_m^p \Leftrightarrow \xi^*\in\mathcal{G}_{-m}^p$, $p\in\{e,o\}$, where ξ^* is the adjoint of the operator ξ.
(2) The linear spaces $\mathcal{G}_m^p$ are orthogonal in $L_2(h)$ and

$$L_2(h) = \oplus\{\mathcal{G}_m^p : p \in \{o,e\}, m \in \mathbb{Z}\}.$$

(3) Each $\mathcal{G}_m^p$ is invariant for the generator L and so also for the semigroup T.
(4) Each $\mathcal{G}_m^p$ is isometrically isomorphic to the space $l^2(\mathbb{N})$ of square summable sequences.

Proposition 4:

$$\text{gap } L = \inf_{m\geq 0} \inf_{p=e,o} A_m^p,$$

$$\textit{where, for } p \in \{e,o\}, \quad A_m^p : \begin{cases} \inf\{\mathcal{E}(\xi), \|\xi\| = 1, \xi \in \mathcal{G}_m^p\} & \textit{for } m \neq 0 \\ \inf\{\mathcal{E}(\xi), \|\xi\| = 1, \xi \in \mathcal{G}_0^p, \xi \perp \rho_p^{1/2}\} & \textit{for } m = 0. \end{cases} \tag{10}$$

Proof: Let $m\in\mathbb{Z}$, $p\in\{e,o\}$ and $\xi\in L_2(h)$ be fixed. Let us denote by $\mathcal{G}_m^p(\xi)$ the orthogonal projection of ξ on $\mathcal{G}_m^p$. Then, due to the orthogonality of the family of subspaces $\mathcal{G}_m^p$ and their invariance under L, we have

$$\mathcal{E}(\xi) = \sum_{m\in\mathbb{Z}} \sum_{p\in\{e,o\}} \mathcal{E}(\mathcal{G}_m^p(\xi))$$

and

$$\|\xi\|^2 = \sum_{m\in\mathbb{Z}} \sum_{p\in\{e,o\}} \|\mathcal{G}_m^p(\xi)\|^2.$$

Then we have,

$$\begin{aligned} \text{gap } L &= \inf_{\xi\perp \text{Ker } L} \frac{\mathcal{E}(\xi)}{\|\xi\|^2} = \inf_{\xi\perp\text{Ker } L} \frac{\Sigma_{m\in\mathbb{Z}}\Sigma_{p\in\{e,o\}}\mathcal{E}(\mathcal{G}_m^p(\xi))}{\Sigma_{m\in\mathbb{Z}}\Sigma_{p\in\{e,o\}}\|\mathcal{G}_m^p(\xi)\|^2} \overset{(*)}{=} \inf_{\xi\perp\text{Ker } L} \inf_{m\in\mathbb{Z}} \inf_{p\in\{e,o\}} \frac{\mathcal{E}(\mathcal{G}_m^p(\xi))}{\|\mathcal{G}_m^p(\xi)\|^2} \\ &= \inf_{m\in\mathbb{Z}} \inf_{p\in\{e,o\}} \inf_{\xi\perp\text{Ker } L} \frac{\mathcal{E}(\mathcal{G}_m^p(\xi))}{\|\mathcal{G}_m^p(\xi)\|^2}, \end{aligned} \tag{11}$$

where in $(*)$ inequality follows from the elementary relation

$$\frac{a+b}{c+d} \geq \inf\left\{\frac{a}{c}, \frac{b}{d}\right\}$$

for all non-negative real numbers a,b,c,d, and equality is trivial since, when ξ is in $\mathcal{G}_m^p$, we have $\xi=\mathcal{G}_m^p(\xi)$.

Now we consider the partial infimums appearing in (11) and define, always for m integer and $p=e,o$,

$$\tilde{A}_m^p := \inf_{\xi\perp\text{Ker } L} \frac{\mathcal{E}(\mathcal{G}_m^p(\xi))}{\|\mathcal{G}_m^p(\xi)\|^2} = \inf_{\xi\perp\text{Ker } L, \xi\in\mathcal{G}_m^p} \frac{\mathcal{E}(\xi)}{\|\xi\|^2} = \inf_{\xi\perp\text{Ker } L, \xi\in\mathcal{G}_m^p, \|\xi\|=1} \mathcal{E}(\xi).$$

We want to see that $\tilde{A}_m^p$ coincide (for $m\geq 0$) with the coefficient A_m^p defined in the statement of this theorem. First notice that the orthogonality condition in $\tilde{A}_m^p$ is necessary only when $m=0$, while, for $m\neq 0$, the entire space $\mathcal{G}_m^p$ is orthogonal to Ker $L=\text{span}\{\rho_o^{1/2},\rho_e^{1/2}\}\subset\mathcal{G}_0^o\oplus\mathcal{G}_0^e$. Moreover, for $m=0$, we can write the orthogonality condition in a simpler way since $\mathcal{G}_0^o$ is orthogonal to $\rho_e^{1/2}$ and $\mathcal{G}_0^e$ is orthogonal to $\rho_o^{1/2}$. Summing up, we have

$$m \neq 0, \quad p = e, \quad o \text{ any } \xi \in \mathcal{G}_m^p \text{ is orthogonal to Ker } L,$$

$$m = 0, \quad p = e \quad \xi \in \mathcal{G}_m^e \text{ is orthogonal to Ker } L \text{ iff } \xi \perp \rho_e^{1/2},$$

$$m=0, \quad p=o \quad \xi \in \mathcal{G}^o_m \text{ is orthogonal to Ker } L \text{ iff } \xi \perp \rho_o^{1/2}.$$

