Spectra of Random Stochastic Matrices and Relaxation in Complex Systems

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Abstract – We compute spectra of large stochastic matrices W, defined on sparse random graphs in the configuration model class, i.e. on graphs that are maximally random subject to a given degree distribution. Edges (i, j) of the graph are given positive random weights $W_{ij} > 0$ in such a fashion that column sums are normalized to one. We compute spectra of such matrices both in the thermodynamic limit, and for single large instances. Our results apply to arbitrary graphs in the configuration model class, as long as the mean vertex degree remains finite in the thermodynamic limit. Edge weights W_{ij} can be largely arbitrary but we require the W_{ij} to satisfy a detailed balance condition, or in other words that the Markov chains described by them are reversible. Knowing the spectra of stochastic matrices is tantamount to knowing the complete spectrum of relaxation times of stochastic processes described by them, so our results should have many interesting applications for the description of relaxation in complex systems. Contributions to the spectral density related to extended states can be disentangled from those related localized states allowing time scales associated with transport processes and those associated with the dynamics of local rearrangements to be differentiated.

There are numerous processes, both natural and artificial, which can be understood in terms of random walks on complex networks [1–3], including the spread of diseases in social networks [4,5], the transmission of information in communication networks (e.g. [6]), search algorithms [7,8], the out-of-equilibrium dynamics of glassy systems at low temperatures as described in terms of hopping between long-lived states in state space [9–11] and – in a similar spirit – the dynamics of major conformational changes in macro-molecules [12], or cell-signalling through protein-protein interaction networks [13], to name but a few. For reviews that cover several of these topics, see e.g. [14–16].

The purpose of the present letter is to use random matrix theory to contribute to the understanding of systems of this type. We compute spectra of transition matrices for discrete Markov chains describing stochastic dynamics in complex systems. We construct these in terms of sparse random graphs in such a way that an edge (i, j) in a graph corresponds to a possible transition $j \to i$, with the edge weight $W_{ij} > 0$ quantifying the associated transitions probability, requiring $\sum_i W_{ij} = 1$ for all j. We are interested in the limit, where the number N of possible states becomes large, with the average number of possible transitions at each state remaining finite in the thermodynamic limit ($N \to \infty$).

Given a time-dependent probability vector $\boldsymbol{p}(t) = (p_i(t))$, we have an evolution equation of the form

$$\boldsymbol{p}(t+1) = W\boldsymbol{p}(t) \; . \tag{1}$$

The condition $W_{ij} \geq 0$ for all (i, j) and the column sum constraint together entail that the spectrum of W is contained in the unit disc of the complex plane, $\sigma(W) \subseteq \{z; |z| \leq 1\}$. If W satisfies a detailed balance condition with an equilibrium distribution, $p_i = p_i^{\rm eq}$, such that $W_{ij}p_j = W_{ji}p_i$ for all pairs (i, j), then W can be symmetrized by a similarity transformation — $\mathcal{W}_{ij} = p_i^{-1/2} W_{ij} p_j^{1/2} = \mathcal{W}_{ji}$ — implying that the spectrum of W is real, and $\sigma(W) \subseteq [-1, 1]$.

Our main interest here is the relation between eigenvalues of W and relaxation times of the Markov chain it describes. It is easily understood by following the evolution of an initial probability vector $\boldsymbol{p}(0)$ over t time steps, i.e. by considering $\boldsymbol{p}(t) = W^t\boldsymbol{p}(0)$. Using a spectral decomposition of W, and assuming the system to be irreducible

and free of cycles, one obtains

$$\boldsymbol{p}(t) = \boldsymbol{p}^{\rm eq} + \sum_{\alpha(\neq 1)} \lambda_\alpha^t \; \boldsymbol{v}_\alpha \; \big(\boldsymbol{w}_\alpha, \boldsymbol{p}(0)\big) \tag{2}$$

where we have used that $1 = \lambda_1 > |\lambda_\alpha|$ for $\alpha \neq 1$, given the assumptions [17], and where $\boldsymbol{v}_\alpha$ and $\boldsymbol{w}_\alpha$ denote the right and left eigenvectors of W, respectively, with $\boldsymbol{v}_1 = \boldsymbol{p}^{\rm eq}$, and $\boldsymbol{w}_1 = (1, \ldots, 1)$. Eq. (2) relates relaxation times of the system to eigenvalues of W via $\tau_\alpha = -1/\ln|\lambda_\alpha|$ for $\alpha \neq 1$.

