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Spectral problem for quasi-uniform nearest-neighbor chains

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One-dimensional arrays with nearest-neighbor interactions occur in several physical contexts: magnetic chains, Josephson-junction and quantum-dot arrays, 1D boson and fermion hopping models, and random walks. When the interactions at the boundaries differ from the bulk ones, these systems are represented by quasi-uniform tridiagonal matrices. We show that their diagonalization is almost analytical: the spectral problem is expressed as a variation of the uniform one, whose eigenvalues constitute a band. A density of in-band states can be introduced, making it possible to treat large matrices, while few discrete out-of-band localized states can show up. The general procedure is illustrated with examples. © *2013 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4797477]

I. INTRODUCTION

The need of diagonalizing quasi-uniform tridiagonal (QUT) matrices, namely tridiagonal matrices which are uniform except at the boundaries, appears in many branches of physics and mathematics.[1–5] In particular, tridiagonal matrices generally occur in the theory of one-dimensional lattices with nearest-neighbor interactions. In this context, quasi-uniform tridiagonal matrices have been recently applied for achieving high quality quantum communication between distant parts[6–12] and for describing spin systems in a spin environment.[13–15]

In this paper we put forward a general method for calculating the eigenvalues and the eigenvectors of symmetric tridiagonal matrices by exploiting the property of bulk uniformity. This allows us to put the eigenvalues in the form of deformations, defined by suitable *shifts*, of those of the fully uniform case, which are known to form a band. The modified density of the eigenmodes in the band is expressed in terms of functions which can be analytically evaluated and depend on the non-uniform matrix elements. Particular examples of this technique can be found in Refs. 6 and 16. In addition, a small number of localized eigenstates could emerge from the band and have to be accounted for separately: we give a general criterion for establishing the presence of out-of-band states by means of the normalization integral for the in-band ones.

Section II is devoted to briefly set up the notations used in this paper; the method for dealing with quasi-uniform tridiagonal matrices is developed in Sec. III; eventually, Sec. IV proposes a few illustrative examples.

II. TRIDIAGONAL MATRICES

A symmetric $\ell \times \ell$ tridiagonal matrix $T = \{T_{\mu\nu}\}$ has $2\ell - 1$ independent real elements, namely $T_{\mu\mu} \equiv a_\mu$ ($\mu = 1, \ldots, \ell$) and $T_{\mu,\mu+1} = T_{\mu+1,\mu} \equiv b_\mu$ ($\mu = 1, \ldots, \ell - 1$). Its spectral decomposition is $T = O^\dagger \Lambda O$, where $O = \{O_{k\mu}\}$ is orthogonal, its rows being the ℓ eigenvectors of T with eigenvalues λ_k, and $\Lambda = \mathrm{diag}(\{\lambda_k\})$.

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T is said to be *mirror-symmetric* if it is also symmetric with respect to the skew diagonal, namely $[T, J] = 0$, where $J_{\mu\nu} = \delta_{\mu,\ell+1-\nu}$ is the mirroring matrix. In the mathematical language, such matrices are both *persymmetric* ($JTJ = T^t$) and *centrosymmetric* ($JTJ = T$). It is known that the eigenvectors of a mirror-symmetric T are either symmetric or antisymmetric,[17]

$$O_{k,\ell+1-\mu} = (-)^{k+1} O_{k\mu}, \tag{1}$$

this formula assumes that $b_\mu > 0$ and the eigenvalues $\{\lambda_k\}$ are listed in decreasing order.

The eigenvectors can be completely expressed in terms of characteristic polynomials of submatrices of T, evaluated at the eigenvalues. In order to prove this, let us introduce the following notation for tridiagonal submatrices:

$$T_{\mu:\nu} = \begin{pmatrix} a_\mu & b_\mu & & & & \\ b_\mu & a_{\mu+1} & b_{\mu+1} & & & \\ & b_{\mu+1} & \ddots & \ddots & & \\ & & \ddots & \ddots & & \\ & & & & a_{\nu-1} & b_{\nu-1} \\ & & & & b_{\nu-1} & a_\nu \end{pmatrix} \tag{2}$$