This implies that $\widetilde{A}^p_m = A^p_m$ for $m \geqslant 0$. Moreover, since $\xi \in \mathcal{G}^p_m$ if and only if $\xi^* \in \mathcal{G}^p_{-m}$ $(p=o,e)$ and $\mathcal{E}(\xi)=\mathcal{E}(\xi^*)$, then, always for positive m, $\widetilde{A}^p_{-m}=\widetilde{A}^p_m=A^p_m$ and we can restrict our analysis to the main and the upper diagonals. In other words, relation (11) becomes

$$\text{gap } L = \inf_{m \geqslant 0} \inf_{p=e,o} A^p_m.$$

□

Remark: The A^p_m's satisfy a relation similar to (9). Indeed, rewriting the usual computations which lead to (9), one has

$$\frac{d}{dt} \lg \|T_t x\|^2 = -\frac{2}{\|T_t x\|^2} \mathcal{E}(T_t x),$$
$$\|T_t x\| = \|x\| \exp\left(\int_0^t \frac{1}{2} \frac{d}{ds} \lg \|T_s x\|^2 ds \right) = \|x\| \exp\left(-\int_0^t \frac{\mathcal{E}(T_s x)}{\|T_s x\|^2} ds \right). \tag{12}$$

We can write then

$$\|T_t x\| \leqslant \|x\| e^{-tA^p_m}, \quad \text{for } x \text{ in } \mathcal{G}^p_m, \quad m \geqslant 1,$$
$$\|T_t x\| \leqslant \|x\| e^{-tA^p_0}, \quad \text{for } x \text{ in } \mathcal{G}^p_0 \text{ and } x \perp \rho_p^{1/2}. \tag{13}$$

We have reduced the computation of the quantum spectral gap to a sequence of minimum problems on $l^2(\mathbb{N})$ (with constraints only when $m=0$), which will be faced in the next two sections. For $m=0$, we will see that the minimum problems are the computation of the spectral gaps for two classical birth and death processes.

IV. OFF-DIAGONAL MINIMUM PROBLEMS

First we give an estimate of the minima outside the diagonal ($m>0$), and we obtain the exact value of these minima for $m=1$. We will see this is all we need in this case to get the exact value of the spectral gap.

Fix $m>0$. For ξ in $\mathcal{G}^e_m$, we can write, for some sequence $y=(y_j)_{j\geqslant 0}$ in $l^2(\mathbb{N})$ [remember $[k]_2 = k(k-1)$],

$$\xi = \sum_j y_j |e_{2j}\rangle\langle e_{2j+m}|,$$

where $y_j = \xi_{2j,2j+m}$, and

$$\mathcal{E}(\xi) = \frac{\mu^2}{2}[m]_2 |y_0|^2 + \frac{1}{2}\sum_{k\geqslant 1} \{ |\mu\sqrt{[2k+m]_2}y_k - \lambda\sqrt{[2k]_2}y_{k-1}|^2 + |\mu\sqrt{[2k]_2}y_k - \lambda\sqrt{[2k+m]_2}y_{k-1}|^2 \}. \tag{14}$$

For $\xi \in \mathcal{G}^o_m$,

$$\xi = \sum_j y_j |e_{2j+1}\rangle\langle e_{2j+1+m}|,$$

where $y_j = \xi_{2j+1,2j+1+m}$, and

$$\mathcal{E}(\xi) = \frac{\mu^2}{2}[m+1]_2|y_0|^2 + \frac{1}{2}\sum_{k\geq 1}\{|\mu\sqrt{[2k+m+1]_2}y_k - \lambda\sqrt{[2k+1]_2}y_{k-1}|^2 + |\mu\sqrt{[2k+1]_2}y_k - \lambda\sqrt{[2k+m+1]_2}y_{k-1}|^2\}. \tag{15}$$

In both cases $\|\xi\|^2_{L^2(\mathsf{h})} = \Sigma_k |y_k|^2 = \|y\|^2_{l^2(\mathbb{N})}$.

We have the following.

Proposition 5: For any $m \geq 1$

$$A_m^e \geq \frac{\lambda^2}{2}m^2\left(2 + \frac{1-m^2}{3m+4+m^2}\right) \quad \text{and } A_m^o \geq \frac{m(m+1)}{2}\mu^2,$$

with equality when $m=1$, i.e., $A_1^e = \lambda^2$ *and* $A_1^o = \mu^2$.

Notice that the inequalities are optimal for $m=1$ but not for $m>1$. This is obvious from the proof.

Proof: Fix $m \geq 1$ and $\xi \in \mathcal{G}_m^e$. To get shorter notations in writing the quadratic forms of Eq. (14), let $y_j = \xi_{2j,2j+m}$ as before. With these notations, grouping the jth summands in the quadratic form (14), we have

$$\mathcal{E}(\xi) = \tfrac{1}{2}[m]_2\mu^2 y_0^2 + \tfrac{1}{2}\sum_{j\geq 1}([2j+m]_2 + [2j]_2)(\mu^2 y_j^2 + \lambda^2 y_{j-1}^2) - 4\lambda\mu\sqrt{[2j+m]_2[2j]_2}y_{j-1}y_j.$$

Now, using the following inequality,

$$4\lambda\mu\sqrt{[2j+m]_2[2j]_2}y_j y_{j-1} \leq \mu^2([2j+m]_2 + [2j]_2)y_j^2 + 4\lambda^2\frac{[2j+m]_2[2j]_2}{[2j+m]_2+[2j]_2}y_{j-1}^2, \tag{16}$$

we have

$$\mathcal{E}(\xi) \geq \frac{\lambda^2}{2}\sum_{j\geq 1}\frac{([2j+m]_2 - [2j]_2)^2}{[2j+m]_2+[2j]_2}y_{j-1}^2 = \frac{\lambda^2}{2}m^2\sum_{j\geq 1}\left(2 + \frac{1-m^2}{8j^2+(m-1)(4j+m)}\right)y_{j-1}^2. \tag{17}$$