We construct random stochastic matrices in terms of unnormalized transition matrices $\Gamma = (\Gamma_{ij}) = (c_{ij}K_{ij})$, with connectivity matrix elements $c_{ij} \in \{0, 1\}$ (and $c_{ii} = 0$) specifying the network structure of possible transitions, and positive edge weights $K_{ij} > 0$, and setting $W_{ij} = \Gamma_{ij}/\Gamma_j$ if $\Gamma_j \equiv \sum_i \Gamma_{ij} \neq 0$, and $W_{ii} = 1$ for isolated sites for which $\Gamma_i = 0$. The present investigation will be restricted to the case where W satisfies a detailed balance condition, and can thus be symmetrized by a similarity transformation, as discussed above. The spectrum of fully connected matrices of this type was shown to converge to a semi-circular law [18] in the large system limit, and to a circular law, if the detailed balance condition is dropped [19]. Asymptotic results related to the circular law were obtained for Erdös-Renyi graphs with mean connectivity diverging in the thermodynamic limit [20]. While there are some recent related results concerning spectra of graph Laplacians (e.g. [21–23]), solutions do involve mean-field [21] or large mean degree [22] approximations, or rely on a strictly self-similar construction of the underlying graph [23]. We are not aware of general exact solutions of the spectral problem for Markov matrices or their corresponding master-equation operators.

We follow [24] and express the spectral density $\rho_W(\lambda)$ of the stochastic matrix W in terms of a derivative

$$\rho_W(\lambda) = -\lim_{\varepsilon\to 0} \frac{2}{\pi N} \,{\rm Im}\, \frac{\partial}{\partial\lambda} \,\log Z_W(\lambda) \;, \tag{3}$$

of the logarithm of a Gaussian integral

$$Z_W(\lambda) = \int \prod_{i=1}^N \frac{{\rm d}u_i}{\sqrt{2\pi/{\rm i}}} \;\exp\big\{ -{\rm i}H_W(\lambda_\varepsilon, \boldsymbol{u})\big\} \tag{4}$$

defined in terms of the quadratic form

$$H_W(\lambda_\varepsilon, \boldsymbol{u}) = \frac{1}{2}\sum_{i,j} \big(\lambda_\varepsilon\delta_{ij} - \mathcal{W}_{ij}\big) \; u_i u_j \;, \tag{5}$$

with $\lambda_\varepsilon = \lambda - {\rm i}\varepsilon$. Here, $\mathcal{W}$ is the symmetrized version of W, obtained via a similarity transform that involves the equilibrium distribution $\boldsymbol{p}^{\rm eq}$ as discussed above. The representation (3) allows one to interpret the spectral density as a sum over single-site variances

$$\rho_W(\lambda) = {\rm Re}\,\frac{1}{\pi N}\sum_i \langle u_i^2\rangle \tag{6}$$

of the complex Gaussian measure

$$P_W(\boldsymbol{u}) = \frac{1}{Z_W}{\rm e}^{-{\rm i}H_W(\lambda_\varepsilon,\boldsymbol{u})} \;. \tag{7}$$

Here and in what follows we shall omit explicitly writing the $\lim_{\varepsilon\to 0}$, and take it to be understood.

In the thermodynamic limit, the spectral density is expected to be non-random and is obtained by averaging Eq. (3) over the matrix ensemble in question, using the replica method to perform averages as proposed in [24], and taking the limit $N \to \infty$. Methods developed in [25] can be used to efficiently deal with the sparsity of the ensemble of matrices considered in the present letter. Alternatively, one can analyse single large instances using a cavity approach proposed in [26] to obtain the single-instance spectral density in terms of variances of single-site marginals. In the thermodynamic limit, recursion relations for the cavity-variances obtained within that approach can be interpreted as stochastic recursions, allowing to formulate self-consistency relations for their distributions, which turn out to be equivalent to those obtained using replica. This is the approach we shall briefly outline in what follows.

In order not to overburden the present exposition with technicalities, we shall restrict our attention here to cases where the unnormalized transition matrix Γ is symmetric, in which case the symmetrized normalized Markov matrix is of the form

$$\mathcal{W}_{ij} = \frac{\Gamma_{ij}}{\sqrt{\Gamma_i\Gamma_j}} \tag{8}$$

for $\Gamma_{ij} > 0$, hence $\Gamma_i > 0$ and $\Gamma_j > 0$, and $\mathcal{W}_{ii} = 1$ for isolated sites.

