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Asymptotic lower bound for the gap of Hermitian matrices having ergodic ground states and infinitesimal off-diagonal elements

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Abstract – Given a $M \times M$ Hermitian matrix $\boldsymbol{\mathcal{H}}$ with possibly degenerate eigenvalues $\mathcal{E}_1 < \mathcal{E}_2 < \mathcal{E}_3 < \ldots$, we provide, in the limit $M \to \infty$, a lower bound for the gap $\mu_2 = \mathcal{E}_2 - \mathcal{E}_1$ assuming that i) the eigenvector (eigenvectors) associated to $\mathcal{E}_1$ is ergodic (are all ergodic) and ii) the off-diagonal terms of $\boldsymbol{\mathcal{H}}$ vanish for $M \to \infty$. Under these hypotheses, we find $\underline{\lim}_{M\to\infty} \mu_2 \geq \overline{\lim}_{M\to\infty} \min_n \mathcal{H}_{n,n}$. This general result turns out to be important for upper bounding the relaxation time of linear master equations characterized by a matrix equal, or isospectral, to $\boldsymbol{\mathcal{H}}$. As an application, we consider symmetric random walks with infinitesimal jump rates and show that the relaxation time is upper bounded by the configurations (or nodes) with minimal degree.

editor's choice

Introduction. – In classical and quantum physics, as well as in applied sciences, many systems can be effectively described by linear master equations [1–6]. If the system is characterized by M states that we can label with an index $n \in \{1, \ldots, M\}$, the master equation reads

$$\frac{\mathrm{d}\boldsymbol{p}(t)}{\mathrm{d}t} = -\boldsymbol{\mathcal{L}}\, \boldsymbol{p}(t), \tag{1}$$

where $\boldsymbol{p}(t)^T = (p_1(t), \ldots, p_n(t))$ is a row vector in which each component $p_n(t)$ represents the probability that the system is in the state n at time t. The matrix $\boldsymbol{\mathcal{L}}$ (a weighted Laplacian) is a singular $M \times M$ real matrix having the property $\sum_m \mathcal{L}_{m,n} = 0$, $n \in \{1, \ldots, M\}$, which stems from the conservation of the total probability $\sum_m p_m(t) = 1$, and where, for $m \neq n$, $-\mathcal{L}_{m,n} \geq 0$ represents the transition rate from state n to state m.

In some cases $\boldsymbol{\mathcal{L}}$ is symmetric and, therefore, has real distinct eigenvalues $\mu_1 = 0, \mu_2, \mu_3, \ldots$. Furthermore, if the associated stochastic matrix $\boldsymbol{\mathcal{S}} = \mathbf{1} - r^{-1}\boldsymbol{\mathcal{L}}$, where $r = \max_n \mathcal{L}_{n,n}$, is irreducible, the Perron-Frobenious theorem [7] implies that $\mu_1 = 0$ is the minimal eigenvalue, it is simple (because μ_1 is real), and $\mu_k > 0$ for $k \geq 2$. Finally, we have that $p_m^{(\mathrm{eq})} = 1/M$ is the m-th component of the normalized eigenvector $\boldsymbol{p}^{(\mathrm{eq})}$ corresponding to the eigenvalue $\mu_1 = 0$.

If $\boldsymbol{\mathcal{L}}$ is asymmetric, we expect, in general, complex eigenvalues. However, if we assume that a detailed balance condition holds, *i.e.* there exist M positive values, $p_m^{(\mathrm{eq})} > 0$, such that $\mathcal{L}_{m,n} p_n^{(\mathrm{eq})} = \mathcal{L}_{n,m} p_m^{(\mathrm{eq})}$, then $\boldsymbol{\mathcal{L}}\boldsymbol{p}^{(\mathrm{eq})} = 0$ ($\boldsymbol{p}^{(\mathrm{eq})}$ is a right eigenvector), and the spectrum of $\boldsymbol{\mathcal{L}}$ is still real and non-negative. In fact, $\boldsymbol{\mathcal{L}}$ is similar (and therefore isospectral) to the real symmetric matrix $\boldsymbol{\mathcal{L}}_s = \boldsymbol{\mathcal{R}}^{-1}\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{R}}$, where $\boldsymbol{\mathcal{R}}$ is the diagonal matrix defined by the elements $\mathcal{R}_{m,n} = \delta_{m,n}(p_m^{(\mathrm{eq})})^{1/2}$. Note that the condition $p_m^{(\mathrm{eq})} > 0$ for any m, which ensures the existence of the inverse $\boldsymbol{\mathcal{R}}^{-1}$, guarantees that both $\mathcal{L}_{m,n}$ and $\mathcal{L}_{n,m}$ are 0 if one of the two is so.