But the map $j \mapsto (1-m^2)/[8j^2+(m-1)(4j+m)]$ attains its global minimum at $j=1$, hence by (17), we have

$$\mathcal{E}(\xi) \geq \frac{\lambda^2}{2}m^2\left(2+\frac{1-m^2}{3m+4+m^2}\right)\sum_{j\geq 0}y_j^2 \geq \frac{\lambda^2}{2}m^2\left(2+\frac{1-m^2}{3m+4+m^2}\right)\|\xi\|^2.$$

These estimates show that $A_m^e \geq (\lambda^2/2)m^2(2+(1-m^2)/(3m+4+m^2))$. To prove that equality holds for $m=1$, let us notice that, in this case, inequality (16) is equality if and only if, for all $j \geq 1$,

$$\mu([2j+1]_2 + [2j]_2)y_j = 2\lambda\sqrt{[2j]_2[2j+1]_2}y_{j-1} \Leftrightarrow y_j = \nu\frac{\sqrt{(2j+1)(2j-1)}}{2j}y_{j-1},$$

which is equivalent to one (and only one) of the following conditions:

(i) $\xi = 0$.

(ii) For all $j \geq 0$, $y_j \neq 0$, and $\xi = \bar{\xi} := \Sigma_j \nu^j 2^{-j}\sqrt{2j+1}(2j-1)!!/j!|e_{2j}\rangle\langle e_{2j+1}|$.
Notice that, in this case, $\lim_j y_j/y_{j-1}\nu < 1$, so $\Sigma_{j\geq 0}y_j^2 < \infty$ and $\bar{\xi} \in \mathcal{G}_1^e$. Moreover, $\mathcal{E}(\bar{\xi}) = \lambda^2\|\bar{\xi}\|^2$, so the infimum is attained.

To prove the claims for A_m^o, we proceed in a similar way. Let $\xi \in \mathcal{G}_m^o$. Again, we use $y_j = \xi_{2j+1,2j+1+m}$ as for (15). Grouping the jth summands in (15), and proceeding as before,

$$\mathcal{E}(\xi) = \frac{[m+1]_2}{2}\mu^2 y_0^2 + \frac{1}{2}\sum_{j\geq 1}([2j+m+1]_2+[2j+1]_2)(\mu^2 y_j^2+\lambda^2 y_{j-1}^2) - 4\lambda\mu\sqrt{[2j+m+1]_2[2j+1]_2}y_{j-1}y_j \geq \frac{1}{2}\mu^2\sum_{j\geq 1}\left(\frac{([2j+m+1]_2-[2j+1]_2)^2}{[2j+m+1]_2+[2j+1]_2}\right)y_j^2. \tag{18}$$

But

$$\frac{([2j+m+1]_2-[2j+1]_2)^2}{[2j+m+1]_2+[2j+1]_2} = m^2\left(2+\frac{1-m^2}{8j^2+4j(m+1)+m+m^2}\right),$$

and this expression, as a function of j, attains its global minimum at $j=1$, so it is greater than or equal to $2+(1-m^2)/(5m+12+m^2)$. Since $m(m+1)\geq m^2(2+(1-m^2)/(5m+12+m^2))$, by (18) we have

$$\mathcal{E}(\xi) \geq \frac{1}{2}\mu^2 m^2\left(2+\frac{1-m^2}{5m+12+m^2}\right)\sum_{j\geq 0} y_j^2 \geq \frac{\mu^2 m(m+1)}{2}\|\xi\|^2.$$

These estimates show that $A_m^o \geq [m(m+1)/2]\mu^2$. To prove that equality holds for $m=1$, let us notice that, in this case, inequality (18) is equality if and only if, for all $j\geq 0$,

$$\lambda([2j+1]_2+[2j+2]_2)y_{j-1} = 2\mu\sqrt{[2j+1]_2[2j+2]_2}y_j \Leftrightarrow y_j = \nu\frac{2j+1}{2\sqrt{j(j+1)}}y_{j-1},$$

which is equivalent to one (and only one) of the following conditions:

(i) $\xi=0$.

(ii) $y_j\neq 0$ for all $j\geq 0$ and $\xi=\tilde{\xi}:=\sum_j \nu^j 2^j\sqrt{j+1}\,j!/(2j+1)!!|e_{2j+1}\rangle\langle e_{2j+2}|$. Notice that, in this case, $\lim_j[y_j/(y_{j-1})]\nu<1$, so $\sum_{j\geq 0}y_j^2<\infty$ and $\tilde{\xi}\in\mathcal{G}_1^o$. Moreover $\mathcal{E}(\tilde{\xi})=\mu^2\|\tilde{\xi}\|^2$.

□

V. DIAGONAL MINIMA AND BIRTH AND DEATH PROCESSES

In this section we will deduce an estimate for the constants A_0^p, in order to conclude the computation of the quantum spectral gap. Indeed, Propositions 4 [relation (10)] and 5 guarantee that

$$\text{gap } L = \lambda^2 \wedge A_0^e \wedge A_0^o. \tag{19}$$

It is important to underline that $A_0^e \wedge A_0^o$ is the spectral gap of the diagonal restriction of the semigroup, which is a classical Markov process. This classical process is given by the restriction of the semigroup generated by £ to the subalgebra of multiplication operators and it can be described by introducing its infinitesimal generator, say $\mathcal{A}$, acting on the space $l^\infty(\mathbb{N})$ of bounded sequences.

For any f in $l^\infty(\mathbb{N})$, let us denote by $M_f\in\mathcal{B}(h)$ the multiplication operator by f, $M_f=\sum_j f(j)|e_j\rangle\langle e_j|$, then the classical generator $\mathcal{A}$ is the (unique) operator satisfying

$$£(M_f) = M_{\mathcal{A}f} \quad \text{for } f\in D(\mathcal{A}) := \{f\in l^\infty(\mathbb{N}): M_f\in D(£)\}.$$

Then we can write a formal explicit expression for $\mathcal{A}$,

TABLE I. Birth and death rates.