To obtain the single-site marginals of (7) required to evaluate $\rho_W(\lambda)$ according to (6), we have to distinguish between single-site marginals on isolated sites, which are of the form $P_i^{\rm is}(u_i) \propto {\rm e}^{-\frac{\rm i}{2}(\lambda_\varepsilon - 1)\,u_i^2}$, and those for sites that are not isolated.

On the latter, we perform a transformation of variables, $\frac{u_i}{\sqrt{\Gamma_i}} \to u_i$ in Eqs. (4) and (7). This step turns out to be crucial to avoid having to average over sets of correlated variables when obtaining ensemble results valid in the thermodynamic limit later on. In terms of the transformed variables, we have

$$\rho_W(\lambda) = p_N(0)\delta(\lambda - 1) + {\rm Re}\,\frac{1}{\pi N}\sum_i \Gamma_i\langle u_i^2\rangle \;, \tag{9}$$

with $p_N(0) = \frac{N^{\rm is}}{N}$ denoting the fraction of isolated sites, and only non-isolated sites with $\Gamma_i > 0$ contributing to the second sum.

The remainder of the analysis closely follows [26]. It is based on the observation that single-site marginals of (7) will be Gaussian, that these can be expressed in terms of Gaussian cavity marginals, and that one can derive self-consistency equations for the complex (inverse) cav-

ity variances $\{\omega_j^{(i)}\}$ of these, which read

$$\omega_j^{(i)} = \mathrm{i}\lambda_\varepsilon\,\Gamma_j + \sum_{\ell\in\partial j\setminus i}\frac{K_{j\ell}^2}{\omega_\ell^{(j)}}\ . \tag{10}$$

These are exact on trees; for finitely coordinated random graphs in the configuration model class they become asymptotically exact in the thermodynamic limit. They can be solved iteratively on large single instances. Inverse variances of single-site marginals can be expressed in terms of solutions of (10) as $\omega_i = \mathrm{i}\lambda_\varepsilon\,\Gamma_i + \sum_{j\in\partial i} K_{ij}^2/\omega_j^{(i)}$. In terms of these, we have

$$\rho_W(\lambda) = p_N(0)\delta(\lambda-1) + \mathrm{Re}\,\frac{1}{\pi N}\sum_i\frac{\Gamma_i}{\omega_i}\ . \tag{11}$$

Specializing to the case of unbiased random walk, we have $\Gamma_{ij} = c_{ij}$, hence $\Gamma_j = k_j$ and $\mathcal{W}_{ij} = c_{ij}/\sqrt{k_i k_j}$ for non-isolated sites, where k_i and k_j are degrees of vertices i and j. In this case, Eqs. (10)-(11) readily lend themselves for averaging over a graph ensemble in the thermodynamic limit, giving rise to an integral equation for a probability density function $\pi(\omega)$ for inverse cavity variances of a form similar to those obtained earlier [25]. We will not produce equations for this special case here but instead refer to a forthcoming extended version of the present letter [27].

For Markov processes other than the unbiased random walk, straightforward averaging of cavity recursions over the ensemble of Markov matrices is prevented by the fact that the $K_{j\ell}$ in (10) are not independent due to column sum constraints, in a way that extends beyond degree. In order to deal with this issue we return to the Gaussian integral in terms of which the problem was originally formulated, and rewrite the quadratic form (using transformed variables on non-isolated sites) as $H_W = \frac{1}{2}\sum_i^{\mathrm{is}}(\lambda_\varepsilon-1)u_i^2 + \frac{1}{2}\sum_{i,j}c_{ij}\left[\frac{1}{2}\lambda_\varepsilon K_{ij}(u_i^2+u_j^2) - K_{ij}\ u_iu_j\right]$.