Whether $\boldsymbol{\mathcal{L}}$ is symmetric or not, but satisfies a detailed balance condition and has an associated irreducible stochastic matrix $\boldsymbol{\mathcal{S}}$, its spectrum consists of real eigenvalues $0 = \mu_1 < \mu_2 < \mu_3 < \ldots$. The eigenvalue $\mu_1 = 0$ is simple and the corresponding eigenvector $\boldsymbol{p}^{(\mathrm{eq})}$ is necessarily an ergodic ground state, *i.e.* all its components are positive, and represents the unique stationary state of eq. (1) toward which the system eventually converges. For almost all initial conditions, up to terms exponentially smaller, we have $\|\boldsymbol{p}(t) - \boldsymbol{p}^{(\mathrm{eq})}\| \sim C \exp(-\mu_2 t)$, where C is a constant. In other words, μ_2, the minimal non-zero eigenvalue of $\boldsymbol{\mathcal{L}}$, provides the inverse of the relaxation time to equilibrium. Determining μ_2 is evidently of crucial importance.

In particular, the existence of a finite lower bound to μ_2 in the limit of $M \to \infty$ is pivotal in establishing if $\boldsymbol{\mathcal{L}}$ represents a gapped system [8].

Motivated by the above remarks, we consider a generic real symmetric or, more in general, Hermitian matrix $\boldsymbol{\mathcal{H}}$ and let $\mathcal{E}_1 < \mathcal{E}_2 < \mathcal{E}_3 < \dots$ be its distinct, possibly degenerate, eigenvalues. We are interested in evaluating $\mu_2 = \mathcal{E}_2 - \mathcal{E}_1$. The matrix $\boldsymbol{\mathcal{H}}$ can be seen as a M-dimensional Hamiltonian operator. In fact, we can always split $\boldsymbol{\mathcal{H}}$ as

$$\boldsymbol{\mathcal{H}} = \boldsymbol{\mathcal{V}} + \boldsymbol{\mathcal{K}}, \tag{2}$$

where, on the chosen base $\{|n\rangle\}$, $n \in \{1, \dots, M\}$,

$$\mathcal{V}_{m,n} = \delta_{m,n} \mathcal{V}_n, \tag{3}$$

and

$$\mathcal{K}_{m,n} = -\left(1 - \delta_{m,n}\right) \sigma_{m,n}, \tag{4}$$

the definitions of the vector $\mathcal{V}_n$ and matrix $\sigma_{m,n}$ being implicit. Note that $\sigma_{m,n}$ is an Hermitian matrix with $\sigma_{m,m} = 0$ and its off-diagonal elements have non-defined signs or phases. With such a decomposition, $\boldsymbol{\mathcal{V}}$ and $\boldsymbol{\mathcal{K}}$ play the role of "potential" and "kinetic" operators, respectively. Suppose that the lowest eigenstate $\mathcal{E}_1$ is k-fold degenerate, with k finite, and let $|\mathcal{E}_1^{(1)}\rangle, \dots, |\mathcal{E}_1^{(k)}\rangle$ be the corresponding orthonormalized eigenstates. We represent the components of each ground state (GS) in the form

$$\langle n|\mathcal{E}_1^{(i)}\rangle = \frac{u_n^{(i)}}{\sqrt{Z^{(i)}}}, \quad Z^{(i)} = \sum_n |u_n^{(i)}|^2, \quad i = 1, \dots, k. \tag{5}$$

In case $\mathcal{E}_1$ is simple, *i.e.* $k = 1$, we will omit the superscript $^{(i)}$.