	$\mathcal{A}^e$	$\mathcal{A}^o$	$\mathcal{A}^{\text{linear}}$
Birth rates b_j	$\lambda^2(2j+1)(2j+2)$	$\lambda^2(2j+2)(2j+3)$	$\lambda^2(j+1)$
Death rates d_j	$2\mu^2 j(2j-1)$	$2\mu^2 j(2j+1)$	$\mu^2 j$

$$\mathcal{A}f = \sum_j e_j\{\lambda^2(j+1)(j+2)(f_{j+2}-f_j) - \mu^2 j(j-1)(f_j - f_{j-2})\}.$$

Following the same ideas of the previous sections, we can distinguish the action of the generator on even and odd indices. For f in $l^\infty(\mathbb{N})$, we denote by f^e and f^o the bounded sequences containing, respectively, the even and odd components of f, i.e., with components

$$f_j^e = f_{2j}, \quad f_j^o = f_{2j+1}.$$

We also introduce the operators $\mathcal{A}^e$ and $\mathcal{A}^o$, formally defined on a dense subspace of $l^\infty(\mathbb{N})$ by

$$\mathcal{A}^e f = \sum_j e_j\{\lambda^2(2j+1)(2j+2)(f_{j+1}-f_j) - \mu^2 2j(2j-1)(f_j - f_{j-1})\},$$

$$\mathcal{A}^o f = \sum_j e_j\{\lambda^2(2j+2)(2j+3)(f_{j+1}-f_j) - \mu^2 2j(2j+1)(f_j - f_{j-1})\}.$$

Then a straightforward computation shows that $\mathcal{A}^e$ and $\mathcal{A}^o$ describe the action of $\mathcal{A}$ on even and odd indices, respectively, in the sense that

$$\mathcal{A}f = \sum_j \{(\mathcal{A}^e f^e)_j e_{2j} + (\mathcal{A}^o f^o)_j e_{2j+1}\}.$$

$\mathcal{A}^e$ and $\mathcal{A}^o$ are the generators of two birth and death processes with quadratic rates.

In the following table we write, in the first two columns, the birth and death rates of these two generators and a third one with linear rates, for which the spectral gap is known and that we will use for comparison. By standard well-known results, see Ref. 5 or,[13] we know that, for a birth and death process with strictly positive rates b_j and d_j, we can immediately write the following.

Notice that the three generators described in Table I have the same invariant probability measure,

$$\pi_u = (1-\nu^2)\nu^{2u}, \quad \nu = \lambda/\mu.$$

Proposition 6: $A_0^p = \text{gap}\,\mathcal{A}^p$ $(p=e,o)$.

Proof: By restricting $\mathcal{T}$ to the subalgebra of diagonal operators, the invariant state ρ_p can be identified with the invariant measure π_p, $p \in \{e,o\}$, where π_e and π_o are mutually singular and $\pi_e(2j) = \pi_o(2j+1) = (1-\nu^2)\nu^{2j}$. Take the case of even indices, so $p=e$ (for $p=o$ it will be the same). It is sufficient to use the definitions of A_o^e (Proposition 4) of gap $\mathcal{A}^e$ (in the Table II) and observe that they are infima of the same quantities.

TABLE II. Birth and death processes.

Invariant measures	$\pi = \Sigma_{u\geq 0}\pi_u e_u$, with $\pi_u = \pi_0 \Pi_{j=0}^{u-1} b_j/(d_{j+1})$ for $u \geq 1$ (not necessarily finite!)
Infinitesimal generator	$\mathcal{A}(f) = b_j(f_{j+1}-f_j) - d_j(f_j - f_{j-1})$
Quadratic form	$\mathcal{E}(\pi^{1/2}f) = \Sigma_{u\geq 0} b_u (f_{u+1}-f_u)^2 \pi_u$
Spectral gap	gap $\mathcal{A} = \inf\{\mathcal{E}(\pi^{1/2}f), \|f\|_\pi^2 = 1, \Sigma f_j \pi_j = 0\}$ where $\|f\|_\pi^2 = \Sigma_{u\geq 0}|f_u|^2 \pi_u$

Indeed, denote by $\mathcal{E}^e$ the quadratic form on $l^2(\mathbb{N})$ associated with $\mathcal{A}^e$, take f in $l^\infty(\mathbb{N})$, and introduce $\xi^f := \sum_{j\geq 0}\nu^j f_j |e_{2j}\rangle\langle e_{2j}| \in \mathcal{G}_0^e$; then notice that

$$\|f\|_\pi^2 = \sum_j \pi_j |f_j|^2 = \|\xi^f\|^2$$

and

$$\sum_j \pi_j f_j = 0 \quad \text{iff } \xi^f \perp \rho_e^{1/2}.$$

By the previous Table II,

$$\mathcal{E}^e(\pi^{1/2}f) = \sum_{u\geq 0} (2u+1)(2u+2)(f_{u+1}-f_u)^2(1-\nu^2)\nu^{2u} = \mathcal{E}(\xi^f),$$

where $\mathcal{E}$ is as usual the quadratic form associated with L and we have written the explicit expression of $\mathcal{E}(\xi^f)$ given by (14) with $m=0$. □

Remark: Comparison with the linear birth and death process. We recall that, for a birth and death generator $\mathcal{A}$ with birth rates $b_j = \lambda^2(j+1)$ and death rates $d_j = \mu^2 j$, we have called it linear in Table I, it is known (see again Ref. 3 or,[5] Sec. 9.3) that

$$\text{gap } (\mathcal{A}^{\text{linear}}) = \mu^2 - \lambda^2.$$

Now, using the relations written before for the birth and death generators, we have that the spectral gaps of the three generators we have considered are the minimum of their quadratic forms on the same set of functions because they have the same invariant measure. So, since, with obvious notations,

$$\mathcal{E}^o(\pi^{1/2}f) \geq \mathcal{E}^e(\pi^{1/2}f) \geq 2\mathcal{E}^{\text{linear}}(\pi^{1/2}f),$$

then the same inequalities hold for the spectral gaps

$$\text{gap } (\mathcal{A}^o) \geq \text{gap } (\mathcal{A}^e) \geq 2 \text{ gap } (\mathcal{A}^{\text{linear}}) = 2(\mu^2 - \lambda^2).$$

This comparison, relation (19) and the previous proposition together imply

$$\text{gap } L = \lambda^2 \wedge \text{gap } (\mathcal{A}^e) \geq \lambda^2 \wedge (2(\mu^2 - \lambda^2)).$$

So we conclude the following.