Using this setup, one easily obtains the following reformulated recursion for inverse variances of cavity marginals

$$\omega_j^{(i)} = \sum_{\ell\in\partial j\setminus i}\left(\mathrm{i}\lambda_\varepsilon K_{j\ell} + \frac{K_{j\ell}^2}{\omega_\ell^{(j)}+\mathrm{i}\lambda_\varepsilon K_{j\ell}}\right)\ . \tag{12}$$

This version can be averaged over the ensemble of random matrices in question which gives rise to a self-consistency equation for cavity variances which is structurally very similar to that obtained for the case of unbiased random walks,

$$\pi(\omega) = \sum_{k\geq1}p(k)\frac{k}{c}\int\prod_{\nu=1}^{k-1}\mathrm{d}\pi(\omega_\nu)\left\langle\delta(\omega-\Omega_{k-1})\right\rangle_{\{K_\nu\}} \tag{13}$$

albeit with a very different expression for the Ω_{k-1}, viz.

$$\Omega_{k-1} = \sum_{\nu=1}^{k-1}\left(\mathrm{i}\lambda_\varepsilon K_\nu + \frac{K_\nu^2}{\omega_\nu+\mathrm{i}\lambda_\varepsilon K_\nu}\right)\ . \tag{14}$$

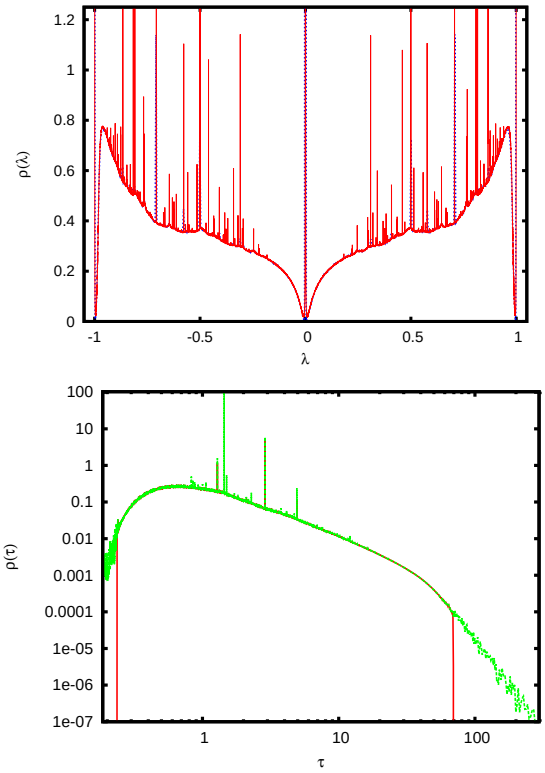

Fig. 1: (Colour online) Top panel: Spectral density of the transition matrix for an unbiased random walk on an Erdös-Renyi graph of mean coordination $c = 2$, comparing results of numerical diagonalization of an ensemble of 1000×1000 matrices (blue dashed curve) and analytic results obtained via population dynamics (red solid curve). Bottom panel: relaxation time distribution for this system (green dashed curve); red vertical lines separate a central part of the relaxation time spectrum corresponding to extended modes from regions corresponding to localized modes at small and large τ. Isolated δ-peaks in the central part of the spectrum also correspond to localized modes

It is efficiently solved using a population dynamics algorithm. In terms of its solution, the spectral density in the thermodynamic limit is given by

$$\begin{aligned}\rho(\lambda) \quad &= \quad p(0)\delta(\lambda-1)\\ &+\frac{1}{\pi}\,\mathrm{Re}\sum_{k\geq1}p(k)\int\prod_{\nu=1}^{k}\mathrm{d}\pi(\omega_\nu)\left\langle\frac{\sum_{\nu=1}^k K_\nu}{\Omega_k}\right\rangle_{\{K_\nu\}}\end{aligned} \tag{15}$$

Finally, given the relation between eigenvalues of a transition matrix and relaxation times of the stochastic process it describes, we can translate spectral densities into spectra of relaxation times. Using the notation ρ_λ and ρ_τ to distinguish eigenvalue densities and relaxation time distributions, we have

$$\rho_\tau(\tau) = \left[\rho_\lambda(\mathrm{e}^{-1/\tau}) + \rho_\lambda(-\mathrm{e}^{-1/\tau})\right]\frac{\mathrm{e}^{-1/\tau}}{\tau^2}\ . \tag{16}$$

Figure 1 shows the spectrum of the transition matrix for an unbiased random walk on an Erdös-Renyi graph