In this paper, we state and prove a general lower bound for the gap $\mu_2 = \mathcal{E}_2 - \mathcal{E}_1$ valid for a large class of Hermitian matrices $\boldsymbol{\mathcal{H}}$ whose unique or multiple ground states are all ergodic. By an ergodic GS here we mean that, for any M, each component of the GS is non-zero, and finite (apart from the normalization condition). More precisely, we say that the GS $|\mathcal{E}_1\rangle$ is ergodic if

$$\exists\ M_0: \quad \forall M \geq M_0, \quad 0 < |u_n|, \quad \forall n. \tag{6}$$

In other words, $|\mathcal{E}_1\rangle$ is ergodic if all the states $|n\rangle$ tend to be populated. In the next section, we precisely state and prove the lower bound in the form of a theorem valid for arbitrary finite degeneracy of $\mathcal{E}_1$. Note that the index k of this degeneracy is thought to be a constant independent of the size M. Then we apply the result to symmetric random walks characterized by infinitesimal jump rates, and show that the relaxation time τ is upper bounded by the minimal degree of the configurations (called nodes in graph theory).

Lower bound for μ_2. – We shall make use of the definitions (2)–(6) previously introduced and assume that the following fair condition always applies: $\overline{\lim}_{M\to\infty} \mathcal{E}_1/Z = 0$.

Theorem 1 *(Non-degenerate case). Let $\boldsymbol{\mathcal{H}}$ be a $M \times M$ Hermitian matrix with distinct, possibly degenerate, eigenvalues $\mathcal{E}_1 < \mathcal{E}_2 < \mathcal{E}_3 < \dots$. Let us suppose that the GS of $\boldsymbol{\mathcal{H}}$ is unique, ergodic, and that there exists a positive function $g(M)$ such that*

$$\sigma = \max_{m,n} \frac{|\sigma_{m,n}|}{|u_n u_m|} < g(M), \tag{7}$$

$$\lim_{M\to\infty} g(M) = 0, \quad \lim_{M\to\infty} \frac{1}{Z^2 g(M)} = 0. \tag{8}$$

Then, for the gap $\mu_2 = \mathcal{E}_2 - \mathcal{E}_1$, we have

$$\underline{\lim}_{M\to\infty} \mu_2 \geq \overline{\lim}_{M\to\infty} \min_n \mathcal{V}_n. \tag{9}$$

The same result holds essentially unchanged if $\mathcal{E}_1$ is k-fold degenerate, with k finite and independent of M, and each one corresponding GS is ergodic.

Theorem 2 *(Finite degenerate case). Let $\boldsymbol{\mathcal{H}}$ be a $M \times M$ Hermitian matrix with distinct, possibly degenerate, eigenvalues $\mathcal{E}_1 < \mathcal{E}_2 < \mathcal{E}_3 < \dots$. Let us suppose that we have k degenerate ergodic GSs and there exists a positive function $g(M)$ such that*

$$\sigma = \max_i \max_{m,n} \frac{|\sigma_{m,n}|}{|u_n^{(i)} u_m^{(i)}|} < g(M), \tag{10}$$

$$\lim_{M\to\infty} g(M) = 0, \quad \lim_{M\to\infty} \frac{1}{(Z^{(i)})^2 g(M)} = 0. \tag{11}$$

Then, for the gap $\mu_2 = \mathcal{E}_2 - \mathcal{E}_1$, we have

$$\underline{\lim}_{M\to\infty} \mu_2 \geq \overline{\lim}_{M\to\infty} \min_n \mathcal{V}_n. \tag{12}$$

Proof. We shall make use of the following short-hand notation: given a Hermitian operator $\boldsymbol{C}$, $GSL[\boldsymbol{C}]$ stands for the GS level of $\boldsymbol{C}$ (*i.e.*, the minimal eigenvalue of $\boldsymbol{C}$).

Let us first suppose that the GS of $\boldsymbol{\mathcal{H}}$ is unique and that $\mathcal{E}_1 = 0$ (so that $\mu_2 = \mathcal{E}_2$). Let us introduce the following new Hamiltonian:

$$\boldsymbol{\mathcal{F}}(\lambda) = \boldsymbol{\mathcal{H}} + \lambda |\mathcal{E}_1\rangle\langle\mathcal{E}_1|. \tag{13}$$

We have

$$GSL\left[\boldsymbol{\mathcal{F}}(\lambda)\right] = \begin{cases} \lambda, & \lambda < \mu_2, \\ \mu_2, & \lambda \geq \mu_2. \end{cases} \tag{14}$$

Equation (14) in particular implies that (the limit exists due to the monotonicity)

$$\mu_2 = \lim_{\lambda\to\infty} GSL\left[\boldsymbol{\mathcal{F}}(\lambda)\right]. \tag{15}$$