(1) At least in the case when $\lambda^2 < 2(\mu^2 - \lambda^2)$ (i.e., when $\nu^2 < 2/3$) gap $L = \lambda^2$.
(2) In order to get the same conclusion in the general case, it will be enough to prove that gap$(\mathcal{A}^e)$ is always bigger than λ^2. This will be our next step; better, we shall prove that gap$(\mathcal{A}^e) \geq \mu^2 \geq \lambda^2$.

Since we cannot achieve the desired estimate by the usual well-known methods, we recover a technique used by Liggett (see Ref. 13, proof of Proposition 3.5) introducing a slight variation and trying to make the computations optimal for the generator $\mathcal{A}^e$; we deduce the estimate written in the following proposition, which is essentially obtained by an elementary Schwarz inequality and by using the exponential form of the invariant measure.

Proposition 7: For any positive sequence $(a_n)_n$, define the (strictly positive) constant

$$B(\nu) := \sup_{u\geq 0} \frac{(\mu^2(1-\nu^2))^{-1}}{a_u(2u+1)(2u+2)} \left\{ \sum_{v\leq u} (1-\nu^{2(v+1)})a_v + (\nu^{-2(u+1)}-1)\sum_{v>u} \nu^{2(v+1)}a_v \right\}.$$

Then gap$(\mathcal{A}^e) \geq (B(\nu))^{-1}$.

Proof: We recall that the quadratic form, for f in $D(\mathcal{A}^e) \subset l^\infty(\mathbb{N})$, can be written

$$\mathcal{E}^e(\pi^{1/2}f) = \sum_{u\geq 0} \lambda^2(2u+1)(2u+2)(f_{u+1}-f_u)^2\pi_u.$$

For any positive sequence $(a_n)_n$ we have

$$(f_y - f_x)^2 \leq \sum_{u=x}^{y-1}(f_{u+1}-f_u)^2(a_u)^{-1}\sum_{v=x}^{y-1} a_v. \tag{20}$$

So, rearranging the proof of Proposition 3.5 in Ref. 13,

$$\begin{aligned}
1 = \|f\|_\pi^2 &= \sum_{x<y}\pi_x\pi_y(f_y-f_x)^2 \leq (1-\nu^2)^2\sum_{x<y}\nu^{2x}\nu^{2y}\sum_{u=x}^{y-1}(f_{u+1}-f_u)^2(a_u)^{-1}\sum_{v=x}^{y-1}a_v\\
&= (1-\nu^2)^2\sum_{u\geq 0}(f_{u+1}-f_u)^2(a_u)^{-1}\sum_{v\geq 0}a_v\sum_{x\leq u\wedge v}\nu^{2x}\sum_{y>u\vee v}\nu^{2y}\\
&= \sum_{u\geq 0}(f_{u+1}-f_u)^2(a_u)^{-1}\sum_{v\geq 0}(1-\nu^{2(u\wedge v+1)})\nu^{2(u\vee v+1)}a_v\\
&= \sum_{u\geq 0}(f_{u+1}-f_u)^2(a_u)^{-1}\left\{\sum_{v\leq u}(1-\nu^{2(v+1)})\nu^{2(u+1)}a_v + \sum_{v>u}(1-\nu^{2(u+1)})\nu^{2(v+1)}a_v\right\}\\
&= \sum_{u\geq 0}(f_{u+1}-f_u)^2(2u+1)(2u+2)\nu^{2(u+1)}\cdot\frac{1}{a_u(2u+1)(2u+2)}\\
&\quad\times\left\{\sum_{v\leq u}(1-\nu^{2(v+1)})a_v + (\nu^{-2(u+1)}-1)\sum_{v>u}\nu^{2(v+1)}a_v\right\} \leq B(\nu)\mathcal{E}^e(f),
\end{aligned}$$

and we conclude simply by the definition of spectral gap. □

Lemma 8: Take a positive summable sequence $(a_n)_{n\geq 0}$ *and define the positive decreasing "tail" sequence* $(A_k)_{k\geq 0}$ *by* $A_k = \Sigma_{n\geq k}a_k$. *Then*

$$B(\nu) = \sup_{u\geq 0}\frac{1}{\mu^2 a_u(2u+1)(2u+2)}\sum_{k\geq 0}\nu^{2k}(A_k - A_{k+u+1}).$$

Proof: Just note that the sums appearing in the definition of $B(\nu)$ can be written in the following form:

$$\begin{aligned}
&(1-\nu^2)^{-1}\sum_{v\leq u}(1-\nu^{2(v+1)})a_v + (\nu^{-2(u+1)}-1)\sum_{v>u}\nu^{2(v+1)}a_v\\
&= \sum_{v\leq u}\sum_{k\leq v}\nu^{2k}a_v + (\nu^{-2(u+1)}-1)\sum_{v>u}\sum_{k\geq v+1}\nu^{2k}a_v = \sum_{k\leq u}\nu^{2k}\sum_{v=k}^{u}a_v + (\nu^{-2(u+1)}-1)\sum_{k>u+1}\nu^{2k}\sum_{v=u+1}^{k-1}a_v\\
&= \sum_{k\leq u}\nu^{2k}(A_k - A_{u+1}) + (\nu^{-2(u+1)}-1)\sum_{k>u+1}\nu^{2k}(A_{u+1}-A_k)\\
&= \sum_{k\neq u+1}\nu^{2k}A_k - \nu^{-2(u+1)}\sum_{k>u+1}\nu^{2k}A_k - (1-\nu^{2(u+1)})A_{u+1} = \sum_{k\geq 0}\nu^{2k}A_k - \nu^{-2(u+1)}\sum_{k\geq u+1}\nu^{2k}A_k\\
&= \sum_{k\geq 0}\nu^{2k}(A_k - A_{k+u+1}).
\end{aligned}$$