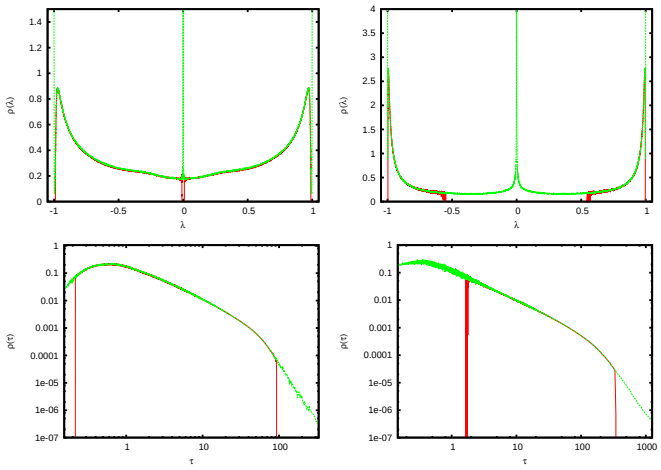

Fig. 2: (Colour online) Spectra (first row) and relaxation time distributions (second row) for transition matrices with Kramers transition rates on an Erdös-Renyi graph of mean coordination $c = 2$; shown are results obtained via population dynamics, separately for the total density of states (green dashed curve) and the density of extended states (red solid lines). Left column: $\beta = 2$. Right column: $\beta = 5$.

of mean connectivity $c = \langle k \rangle = 2$, comparing results obtained for the thermodynamic limit with simulations averaged over 5000 realizations of 1000×1000 matrices, showing excellent agreement — with analytic results lying virtually on top of simulation results — except that our population dynamics algorithm picks up many more of the localized states which appear as δ-peaks in the diagram. The second panel shows the relaxation time spectrum corresponding to the density of states via (16). We note that the relaxation time spectrum for this system is very broad, with significant contributions over more than four orders of magnitude in relaxation times. As explained in [25] one can identify contributions to the spectral density corresponding to extended and localized states and we use this in the second panel of fig. 1 to separately exhibit the contribution of the extended modes to the relaxation time spectrum, demonstrating that both very fast and very slow modes correspond to localized states in the system.

In the eigenvalue density itself these features are a consequence of the existence of mobility edges at $\pm\lambda_c$ with $\lambda_c \simeq 0.986$, with states corresponding to eigenvalues $|\lambda| \geq \lambda_c$ forming bands localized modes (with large relaxation times), whereas a very narrow band of localized states for very small λ at $|\lambda| \lesssim 1.4 \times 10^{-2}$ gives rise to localized modes with very short relaxation times.

In fig. 2 we present results for systems with unnormalized transition matrix elements taking the form of Kramers transition rates $\Gamma_{ij} = c_{ij} \mathrm{e}^{-\beta(V_{ij} - E_j)}$, with barrier heights V_{ij} randomly chosen from an exponential distribution of mean 1; the distribution of initial energies is arbitrary, as initial energies cancel in properly normalized stochastic matrices, so that $W_{ij} = c_{ij} \mathrm{e}^{-\beta V_{ij}} / \sum_i c_{ij} \mathrm{e}^{-\beta V_{ij}}$. Systems of this type were studied within a heterogeneous mean-field approximation to dynamics in [11], generalizing earlier work [9, 10] to include barrier height distributions and incompletely connected networks of traps. Two aspects are particularly notable: (i) as β is increased the spectral density gives more weight to regions near $\lambda = \pm 1$, i.e. to slow modes; (ii) the narrow region of localized states near $\lambda = 0$ broadens considerably, as β is increased from 2 to 5, implying that many more modes have become localized. Both features have their analogues in the relaxation time spectra, the latter implying in particular that the lower cutoff of the relaxation time distribution corresponding to extended modes is being shifted to larger τ by roughly an order of magnitude as β is increased. Once more, we found excellent agreement with simulation results (not shown).

For the unbiased random walk problem on a regular random graph with $p(k) = \delta_{k,c}$, the integral equation for the distribution of inverse cavity variances is solved by a δ-function, $\pi(\omega) = \delta(\omega - \bar{\omega})$, giving rise to a quadratic self-consistency equation $\bar{\omega} = \mathrm{i}\lambda_\varepsilon c + \frac{c-1}{\bar{\omega}}$ for $\bar{\omega}$; its solution allows one to obtain a closed-form expression for the spectral density

$$\rho(\lambda) = \frac{c}{2\pi} \frac{\sqrt{4\frac{c-1}{c^2} - \lambda^2}}{1 - \lambda^2} \ , \tag{17}$$

which is readily recognised as a variant of the Kesten-McKay distribution [28], adapted to capture the spectral problem of the Markov transition matrix for an unbiased random walk on random regular graphs. The same result is found to provide an accurate approximate description for Erdös-Renyi random graphs at large mean degree c, for which the degree distribution becomes sharply peaked at the mean degree c. The approximation becomes asymptotically exact as $c \to \infty$, where fluctuations of the degree distribution become negligible, and (17) approaches a semicircular law.