and for the corresponding characteristic polynomials,

$$\chi_{\mu:\nu}(\lambda) = \det[\lambda - T_{\mu:\nu}], \tag{3}$$

where $\mu \le \nu$; then $T_{1:\ell} \equiv T$ and $\chi_{1:\ell}(\lambda) \equiv \chi(\lambda)$; the eigenvalues are the ℓ solutions of the secular equation $\chi(\lambda_k) = 0$. By expanding from the bottom (upper) corners, these polynomials are found to satisfy the recurrence relations

$$\chi_{\mu:\nu}(\lambda) = (\lambda - a_\nu)\ \chi_{\mu:\nu-1}(\lambda) - b_{\nu-1}^2\ \chi_{\mu:\nu-2}(\lambda), \tag{4a}$$

$$\chi_{\mu:\nu}(\lambda) = (\lambda - a_\mu)\ \chi_{\mu+1:\nu}(\lambda) - b_\mu^2\ \chi_{\mu+2:\nu}(\lambda). \tag{4b}$$

The following important and useful formula (see, e.g., Ref. 18) expresses the product of two components of the same eigenvector:

$$\chi'(\lambda_k)\ O_{k\mu} O_{k\nu} = \chi_{1:\mu-1}(\lambda_k) \left(\prod_{\sigma=\mu}^{\nu-1} b_\sigma \right) \chi_{\nu+1:\ell}(\lambda_k), \tag{5}$$

which holds for $\mu \le \nu$ if one defines $\chi_{1:0}(\lambda_k) = \chi_{\ell+1:\ell}(\lambda_k) \equiv 1$. One can assume $b_\mu \ne 0$ for all $\mu = 1, \ldots, \ell - 1$, as otherwise the diagonalization of T would split into the diagonalization of independent submatrices, so that the eigenvalues of T are nondegenerate. Hence, the derivatives of the characteristic polynomial at the eigenvalues do not vanish, $\chi'(\lambda_k) \ne 0$, and Eq. (5) can be solved for the eigenvector components, for example,

$$O_{k1}^2 = \frac{\chi_{2:\ell}(\lambda_k)}{\chi'(\lambda_k)}, \qquad O_{k\ell}^2 = \frac{\chi_{1:\ell-1}(\lambda_k)}{\chi'(\lambda_k)} \tag{6}$$

and from one of these (one can arbitrarily choose the positive root) the remaining elements of the kth eigenvector follow by means of Eq. (5); for instance, taking $\mu = 1$,

$$O_{k\nu} = O_{k1} b_1 \cdots b_{\nu-1} \frac{\chi_{\nu+1:\ell}(\lambda_k)}{\chi_{2:\ell}(\lambda_k)}, \tag{7}$$

note that the assumption that T is unreduced (i.e., all b's are nonzero) implies that O_{k1} does not vanish, so also $\chi_{2:\ell}(\lambda_k) \ne 0$: indeed, from Eq. (5) one has $O_{k1}O_{k\ell} = b_1 ... b_{\ell-1}/\chi'(\lambda_k) \ne 0$. This shows that the orthogonal matrix O can be fully expressed in terms of characteristic polynomials.

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Note also that the recurrence equations (4) give

$$O_{k,\nu+1} = \frac{\lambda_k - a_\nu}{b_\nu}\, O_{k\nu} - \frac{b_{\nu-1}}{b_\nu}\, O_{k,\nu-1} \quad (\nu = 1, \ldots, \ell{-}1) \tag{8}$$

with the assumption $O_{k0} = 0$; these equations can be used for a sequential computation of the eigenvectors' components once the eigenvalues are known. An important consequence of this construction is that, once the first components of the eigenvectors (O_{k1}) are determined from Eq. (6), the eigenvectors come out already normalized, i.e., the matrix O is orthogonal, making the explicit normalization unnecessary and tremendously simplifying the analytical calculations.

When the matrix size ℓ is large, the characteristic polynomials $\chi_{\mu:\nu}(\lambda_k)$ have a high degree and the analytical evaluation of the eigenvalue decomposition is very demanding. In Sec. III, we provide general simplified formulas for the eigenvalues and for the eigenvector elements, Eqs. (6) and (7), in the case of a quasi-uniform matrix T.