Uniform ergodic state. For the moment being, let us suppose that $\langle n|\mathcal{E}_1\rangle = 1/\sqrt{Z} = \sqrt{M}$ (such a situation occurs, for example, when we are considering a random walk, where $\mathcal{V}_n = -\sum_m \mathcal{K}_{m,n}$). In this case, we can rewrite eq. (13) as

$$\boldsymbol{\mathcal{F}}(\lambda) = \boldsymbol{\mathcal{V}} + \frac{\lambda}{Z}\boldsymbol{I} + \boldsymbol{\mathcal{K}} + \frac{\lambda}{Z}\boldsymbol{\mathcal{U}}, \tag{16}$$

where we have introduced

$$\boldsymbol{\mathcal{U}} = Z|\mathcal{E}_1\rangle\langle\mathcal{E}_1| - \boldsymbol{I}, \tag{17}$$

and $\boldsymbol{I}$ is the identity matrix. Note that, in the chosen base, we have $\mathcal{U}_{n,n} = 0$ and $\mathcal{U}_{m,n} = 1$ for $m \neq n$. Furthermore, from

$$\boldsymbol{\mathcal{U}}|\mathcal{E}_1\rangle = (Z-1)|\mathcal{E}_1\rangle, \tag{18a}$$

$$\boldsymbol{\mathcal{U}}|\mathcal{E}_i\rangle = -|\mathcal{E}_i\rangle, \qquad i \neq 1, \tag{18b}$$

it follows that for any $\alpha \in \mathbb{R}$

$$GSL\left[\alpha\boldsymbol{\mathcal{U}}\right] = \begin{cases} -|\alpha|(Z-1), & \alpha < 0, \\ -|\alpha|, & \alpha \geq 0. \end{cases} \tag{19}$$

Equation (19), despite its simplicity, is the key of our proof: when α changes from a negative to a positive value, the GS level of $\alpha\boldsymbol{\mathcal{U}}$ changes from being extensive, *i.e.* of order $O(Z)$, to being intensive, *i.e.* of order $O(1)$. From the first Weyl's inequality [7], we have

$$GSL\left[\boldsymbol{\mathcal{F}}(\lambda)\right] \geq \min_n \mathcal{V}_n + \frac{\lambda}{Z} + f\left(\frac{\lambda}{Z}, \boldsymbol{\sigma}\right), \tag{20}$$

where

$$f\left(\frac{\lambda}{Z}, \boldsymbol{\sigma}\right) = GSL\left[\boldsymbol{\mathcal{K}} + \frac{\lambda}{Z}\boldsymbol{\mathcal{U}}\right]. \tag{21}$$

We are not able to exactly calculate $f\left(\frac{\lambda}{Z}, \boldsymbol{\sigma}\right)$, however, from eq. (19) we see that

$$f\left(\frac{\lambda}{Z}, \boldsymbol{\sigma}\right) \sim \begin{cases} -(Z-1)\dfrac{\lambda}{Z} + GSL\left[\boldsymbol{\mathcal{K}}\right], & \dfrac{\lambda}{Z} \ll \sigma, \\ -\left(\dfrac{\lambda}{Z} - \sigma^*\right), & \dfrac{\lambda}{Z} \gg \sigma, \end{cases} \tag{22}$$

where σ has been defined in eq. (7), and $\sigma^* \in \mathbb{R}$ is some appropriate value of the order of magnitude of $2\sum_{m,n} \sigma_{m,n}/(M(M-1))$ (which is real). We stress that we do not need to know σ^*, nor to assume eq. (22) as an actual equality. However, eq. (22) makes clear that there exists a threshold in λ/Z, which is of order σ, where there occurs a sort of phase transition, the GS of $\boldsymbol{\mathcal{K}} + \boldsymbol{\mathcal{U}}\lambda/Z$ transiting from being extensive to being intensive. In the latter phase, we see that there exists a regime where λ/Z, σ and σ^* tend all to zero. In fact, let us choose $\lambda = \lambda(M)$ such that

$$\frac{\lambda(M)}{Z} = \sqrt{g(M)}. \tag{23}$$

With this choice and due to eqs. (7) and (8), we have that the following limits are simultaneously satisfied