An analogous line of reasoning allows to obtain the spectral density for more general Markov matrices on Erdös-Renyi and random regular graphs in the large-c limit. In this case, the ansatz $\pi(\omega) = \delta(\omega - \bar{\omega})$ gives rise to a self-consistency equation for $\bar{\omega}$ of the form

$$\bar{\omega} \simeq c \left[\mathrm{i}\lambda_\varepsilon \langle K \rangle + \left\langle \frac{K^2}{\bar{\omega} + \mathrm{i}\lambda_\varepsilon K} \right\rangle \right] . \tag{18}$$

obtained by referring to the law of large numbers (LLN) allowing one to replace Ω_{k-1} in (14) by a sum of averages. In terms of its solution $\bar{\omega}$, we can once more invoke the LLN in the expression for the spectral density

$$\begin{aligned} \rho(\lambda) &\simeq \frac{1}{\pi} \mathrm{Re} \left[\frac{\langle K \rangle}{\mathrm{i}\lambda_\varepsilon \langle K \rangle + \left\langle \frac{K^2}{\bar{\omega} + \mathrm{i}\lambda_\varepsilon K} \right\rangle} \right] \\ &= \frac{1}{\pi} \mathrm{Re} \left[\frac{c\langle K \rangle}{\bar{\omega}} \right] , \end{aligned} \tag{19}$$

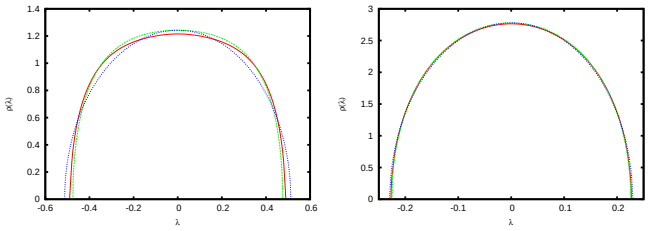

Fig. 3: (Colour online) Spectral density of the transition matrix with Kramers transition rates with $\beta = 2$ on an Erdös-Renyi graph for large values of the mean coordination c. Shown are analytic results obtained via population dynamics (green dashed curve), the analytical approximation based on Eqs. (18), (19) (red aolid curve), as well as the semi-circular approximation (20) (blue dashed curve). Left panel: $c = 20$; right panel: $c = 100$.

Note that this requires (and entails self-consistently) that $\bar{\omega} \propto \langle K \rangle$ for the spectral density to be independent of the K-scale. Moreover, for large c we have $\bar{\omega} \sim c$ which allows us to approximate (18) by a quadratic equation; its solution, when inserted into the final equation for the spectral density gives rise to a Wigner semi-circular distribution of the form

$$\rho(\lambda) = \frac{c}{2\pi} \frac{\langle K \rangle^2}{\langle K^2 \rangle} \sqrt{\frac{4\langle K^2 \rangle}{c\langle K \rangle^2} - \lambda^2} \ . \tag{20}$$

This expression, too, is invariant under rescaling of the edge weights K_{ij} as it should, because K scales are immaterial in normalized Markov transition matrices. As shown in Fig. 3 the analytical large c approximation based on Eqs. (18), (19) is very reasonable already for c as small as $c = 20$, and becomes remarkably accurate for $c = 100$ or larger.

In summary, we computed spectra of random stochastic matrices defined in terms of random graphs as well as the relaxation time spectra of the Markov chains described by these matrices. We need to assume that the transition matrices satisfy a detailed balance condition or, in other words, that the Markov chains under consideration are reversible. We expect our methods and results to be of interest for the study of a broad range of relaxation phenomena in complex systems.

Apart from the detailed balance condition, our solution is valid for graphs in the configuration model class with arbitrary degree distributions, provided only that the mean degree remains finite in the thermodynamic limit. As in the case of adjacency matrices and weighted graph Laplacians our approach is easily generalized to systems exhibiting modular or small-world properties [29]. We expect that a solution for general asymmetric stochastic matrices will be obtainable along the lines of [30].

Of particular relevance is the possible appearance of localized states in systems of the type described in the present letter. Referring to Eq. (2), one can indeed argue that most modes corresponding to localized states will not contribute to the relaxation dynamics, if initial conditions are themselves localized, an issue we have not seen systematically investigated in the literature.

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