□

So we have to find a "good" sequence (a_n) and appropriately estimate the related constant $B(\nu)$. But how to choose the good (a_n)? The estimate of Proposition 7 is obtained by applying a Schwarz inequality in relation (20). At least when the spectral gap is an eigenvalue of the operator, we get the optimal estimate when the sequence f is an eigenvector related to this eigenvalue of the generator and relation (20) is true with identity, so $|f_{k+1}-f_k|=a_k$. Obviously, we do not know such a function f, this is, in general, more difficult than computing the spectral gap, however, we can guess a good sequence considering the behavior of the limit case for $\nu\to 1^-$, i.e., solving the equation $Lf=-f$. This is how we could get it, but it is not necessary to write down all the computations since they would be quite long and the proof of our result is anyway complete also without them.

Lemma 9: Choose $a_n=(2n-1)!!/(2n+2)!!$, $n\geqslant 0$. *Then* $(a_n)_{n\geqslant 0}$ *is a positive summable sequence and (i)* $A_k=\Sigma_{n\geqslant k}a_n(2k-1)!!/(2k)!!=(2k+2)a_k$, *and* $1/2\sqrt{k}\leqslant A_k\leqslant 1/2\sqrt{3/2k+1}$; *(ii)* $\Sigma_{j=0}^{k}A_j=(2k+1)!!/(2k)!!=(2k+2)A_{k+1}$; *(iii)* $\Sigma_{k\geqslant 0}a_k=1$ *and* $\Sigma_{k\geqslant 0}\nu^{2k}a_k=(1-\sqrt{1-\nu^2})/\nu^2$.

Proof:

(i) Notice that

$$\frac{(2k-1)!!}{(2k)!!}=\frac{1}{2}\exp\left(\sum_{j=2}^{k}\ln\frac{2j-1}{2j}\right)=\frac{1}{2}\exp\left(-\sum_{j=2}^{k}\int_{2j-1}^{2j}\frac{dt}{t}\right),$$

but

$$\frac{1}{2}\int_{2j-2}^{2j}\frac{dt}{t}\geqslant\int_{2j-1}^{2j}\frac{dt}{t}\geqslant\frac{1}{2}\int_{2j-1}^{2j+1}\frac{dt}{t},$$

and so

$$\frac{1}{2\sqrt{k}}\leqslant\frac{(2k-1)!!}{(2k)!!}\leqslant\frac{1}{2}\sqrt{\frac{3}{2k+1}}.$$

Then it is obvious that $a_k=[(2k-1)!!/(2k)!!](2k+2)^{-1}$ is the term of a summable sequence. To verify that $((2k-1)!!/(2k)!!)_k$ is indeed the tail sequence of $(a_k)_k$, it is enough to notice that $(2k-1)!!/(2k)!!-(2k+1)!!/(2k+2)!!=a_k$ and take into account that the series $-\Sigma_{j=2}^{\infty}\int_{2j-1}^{2j}$ diverges.

(ii) The relation can be easily verified by induction.

(iii) We denote by T the time of first return in 0 for a symmetric random walk on the integers. The distribution of T is described by

$$\mathbb{P}\{T=2n\}=\frac{(2n-3)!!}{(2n)!!}=a_{n-1},\quad n\geqslant 1$$

(so $\Sigma_{n\geqslant 0}a_n=1$), and its moment generating function is given by

$$\phi(s)=\mathbb{E}[s^T]=1-\sqrt{1-s^2}\tag{21}$$

(see Sec. 20 in Ref. 12, for instance). So

$$\sum_{k\geqslant 0}\nu^{2k}a_k=\sum_{k\geqslant 1}\nu^{2k-2}\mathbb{P}\{T=2k\}=\mathbb{E}[\nu^{T-2}]=\frac{\phi(\nu)}{\nu^2}=\frac{1-\sqrt{1-\nu^2}}{\nu^2}.$$

□

Theorem 10: *For the spectral gap of the diagonal restriction* $\mathrm{gap}(\mathcal{A})=\mathrm{gap}(\mathcal{A}^e)$, *we have*

$$\mu^2(1+\sqrt{1-\nu^2})\leqslant\mathrm{gap}(\mathcal{A}^e)\leqslant\mu^2\left(1-3\frac{2-\dfrac{1-\nu^2}{\nu}\ln\dfrac{1+\nu}{1-\nu}}{4\ln(1-\nu^2)}\right)\leqslant 2\mu^2.$$

Moreover the bound is optimal for ν *close to 0 and 1.*

Proof: The lower bound follows by using Proposition 7 with $a_k=(2k-1)!!/(2k+2)!!$. We are going to prove that, with this choice, we have $B(\nu)=1/\mu^2(1+\sqrt{1-\nu^2})$.

We introduce the map $V:\mathbb{N}\to[0,+\infty)$, $V(u):=(2u)!!/(2u+1)!!\sum_{k\geqslant 0}\nu^{2k}(A_k-A_{k+u+1})$, so that $\mu^2B(\nu)=\sup_{u\geqslant 0}V(u)$ (by Lemma 8). We want to prove that V is a nonincreasing function for all $\nu\in(0,1]$, so the maximum is obtained for $u=0$ and can be explicitly computed since

$$\mu^2B(\nu)=V(0)=\sum_{k\geqslant 0}\nu^{2k}a_k=\frac{1-\sqrt{1-\nu^2}}{\nu^2}=\frac{1}{1+\sqrt{1-\nu^2}},$$

where the sum follows from the previous Lemma.