$$\lim_{M\to\infty} \sigma = \lim_{M\to\infty} \sigma^* = 0, \tag{24}$$

$$\lim_{M\to\infty} \frac{\lambda(M)}{Z} = 0, \tag{25}$$

$$\lim_{M\to\infty} \frac{\sigma}{\frac{\lambda(M)}{Z}} = 0, \tag{26}$$

$$\lim_{M\to\infty} \lambda(M) = +\infty. \tag{27}$$

Equations (24)–(26) plugged into eq. (22) provide

$$\lim_{M\to\infty} f\left(\frac{\lambda(M)}{Z}, \boldsymbol{\sigma}\right) = 0, \tag{28}$$

whereas, by using eq. (27) in eq. (20) we have

$$\underline{\lim}_{M\to\infty} GSL\left[\boldsymbol{\mathcal{F}}(\lambda(M))\right] \geq \overline{\lim}_{M\to\infty} \min_n \mathcal{V}_n. \tag{29}$$

Finally, by using eq. (15) the proof of the theorem in the case of a uniform ergodic state is complete.

General ergodic state. Now we still consider a unique (and ergodic) GS with $\mathcal{E}_1 = 0$, but we have $\langle n|\mathcal{E}_1\rangle = u_n/\sqrt{Z}$ with $u_n \neq 1$. Little changes are necessary to generalize the previous proof to the present case. We define

$$\boldsymbol{\mathcal{F}}(\lambda) = \boldsymbol{\mathcal{V}} + \frac{\lambda}{Z}\boldsymbol{\mathcal{D}} + \boldsymbol{\mathcal{K}} + \frac{\lambda}{Z}\boldsymbol{\mathcal{U}}, \tag{30}$$

where

$$\boldsymbol{\mathcal{U}} = Z|\mathcal{E}_1\rangle\langle\mathcal{E}_1| - \boldsymbol{\mathcal{D}}, \tag{31}$$

and $\boldsymbol{\mathcal{D}}$ is a diagonal matrix with elements

$$\mathcal{D}_{m,n} = |u_n|^2\delta_{m,n}. \tag{32}$$

In the chosen base we have $\mathcal{U}_{n,n} = 0$ and $\mathcal{U}_{m,n} = \overline{u_m}u_n$ for $m \neq n$. Furthermore, from

$$\langle n|\boldsymbol{\mathcal{U}}|\mathcal{E}_1\rangle = (Z - |u_n|^2)\langle n|\mathcal{E}_1\rangle, \tag{33a}$$

$$\langle n|\boldsymbol{\mathcal{U}}|\mathcal{E}_i\rangle = -|u_n|^2\langle n|\mathcal{E}_i\rangle, \qquad i \neq 1, \tag{33b}$$

follows that, for any $\alpha \in \mathbb{R}$, we have

$$GSL\left[\alpha\boldsymbol{\mathcal{U}}\right] = \begin{cases} -|\alpha|(Z - s^*(M)), & \alpha < 0, \\ -|\alpha|s^*(M), & \alpha \geq 0, \end{cases} \tag{34}$$

where $s^*(M)$ is an appropriate value of the order of magnitude of $s(M)$:

$$s(M) = \max_n |u_n|^2. \tag{35}$$

Equation (34) can be verified rigorously by using the "Matrix Determinant Lemma" [7]. More precisely, s^* is the smallest root of the equation in s: $\sum_n |u_n|^2/(|u_n|^2 - s) = 1$.

From the first Weyl's inequality, we have

$$GSL\left[\boldsymbol{\mathcal{F}}(\lambda)\right] \geq \min_n \left(\mathcal{V}_n + \frac{\lambda}{Z}|u_n|^2\right) + f\left(\frac{\lambda}{Z}, \boldsymbol{\sigma}\right), \tag{36}$$

where

$$f\left(\frac{\lambda}{Z}, \boldsymbol{\sigma}\right) = GSL\left[\boldsymbol{\mathcal{K}} + \frac{\lambda}{Z}\boldsymbol{\mathcal{U}}\right]. \tag{37}$$

From eq. (34) we have

$$f\left(\frac{\lambda}{Z},\boldsymbol{\sigma}\right)\sim\begin{cases}-(Z-s^*(M))\dfrac{\lambda}{Z}+GSL\left[\boldsymbol{\mathcal{K}}\right], & \dfrac{\lambda}{Z}\ll\sigma,\\ -\left(\dfrac{\lambda s^*(M)}{Z}-\sigma^*\right), & \dfrac{\lambda}{Z}\gg\sigma,\end{cases} \tag{38}$$

where σ has been defined in eq. (7), and $\sigma^*\in\mathbb{R}$ is some appropriate value of the order of magnitude of $2\sum_{m,n}\sigma_{m,n}/(M(M-1))$ (which is real). As in the uniform case, we do not need to know σ^*, nor to assume eq. (38) as an actual equality. The proof is completed by observing that, as in the uniform case, eqs. (7) and (8) imply the existence of a regime where $\lambda(M)s^*(M)/Z$, σ, and σ^*, tend all to zero.