III. QUASI-UNIFORM TRIDIAGONAL MATRICES

A. Uniform tridiagonal matrices

A uniform tridiagonal matrix has equal elements within each diagonal, namely $a_\mu = a$ and $b_\mu = b$, and without loss of generality one can set $b = 1$ and $a = 0$. In this case the recurrence relations (4) for the characteristic polynomials are found to be equal to those defining the Chebyshev polynomials of the second kind,[19]

$$\mathcal{U}_n(\xi) = \frac{\big(\xi + \sqrt{\xi^2{-}1}\big)^{n+1} - \big(\xi - \sqrt{\xi^2{-}1}\big)^{n+1}}{2\sqrt{\xi^2{-}1}}, \tag{9}$$

the correspondence being $\chi_{1:\ell}(\lambda) = \mathcal{U}_\ell(\lambda/2)$. Setting $\xi \equiv \cos k$ the Chebyshev polynomials of the second kind can be compactly written as

$$\mathcal{U}_n(\cos k) = \frac{\sin[(n{+}1)k]}{\sin k}, \tag{10}$$

so that the secular equation $\chi(\lambda) = \mathcal{U}_\ell(\lambda/2) = 0$ defines the ℓ eigenvalues $\lambda \equiv 2\cos k$ corresponding to

$$k \equiv k_j = \frac{\pi j}{\ell+1}, \quad (j = 1, \ldots, \ell). \tag{11}$$

With no ambiguity we will use, henceforth, the index k as running over such a set of ℓ discrete values, so we may keep the notations introduced for the spectral decomposition and, e.g., write the eigenvectors of the uniform case as

$$O_{k\mu} = \sqrt{\frac{2}{\ell{+}1}}\, \sin \mu k.$$

B. Quasi-uniform tridiagonal matrices

A tridiagonal matrix T is said to be *quasi-uniform* if it is mainly constituted by a large uniform tridiagonal block $T_{u:v}$ of size $n \times n$ (with $n = v{-}u{+}1$), i.e., its elements are $a_u = a_{u+1} = \cdots = a_v \equiv a$ and $b_u = b_{u+1} = \cdots = b_{v-1} \equiv b$. By "large uniform block" it is meant that the number of different elements, sitting at one or both *corners*, is much smaller than the size of the whole matrix T, namely that $\ell - n \ll \ell$. Indeed, the important point of our approach is in taking into account the uniform part of T, which for QUT matrices is almost the whole T, and use the properties of Chebyshev polynomials for reducing the complexity of Eqs. (5) and (6). Again, without loss of generality we set $a = 0$ and $b = 1$ in what follows.

The results we present in this paper are based on the following important statement: the characteristic polynomial of QUT matrices can always be expressed in terms of the Chebyshev polynomials[19]

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of the first and second kind, $\mathcal{T}_{n+1}(\xi)$ and $\mathcal{U}_n(\xi)$,

$$\chi(2\xi) \equiv \chi_{1:\ell}(2\xi) = u(\xi)\,\mathcal{U}_n(\xi) + t(\xi)\,\mathcal{T}_{n+1}(\xi), \tag{12}$$

where $u(\xi)$ and $t(\xi)$ are *low-degree* polynomials: indeed, their degree cannot be larger than $\ell - n$ and $\ell - n - 1$, respectively. Their coefficients involve the nonuniform matrix elements and generally they can be easily calculated by means of Eqs. (4).

In order to prove the above general statement we start from the characteristic polynomial of the uniform tridiagonal submatrix $T_{u:v}$ and calculate the characteristic polynomial of larger submatrices by means of Eq. (4a):

$$\begin{aligned}
\chi_{u:v}(2\xi) &= \mathcal{U}_n(\xi),\\
\chi_{u:v+1}(2\xi) &= (2\xi - a_{v+1})\,\mathcal{U}_n(\xi) - b_v^2\,\mathcal{U}_{n-1}(\xi),\\
\chi_{u:v+2}(2\xi) &= (2\xi - a_{v+2})\,\chi_{u:v+1}(2\xi) - b_{v+1}^2\,\mathcal{U}_n(\xi),\\
&\;\;\vdots\\
\chi_{u:\ell}(2\xi) &= \tilde{p}_0(\xi)\,\mathcal{U}_n(\xi) + \tilde{p}_1(\xi)\,\mathcal{U}_{n-1}(\xi),
\end{aligned} \tag{13}$$