So we just have to prove that the increments of function V,

$$\begin{aligned}V(u+1)-V(u)&=\frac{(2u+2)!!}{(2u+3)!!}\sum_{k\geqslant 0}\nu^{2k}(A_k-A_{k+u+2})-\frac{(2u)!!}{(2u+1)!!}\sum_{k\geqslant 0}\nu^{2k}(A_k-A_{k+u+1})\\&=\frac{(2u)!!}{(2u+1)!!}\sum_{k\geqslant 0}\nu^{2k}\left(-\frac{1}{2u+3}A_k+A_{k+u+1}-\frac{(2u+2)}{(2u+3)}A_{k+u+2}\right)\\&=\frac{(2u)!!}{(2u+3)!!}\sum_{k\geqslant 0}\nu^{2k}(-A_k+(2u+3)A_{k+u+1}-(2u+2)A_{k+u+2}),\end{aligned}\tag{22}$$

are negative. This will be enough to conclude.

First notice that the partial sums with $\nu=1$ are negative for all n and u,

$$\begin{aligned}s_n&:=\sum_{k=0}^{n}(-A_k+(2u+3)A_{k+u+1}-(2u+2)A_{k+u+2})=\sum_{k=0}^{n}(A_{k+u+1}-A_k)+(2u+2)\sum_{k=0}^{n}(A_{k+u+1}-A_{k+u+2})\\&=-\sum_{k=0}^{n}A_k+\sum_{k=u+1}^{n+u+1}A_k+(2u+2)(A_{u+1}-A_{n+u+2})=(2n+2)(A_{n+u+2}-A_{n+1})\leqslant 0,\end{aligned}$$

where we used Lemma 9 (ii) to obtain the last equality (one could also compute the series $\lim_n s_n=0$ similarly). Now define $s_{-1}=0$ and introduce weights depending on ν, then we have

$$\begin{aligned}&\sum_{k=0}^{n}\nu^{2k}(-A_k+(2u+3)A_{k+u+1}-(2u+2)A_{k+u+2})\\&\quad=\sum_{k=0}^{n}\nu^{2k}(s_k-s_{k-1})=\sum_{k=0}^{n}\nu^{2k}s_k-\sum_{k=0}^{n-1}\nu^{2(k+1)}s_k=\nu^{2n}s_n+(1-\nu^2)\sum_{k=0}^{n-1}\nu^{2k}s_k\leqslant 0.\end{aligned}$$

Letting n tend to infinity, we deduce $V(u+1)-V(u)\leqslant 0$ for any u [remember (22)].

The upper bound. By definition of spectral gap, for any bounded sequence h such that $\sum_j\pi_jh_j=0$, we have $\text{gap}(\mathcal{A}^e)\leqslant\mathcal{E}^e(\pi^{1/2}h)/\|h\|_\pi^2$. Take the sequence $(a_k)_k$ (and consequently A_k) as before and choose the sequence h as

$$h_k=A_k-c=\frac{(2k-1)!!}{(2k)!!}-c,$$

where we have to choose the constant c in such a way that $\sum_j\pi_jh_j=0$, hence $c=(1-\nu^2)\sum_j\nu^{2j}A_j$. We can compute c deriving the generating function ϕ introduced in (21); indeed we have

$$\frac{s}{\sqrt{1-s^2}}=\phi'(s)=\mathbb{E}[Ts^{T-1}]=\sum_{n\geqslant 1}2ns^{2n-1}a_{n-1},$$

then

$$c=(1-\nu^2)\sum_{j\geq 0}\nu^{2j}(2j+2)a_j=\sqrt{1-\nu^2}.$$

Now one can easily write

$$\|h\|^2=(1-\nu^2)\sum_{j\geq 1}\nu^{2j}A_j^2,\quad \mathcal{E}^e(\pi^{1/2}h)=\mu^2(1-\nu^2)\sum_{j\geq 1}\nu^{2j}\frac{2j}{2j-1}A_j^2$$

and

$$\frac{\mathcal{E}^e(\pi^{1/2}h)}{\|h\|^2}=\mu^2\left(1+\frac{\Sigma_{j\geq 1}\nu^{2j}\dfrac{1}{2j-1}A_j^2}{\Sigma_{j\geq 1}\nu^{2j}A_j^2}\right).$$

We cannot compute explicitly the sums in the previous expression, so we use the estimates of A_j obtained in Lemma 9 (i) and deduce

$$\frac{\mathcal{E}^e(\pi^{1/2}h)}{\|h\|^2}\leq\mu^2\left(1+3\frac{\Sigma_{j\geq 1}\nu^{2j}\dfrac{1}{2j-1}\dfrac{1}{2j+1}}{\Sigma_{j\geq 1}\nu^{2j}\dfrac{1}{j}}\right)=\mu^2(1+\varphi(\nu)),$$

where

$$\varphi(\nu):=3\frac{\Sigma_{j\geq 1}\nu^{2j}\dfrac{1}{2j-1}\dfrac{1}{2j+1}}{\Sigma_{j\geq 1}\nu^{2j}\dfrac{1}{j}}=\frac{3}{2}\frac{\Sigma_{j\geq 1}\nu^{2j}\left(\dfrac{1}{2j-1}-\dfrac{1}{2j+1}\right)}{\Sigma_{j\geq 1}\nu^{2j}\dfrac{1}{j}}\leq 1$$