So far we have considered, for simplicity, $\mathcal{E}_1=0$. The generalization to the case $\mathcal{E}_1\neq 0$ is immediate. In eq. (13) or in eq. (30), we replace $\lambda|\mathcal{E}_1\rangle\langle\mathcal{E}_1|$ with $(\lambda-\mathcal{E}_1)|\mathcal{E}_1\rangle\langle\mathcal{E}_1|$ and use $\overline{\lim}_{M\to\infty}\mathcal{E}_1/Z=0$.

Degenerate case. Let us consider a two-fold degenerate case. We introduce

$$\begin{aligned}\boldsymbol{\mathcal{F}}(\lambda^{(1)},\lambda^{(2)}) &= \boldsymbol{\mathcal{H}}+\left(\lambda^{(1)}-\mathcal{E}_1\right)|\mathcal{E}_1^{(1)}\rangle\langle\mathcal{E}_1^{(1)}|\\ &\quad+\left(\lambda^{(2)}-\mathcal{E}_1\right)|\mathcal{E}_1^{(2)}\rangle\langle\mathcal{E}_1^{(2)}|.\end{aligned} \tag{39}$$

Instead of eq. (15), we now have to exploit

$$\mu_2=\lim_{\lambda^{(1)}\to\infty,\lambda^{(2)}\to\infty}GSL\left[\boldsymbol{\mathcal{F}}(\lambda^{(1)},\lambda^{(2)})\right]. \tag{40}$$

By defining

$$\boldsymbol{\mathcal{U}}^{(i)}=Z^{(i)}|\mathcal{E}_1^{(i)}\rangle\langle\mathcal{E}_1^{(i)}|-\boldsymbol{\mathcal{D}}^{(i)}, \tag{41}$$

where $\boldsymbol{\mathcal{D}}^{(1)}$ and $\boldsymbol{\mathcal{D}}^{(2)}$ have matrix elements

$$\mathcal{D}^{(i)}_{m,n}=\left(u_n^{(i)}\right)^2\delta_{m,n},\qquad i=1,2, \tag{42}$$

we proceed as in the non-degenerate case. The generalization to a k-fold degeneracy, with k finite and independent of M, is obvious. ■

Weak ergodicity. – From the comments following eq. (38), it is evident that, in order for the theorem to hold, we can ask for a weaker condition on the GSs $|\mathcal{E}_1^{(i)}\rangle$. The following theorem accounts for such a generalization.

Theorem 3 *(Weak ergodicity). Let $\boldsymbol{\mathcal{H}}$ be a $M\times M$ Hermitian matrix with distinct, possibly degenerate, eigenvalues $\mathcal{E}_1<\mathcal{E}_2<\mathcal{E}_3<\ldots$. Let us suppose to have k degenerate GSs and there exists a positive function $g(M)$ such that*

$$\sigma=\max_i\max_{m,n}\frac{|\sigma_{m,n}|}{|u_n^{(i)}u_m^{(i)}|}<g(M), \tag{43}$$

$$\lim_{M\to\infty}g(M)=0,\quad \lim_{M\to\infty}\frac{1}{(Z^{(i)})^2g(M)}=0. \tag{44}$$

Let each GS of $\boldsymbol{\mathcal{H}}$ be weakly ergodic, i.e. $\exists\, M_0$ such that for any $M\geq M_0$ and for any i:

$$0<|u_n^{(i)}|\quad\text{if }\exists\, m:\ \sigma_{m,n}\neq 0\quad\text{or }\sigma_{n,m}\neq 0, \tag{45}$$

and

$$\underline{\lim}_{M\to\infty}\, s^*(M)\sqrt{g(M)}=0, \tag{46}$$

where s^* is the smallest root of the equation in s: $\sum_n|u_n^{(i)}|^2/(|u_n^{(i)}|^2-s)=1$. Then we have

$$\underline{\lim}_{M\to\infty}\,\mu_2\geq\overline{\lim}_{M\to\infty}\,\min_n\mathcal{V}_n. \tag{47}$$