this holds for some polynomials $\tilde{p}_0(\xi) = (2\xi)^{\ell-v} + \dots$ and $\tilde{p}_1(\xi)$, whose coefficients are products of the nonuniform matrix elements $a_{v+1}, \dots, a_\ell$ and $b_v, \dots, b_\ell$. By further enlarging the matrix $T_{u:\ell}$ in the upper corner by means of Eq. (4b) we first obtain

$$\chi_{u-1:\ell}(2\xi) = (2\xi - a_{u-1})\,\chi_{u:\ell}(2\xi) - b_{u-1}^2\,\chi_{u+1:\ell}(2\xi),$$

where $\chi_{u+1:\ell}(2\xi)$ concerns the QUT matrix $T_{u+1:\ell}$ whose uniform block is $(n-1)\times(n-1)$, so its expression analogous to Eq. (13) involves $\mathcal{U}_{n-1}(\xi)$ and $\mathcal{U}_{n-2}(\xi)$. Proceeding further one has

$$\begin{aligned}
\chi_{u-2:\ell}(2\xi) &= (2\xi - a_{u-2})\,\chi_{u-1:\ell}(2\xi) - b_{u-2}^2\,\chi_{u:\ell}(2\xi),\\
&\;\;\vdots\\
\chi_{1:\ell}(2\xi) &= p_0(\xi)\,\mathcal{U}_n(\xi) + p_1(\xi)\,\mathcal{U}_{n-1}(\xi) + p_2(\xi)\,\mathcal{U}_{n-2}(\xi),
\end{aligned} \tag{14}$$

for some polynomials $p_0(\xi)$, $p_1(\xi)$, and $p_2(\xi)$. This expression allows us to recover Eq. (12), using the identities

$$\mathcal{U}_{n-1}(\xi) = \xi\,\mathcal{U}_n(\xi) - \mathcal{T}_{n+1}(\xi), \tag{15a}$$

$$\begin{aligned}
\mathcal{U}_{n-2}(\xi) &= 2\xi\,\mathcal{U}_{n-1}(\xi) - \mathcal{U}_n(\xi),\\
&= (2\xi^2 - 1)\,\mathcal{U}_n(\xi) - 2\xi\,\mathcal{T}_{n+1}(\xi)
\end{aligned} \tag{15b}$$

and identifying

$$u(\xi) = p_0(\xi) + \xi\, p_1(\xi) + (2\xi^2 - 1)\,p_2(\xi), \tag{16a}$$

$$t(\xi) = -p_1(\xi) - 2\xi\, p_2(\xi). \tag{16b}$$

The usefulness of expressing $\chi(\lambda) \equiv \chi_{1:\ell}(\lambda)$ in the form (12) is evident looking at the analog of Eq. (10) for the first-kind Chebyshev polynomials,

$$\mathcal{T}_n(\cos k) = \cos(nk), \tag{17}$$

which turns Eq. (12) into

$$\chi(2\cos k) = u(\cos k)\,\frac{\sin[(n+1)k]}{\sin k} + t(\cos k)\,\cos[(n+1)k], \tag{18}$$

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hence, the secular equation $\chi = 0$ can be written

$$\sin[(n+1)k - 2\phi_k] = 0 \tag{19}$$

with the angle ϕ_k defined by

$$\tan 2\phi_k = -\frac{t(\cos k)}{u(\cos k)} \sin k. \tag{20}$$

Equivalently, the same form of the secular equation can be derived directly by simply rewriting Eq. (10) as $\sin k\, \mathcal{U}_n(\cos k) = \Im\left\{e^{i(n+1)k}\right\}$ and replacing it in Eq. (14), which turns indeed into

$$\Im\left\{e^{i[(n+1)k-2\phi_k]}\right\} = 0, \tag{21}$$

where $2\phi_k$ coincides with the phase of the complex number

$$w_k \equiv p_0(\xi) + e^{-ik}\, p_1(\xi) + e^{-2ik}\, p_2(\xi) = |w_k|\, e^{-2i\phi_k}. \tag{22}$$