[the inequality follows immediately since $((2j-1)(2j+1))^{-1}\leq(3j)^{-1}$]. Moreover, we can explicitly compute the series; simply notice that $\Sigma_{j\geq 1}\nu^{2j}/j=-\ln(1-\nu^2)$, $\Sigma_{j\geq 1}\nu^{2j}/(2j+1)=-1+(1/2\nu)\ln[(1+\nu)/(1-\nu)]$ and $\Sigma_{j\geq 1}\nu^{2j}/(2j-1)=\nu/2\ln[(1+\nu)/(1-\nu)]$, then

$$\varphi(\nu)=-\frac{3}{4}\left(\frac{2-\dfrac{1-\nu^2}{\nu}\ln\dfrac{1+\nu}{1-\nu}}{\ln(1-\nu^2)}\right).$$

Now it is easy to verify that the bounds are optimal for the extreme values of ν since

$$\lim_{\nu\to 0}\varphi(\nu)=1$$

and

$$\lim_{\nu\to 1}\varphi(\nu)=0.$$

□

VI. CONCLUSIONS AND REMARKS

We point out that the diagonal gap, $\mathrm{gap}(\mathcal{A}^e)$, cannot be equal to the bounds found in Theorem 10 for $\nu\in(0,1)$; but the estimates seem good, as the plot in Fig. 1 shows, it represents the upper and lower bounds as functions of ν, with unit$=\mu^2$ in the vertical axis.

We also underline again that the estimate we obtain for the diagonal gap allows us to compute anyway the exact value of the spectral gap for the quantum model we are interested in.

Let us use the notations in the proof of Proposition 5 and let κ be as in (1). Since the elements $\bar{\xi}$ and $\tilde{\xi}$ are partial minimum points of the quadratic form, it is natural to wonder if they are eigenvectors for the generator L of the semigroup acting on $L^2(h)$. A direct computation shows that this is true only for $\kappa=0$. Indeed

$$L(\bar{\xi}) = -\lambda^2\bar{\xi} + 2i\kappa\sum_{n\geq 0} 2n\bar{\xi}_{2n}|e_{2n}\rangle\langle e_{2n+1}|,$$

$$L(\tilde{\xi}) = -\mu^2\tilde{\xi} + 2i\kappa\sum_{n\geq 0}(2n+1)\tilde{\xi}_{2n+1}|e_{2n+1}\rangle\langle e_{2n+2}|.$$

Notice that $\bar{\xi}$ is the only possible eigenvector, up to multiplication by scalar numbers, associated with $-\lambda^2$, since, if x is such an eigenvector ($Lx=-\lambda^2 x$), then $\mathcal{E}(x)=\lambda^2\|x\|^2$ and so, by the proof of Proposition 5, x is a multiple of $\bar{\xi}$. Hence $-\lambda^2$ is an eigenvalue of L if and only if $\kappa=0$.

However, our result assures that

$$\|T_t x\| \leq \|x\| e^{-\lambda^2 t} \tag{23}$$

for any x in $L^2(h)$ orthogonal to $\rho_p^{1/2}$, $p\in\{e,o\}$ and λ^2 is the best constant we can choose for this relation. The constant is optimal in the sense that relation (23) is no more true if we replace λ^2 with any $\varepsilon>\lambda^2$.

Further, for $\kappa=0$, (23) becomes an equality if we choose $x=\bar{\xi}$. But we underline that, for $\kappa\neq 0$, an element x for which (23) becomes an equality does not exist.

(To explain the decay estimates written in the Introduction.) Take y in $\mathcal{B}(h)$ and a state σ_0 in the domain of attraction of ρ [i.e., $\rho=\lim_{t\to\infty}\mathcal{T}_{*t}(\sigma)$] and such that $\rho^{-1/4}\sigma_0\rho^{-1/4}$ is in $L^2(h)$. Notice that we can compute $\lim_{t\to\infty}\mathcal{T}_{*t}(\sigma)=\mathrm{tr}(\sigma_0 p_e)\rho_e+\mathrm{tr}(\sigma_0 p_o)\rho_o$ by Proposition 7.1 in Ref. 6. Then

$$|\mathrm{tr}(y\sigma_t)-\mathrm{tr}(y\rho)| = |\mathrm{tr}\{(\mathcal{T}_t(y-\mathrm{tr}(y\rho)\mathbb{1}))\sigma_0\}| \leq \|T_t(\rho^{1/4}(y-\mathrm{tr}(y\rho)\mathbb{1})\rho^{1/4})\|\|\rho^{-1/4}\sigma_0\rho^{-1/4}\|,$$

where the decay of the first term can be controlled by using relations (9) or (13) and our estimates of the involved exponential rates. In fact, we can write

$$\begin{aligned}|\mathrm{tr}(x\sigma_t)| &\leq e^{-\lambda^2 t}\|\rho^{1/4}x\rho^{1/4}\|\|\rho^{-1/4}\sigma_0\rho^{-1/4}\|,\\ |\mathrm{tr}(y\sigma_t)-\mathrm{tr}(y\rho)| &\leq e^{-gt}\|\rho^{1/4}(y-\mathrm{tr}(y\rho)\mathbb{1})\rho^{1/4}\|\|\rho^{-1/4}\sigma_0\rho^{-1/4}\|,\end{aligned} \tag{24}$$

for every off-diagonal (diagonal) bounded operator x (y) on h. The inequalities show that, when $\rho^{-1/4}\sigma_0\rho^{-1/4}$ is Hilbert–Schmidt, the off-diagonal part of σ_t vanishes with an exponential rate λ^2 in the weak operator topology and the diagonal part converges *faster* toward an invariant state with a bigger exponential rate g.[7]

Inequalities (3) in the Introduction follow from (24) choosing $x=|e_k\rangle\langle e_j|$ with $j\neq k$ and $y=|e_j\rangle\langle e_j|$.

ACKNOWLEDGMENTS

The financial support from CONACYT-México (Grant No. 49510-F), the MIUR-PRIN programme "Quantum Markov Semigroups and Quantum Stochastic Differential Equations" 2006-2007, and the project Mexico-Italia "Dinámica Estocástica con Aplicaciones en Física y Finanzas," are gratefully acknowledged.

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