Application to random walks with infinitesimal jump rates. – A master equation of the form of eq. (1) can be interpreted as a weighted continuous-time random walk taking place on a graph whose adjacency matrix $\boldsymbol{\mathcal{A}}$ is defined by $\mathcal{A}_{m,n}=(1-\delta_{m,n})\theta[-\mathcal{L}_{m,n}]$, where $\theta[\cdot]$ is the Heaviside function. The evolution of the probability $p_n(t)$ goes through random jumps characterized by the jump rates

$$W(n\to m)=-\mathcal{L}_{m,n}(1-\delta_{m,n}). \tag{48}$$

In the case of unweighted random walks, the non-zero off-diagonal elements of $\boldsymbol{\mathcal{L}}$ are uniform, whereas the diagonal elements $\mathcal{L}_{n,n}$ coincide with the degree $k(n)$ of the configuration with label n, namely,

$$\mathcal{L}_{n,n}=k(n)=\sum_{m\neq n}W(n\to m)=-\sum_{m\neq n}\mathcal{L}_{m,n}. \tag{49}$$

Furthermore, if the random walk is symmetric, *i.e.* the induced graph is indirect, we have $\mathcal{L}_{m,n}=\mathcal{L}_{n,m}$. In such a case, we can directly identify $\boldsymbol{\mathcal{L}}$ as the Hamiltonian $\boldsymbol{\mathcal{H}}$. The GS of $\boldsymbol{\mathcal{H}}=\boldsymbol{\mathcal{L}}$ has zero energy, $\mathcal{E}_1=0$, and is uniform, $\langle n|\mathcal{E}_1\rangle=1/\sqrt{M}$ (here $Z=M$).

Consider now a symmetric random walk in which the jump rates are infinitesimal with M. We assume, for instance,

$$|\mathcal{L}_{m,n}|\leq\frac{1}{[\log(M)]^\alpha},\qquad m\neq n,\qquad 0<\alpha<1. \tag{50}$$

Taking into account that the GS is ergodic, we see that for this model the hypotheses of the theorem are satisfied, and we can conclude that (we keep using the symbol $k(n)$ as a weighted degree to include also symmetric weighted random walks because, although these have non-uniform jump rates, their GS is still the uniform one)

$$\underline{\lim}_{M\to\infty}\,\mu_2\geq\overline{\lim}_{M\to\infty}\,\min_n k(n). \tag{51}$$

Equation (51) tells us that, in symmetric random walks having jump rates decaying with the logarithm of the system size M, the relaxation time τ to reach equilibrium is upper bounded by the configuration having minimal degree, namely $\tau\leq 1/\min_n k(n)$. This result is quite intuitive: a necessary condition to observe a fast dynamics is that the configurations (or nodes) have not too small degrees. However, we warn the reader that, in the usual definition of random walk, the jump rates are either $W(n \to m) = 0$ or $W(n \to m) = O(1)$, so that the theorem cannot be directly applied, its hypotheses being not satisfied. Nevertheless, if $\min_n k(n)$ is a function of M which diverges as $1/g(M)$, with $1/(M^2 g(M)) \xrightarrow{M\to\infty} 0$, we can apply the theorem to the matrix $\boldsymbol{\mathcal{H}} = \boldsymbol{\mathcal{L}}/(\min_n k(n))$, and we conclude that

$$\varliminf_{M\to\infty} \frac{\mu_2}{\min_n k(n)} \geq 1. \tag{52}$$

Conclusions. – We have stated and proved a lower bound, in the limit $M \to \infty$, for the gap of Hermitian $M \times M$ matrices characterized by i) ergodic GS, simple or degenerate, and ii) off-diagonal terms which are infinitesimal in M. The "infinitesimal" conditions (7), (8) under which the theorem is satisfied are quite mild, and, in particular, cover the common cases in which the off-diagonal terms decay as the logarithm of the system size M. This includes random-walks models with infinitesimal jump rates, thermalization of classical models characterized by infinitesimal couplings arbitrarily distributed, and the Pauli master equation characterizing the thermalization of open quantum systems [5,6][1].