It is convenient, in order to easily recover the limit of a fully uniform $\ell \times \ell$ matrix T, to use slightly modified versions of Eqs. (19) and (20), namely

$$\sin[(\ell+1)k - 2\varphi_k] = 0 \tag{23}$$

with *shifts* φ_k defined by

$$2\varphi_k = (\ell-n)\,k - \tan^{-1}\left[\frac{t(\cos k)}{u(\cos k)} \sin k\right]. \tag{24}$$

Hence, the eigenvalues of the QUT matrix, parametrized as $\lambda = 2\cos k$, with $k \in [0, \pi]$, can be obtained from the equations

$$k \equiv k_j = \frac{\pi\, j + 2\varphi_{k_j}}{\ell+1}, \quad (j = 1, \ldots, \ell), \tag{25}$$

which determine the *allowed* values of k. Comparing with Eq. (11) it appears that the shifts φ_k represent the deviation from the uniform case, where they vanish. Equation (25) can be solved numerically for any j (except for a few j's if there are out-of-band eigenvalues, see below). Usually, an iterative computation is fast converging; in the limit of $\ell \gg 1$ even the truncation of (25) after the first iteration can be very accurate, as it was verified in the cases considered in Refs. 6 and 16. Note that while Eqs. (19) and (23) are well-defined, there is an ambiguity in expressing their solutions as in Eq. (25), due to the fact that the phase shifts involve the multivalued $\tan^{-1}$ function whose conventional range is $[-\pi/2, \pi/2]$: this can yield π-steps at the zeroes of the argument's denominator, so care has to be taken in choosing a continuous phase for $k \in (0, \pi)$.

Noteworthy, in the limit of large ℓ, Eq. (25) allows us to obtain a useful analytic expression of the *density of states* ρ_k defined in the interval $k \in [0, \pi]$, namely

$$\rho_k^{-1} = \partial_j k = \frac{\pi}{\ell+1 - 2\varphi'_k}, \tag{26}$$

by means of which summations over eigenmodes can be transformed into integrals over k,

$$\sum_j (\cdots) \simeq \int_0^\pi dk \rho_k (\cdots), \tag{27}$$

one can also observe that ρ_k^{-1} represents the spacing between subsequent allowed values of k: the deformation from the equally-spaced k's of the uniform case, $\pi/(\ell + 1)$, is represented by the correction term with φ'_k.

C. Eigenvectors

The boundary elements of the eigenvectors given in Eq. (6) can be calculated using the same formalism. Indeed, following the construction of Subsection III B we can find the polynomials $u^{\ulcorner}(\xi)$,

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$t^{\ulcorner}(\xi)$, $u_{\lrcorner}(\xi)$, $t_{\lrcorner}(\xi)$ such that

$$\chi_{2:\ell}(2\xi) = u^{\ulcorner}(\xi)\,\mathcal{U}_n(\xi) + t^{\ulcorner}(\xi)\,\mathcal{T}_{n+1}(\xi),$$
$$\chi_{1:\ell-1}(2\xi) = u_{\lrcorner}(\xi)\,\mathcal{U}_n(\xi) + t_{\lrcorner}(\xi)\,\mathcal{T}_{n+1}(\xi), \tag{28}$$

where the symbols $^{\ulcorner}$ and $_{\lrcorner}$ clearly refer to the submatrices $T_{2:\,\ell}$ and $T_{1:\,\ell\,-\,1}$, respectively. Accordingly, expressing $\chi'(\lambda)$ as a function of $\mathcal{U}_n$ and $\mathcal{T}_{n+1}$ thanks to the relations

$$\mathcal{T}'_{n+1}(\xi) = (n{+}1)\mathcal{U}_n(\xi), \tag{29a}$$

$$(1{-}\xi^2)\mathcal{U}'_n(\xi) = \xi\mathcal{U}_n(\xi) - (n{+}1)\,\mathcal{T}_{n+1}(\xi), \tag{29b}$$

Eqs. (6) take the form

$$O_{1k}^2 = 2\frac{u^{\ulcorner}(\xi_k)\,\mathcal{U}_n(\xi_k) + t^{\ulcorner}(\xi_k)\,\mathcal{T}_{n+1}(\xi_k)}{u_n^{\star}(\xi_k)\,\mathcal{U}_n(\xi_k) + t_n^{\star}(\xi_k)\,\mathcal{T}_{n+1}(\xi_k)}, \tag{30a}$$

$$O_{\ell k}^2 = 2\frac{u_{\lrcorner}(\xi_k)\,\mathcal{U}_n(\xi_k) + t_{\lrcorner}(\xi_k)\,\mathcal{T}_{n+1}(\xi_k)}{u_n^{\star}(\xi_k)\,\mathcal{U}_n(\xi_k) + t_n^{\star}(\xi_k)\,\mathcal{T}_{n+1}(\xi_k)}, \tag{30b}$$

where $\xi_k \equiv \lambda_k/2 \equiv \cos k$ and

$$u_n^{\star}(\xi) = u'(\xi) + \frac{\xi}{1{-}\xi^2}\,u(\xi) + (n{+}1)\,t(\xi), \tag{31a}$$

$$t_n^{\star}(\xi) = t'(\xi) - \frac{n{+}1}{1{-}\xi^2}\,u(\xi). \tag{31b}$$

As the eigenvalues are the solutions of the secular equation,

$$0 = u(\xi_k)\,\mathcal{U}_n(\xi_k) + t(\xi_k)\,\mathcal{T}_{n+1}(\xi_k), \tag{32}$$

the high-degree polynomials $\mathcal{U}_n(\xi_k)$ and $\mathcal{T}_{n+1}(\xi_k)$ can be removed from (30) and accordingly

$$O_{1k}^2 = 2\frac{u^{\ulcorner}(\xi_k)\,t(\xi_k) - t^{\ulcorner}(\xi_k)\,u(\xi_k)}{u_n^{\star}(\xi_k)\,t(\xi_k) - t_n^{\star}(\xi_k)\,u(\xi_k)}, \tag{33a}$$

$$O_{\ell k}^2 = 2\frac{u_{\lrcorner}(\xi_k)\,t(\xi_k) - t_{\lrcorner}(\xi_k)\,u(\xi_k)}{u_n^{\star}(\xi_k)\,t(\xi_k) - t_n^{\star}(\xi_k)\,u(\xi_k)}. \tag{33b}$$

This shows a remarkable result, namely that, although the eigenvector components generally depend on complicated high-degree polynomials, for QUT matrices one can express the boundary coefficients of the eigenvectors in terms of ratios of low-degree polynomials.

Further simplifications can be obtained by replacing again $\xi_k = \cos k$. In fact, from Eq. (24)

$$2\varphi'_k = (\ell{-}n) - \frac{tu\ \cos k + (t'u - u't)\ \sin^2 k}{u^2 + t^2 \sin^2 k}, \tag{34}$$

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where the argument ξ_k of u and t is understood, so that the eigenvector elements (33) read

$$O_{1k}^2 = \frac{2\sin^2 k}{\ell+1-2\varphi_k'}\;\frac{u^{\ulcorner}(\xi_k)\,t(\xi_k)-t^{\ulcorner}(\xi_k)\,u(\xi_k)}{u^2(\xi_k)+t^2(\xi_k)\;\sin^2 k}, \tag{35a}$$

$$O_{\ell k}^2 = \frac{2\sin^2 k}{\ell+1-2\varphi_k'}\;\frac{u_{\lrcorner}(\xi_k)\,t(\xi_k)-t_{\lrcorner}(\xi_k)\,u(\xi_k)}{u^2(\xi_k)+t^2(\xi_k)\;\sin^2 k}. \tag{35b}$$

These expressions generalize what was found in Refs. 6 and 16.

As for the remaining elements, note that the recurrence relation (8) in the bulk, i.e., for $u < \nu < v$, reads

$$O_{k,\nu+1}+O_{k,\nu-1} = (e^{ik}+e^{-ik})\,O_{k\nu}, \tag{36}$$

whose generic solution is

$$O_{k\nu} = \Im\{e^{ik\nu}\alpha_k\}, \tag{37}$$

for any complex number α_k independent of ν, which has to be determined by requiring that the "boundary" relations (8), i.e., for $\nu = 2, \ldots, u$ and $\nu = v, \ldots, \ell-1$ be satisfied.