The key ingredient of the proof of the present theorem is eq. (19), or its generalization eq. (34). From a physics viewpoint, these equations describe a sort of phase transition between a "bosonic" extensive phase, and a "non-bosonic" intensive phase. Here, the terms "bosonic" and "non-bosonic" come from the observation of the signs of the off-diagonal matrix elements of the operator $\alpha\boldsymbol{\mathcal{U}}$, which, in turn, determine those of the "kinetic" operator $\boldsymbol{\mathcal{K}} + \boldsymbol{\mathcal{U}}\lambda/Z$. Essentially, the proof of the theorem consists in finding a scaling $\lambda(M)$ such that the system stays in the non-bosonic intensive phase, and, at the same time, the parameters characterizing $\boldsymbol{\mathcal{K}} + \boldsymbol{\mathcal{U}}\lambda/Z$ tend to zero.

To compare our theorem with previously known results, a few comments are in order. Consider a symmetric and unweighted Laplacian matrix $\boldsymbol{\mathcal{L}}$, with $\mathcal{L}_{n,n} = k(M)$, where $k(M)$ is a suitable growing function of M. We can apply the theorem to the matrix $\boldsymbol{\mathcal{H}} = \boldsymbol{\mathcal{L}}/k$ obtaining $\varliminf_{M\to\infty} \mu_2 \geq 1$. On the other hand, the graph induced by $\boldsymbol{\mathcal{L}}$ is a regular graph of degree k, and classical results of spectral graph theory applied to $\boldsymbol{\mathcal{H}}$ provide the more accurate estimate $\mu_2 \simeq 1-2/(\sqrt{k-1})$ [9]. This example shows that for matrices associated to graphs satisfying special properties, our lower bound can be somehow not competitive. However, our result may become crucial whenever, besides the above conditions i) and ii), there are no other assumptions or information about $\boldsymbol{\mathcal{H}}$. Notice, in particular, that $\boldsymbol{\mathcal{H}}$ can be quite different from a Laplacian, its matrix elements being weighted and with no definite sign or phase. We are not aware of other lower bounds for such a general case. In ref. [10] general weighted non-symmetric Laplacians $\boldsymbol{\mathcal{L}}$ are considered and the eigenvalues of the standardized Laplacian $\boldsymbol{\mathcal{L}}/M$ are bounded in a region of the complex plane which contains the real segment $[0,1]$. If we assume a Laplacian with real eigenvalues and take $\mathcal{L}_{n,n} = \alpha_n M$, with $0 \leq \alpha_n \leq 1$, and $\mathcal{L}_{m,n} = -\beta_{m,n}$, with $0 \leq \beta_{m,n} \leq 1$, $m \neq n$, for the standardized Laplacian our theorem provides $\varliminf_{M\to\infty} \mu_2 \geq \varlimsup_{M\to\infty} \min_k \alpha_k$, asymptotically localizing, as a function of the values of the set $\{\alpha_k\}$, the second eigenvalue in the same segment $[0,1]$ of ref. [10]. However, we stress that a standardized Laplacian with its off-diagonal elements vanishing as $1/M$ is not of great interest for physics, whereas our theorem covers the widespread cases in which the off-diagonal terms decay as $1/\log M$, *i.e.* linearly with the inverse of the system size N where, typically, N is the number of particles or the physical volume.

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[1] The arbitrariness of the representation of the GS via eq. (5) can play an advantage in applying our theorems, as in the cases in which the GS of $\boldsymbol{\mathcal{H}}$ coincides with the square root of the Gibbs distribution of a system having energy eigenvalues E_n and corresponding eigenvectors $|E_n\rangle$, namely, $\langle E_n|\mathcal{E}_1\rangle = \exp(-\beta E_n/2)/\sqrt{Z}$, where β is an inverse temperature and Z is the usual partition function. By choosing the natural representation $u_n = \exp(-\beta E_n/2)$, $|\mathcal{E}_1\rangle$ is manifestly ergodic. Furthermore, since the E_n are extensive in the system size N, with $N \sim O(\log M)$, and the Gibbs distribution is invariant with respect to an overall energy shift, it is easy to check that, whenever the matrix elements of $\boldsymbol{\mathcal{K}}$ decay polynomially in N, up to a suitable energy shift, conditions (10), (11) of theorem 2 can always be satisfied for a sufficiently large size N.