D. Out-of-band eigenvalues

The fact of setting $\lambda \equiv 2\cos k$ does not imply that *all* eigenvalues are included in the band $[-2, 2]$. For a QUT matrix this is generally true for the largest part of the spectrum, though a few eigenvalues can emerge over or below the band when (the absolute values of) the nonuniform matrix elements are large enough; correspondingly, Eq. (25) cannot be solved for a few values of j, i.e., Eq. (23) has less than ℓ solutions in the interval $k \in [0, \pi]$. On the other hand, the out-of-band eigenvalues are still described by $\lambda \equiv 2\cos k$, but with complex values of $k = q + ip$; for the eigenvalues to be real q must be either 0 or π, i.e.,

$$\lambda = \pm 2\cosh p \tag{38}$$

and $p \geq 0$. Correspondingly, one can take the expression for the Chebyshev polynomials when the absolute value of the argument is larger than one,

$$U_n(\pm\cosh p) = (\pm)^n\frac{\sinh(n+1)p}{\sinh p}. \tag{39}$$

In the large-ℓ limit, the out-of-band eigenvalues have to be considered separately by adding to the integral (27) the sum over the out-of-band states. As for the eigenvectors, the recurrence relation (8) in the bulk, i.e., for $u < \nu < v$, reads

$$O_{p,\nu+1}+O_{p,\nu-1} = \pm(e^{p}+e^{-p})\,O_{p\nu}, \tag{40}$$

where the sign corresponds to that of Eq. (38); the generic solution is

$$O_{p\nu} = (\pm)^\nu\big(\alpha_p\,e^{p\nu}+\beta_p\,e^{-p\nu}\big), \tag{41}$$

where the real numbers α_p and β_p (independent of ν) have to be determined by requiring that the "boundary" relations (8), i.e., for $\nu = 2, \ldots, u$ and $\nu = v, \ldots, \ell-1$ be satisfied.

An example of how to deal with such eigenvalues is given in Sec. IV A.

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IV. EXAMPLES

A. Mirror-symmetric two-edge matrix

As a first example we consider a mirror-symmetric QUT matrix with two non-uniform edges: the uniform block is of size $n = \ell - 2$, so the matrix reads, setting $b = 1$ and $a = 0$,

$$T = T_{1:\ell} = \begin{pmatrix} x & y & & & & & \\ y & 0 & 1 & & & & \\ & 1 & 0 & 1 & & & \\ & & 1 & \ddots & \ddots & & \\ & & & \ddots & & 1 & \\ & & & & 1 & 0 & y \\ & & & & & y & x \end{pmatrix}, \tag{42}$$

and, with the notations of Sec. III, $u = 2$ and $v = \ell{-}1$.

Keeping the notation $\lambda \equiv 2\xi$, thanks to the recursion relations (4) it holds that

$$\begin{aligned} \chi_{2:\ell}(2\xi) &= (2\xi{-}x)\,\mathcal{U}_n(\xi) - y^2\,\mathcal{U}_{n-1}(\xi), \\ \chi_{3:\ell}(2\xi) &= (2\xi{-}x)\,\mathcal{U}_{n-1}(\xi) - y^2\,\mathcal{U}_{n-2}(\xi), \\ \chi_{1:\ell}(2\xi) &= (2\xi{-}x)\;\chi_{2:\ell}(2\xi) - y^2\,\chi_{3:\ell}, \\ &= (2\xi{-}x)^2\,\mathcal{U}_n(\xi) - 2(2\xi{-}x)y^2\,\mathcal{U}_{n-1}(\xi) + y^4\,\mathcal{U}_{n-2}(\xi). \end{aligned} \tag{43}$$

Accordingly, the secular equation for the in-band eigenvalues is given by (23), where the shifts are more easily found from Eq. (22): indeed, thanks to mirror symmetry, w_k turns out to be a square,

$$w_k = (2\xi - x - y^2 e^{-ik})^2 = \big[(2{-}y^2)\cos k - x + i\,y^2\sin k\big]^2, \tag{44}$$

so that

$$\varphi_k = k - \tan^{-1}\frac{y^2\sin k}{(2{-}y^2)\cos k - x}. \tag{45}$$

The expression (43) can be rewritten in the form (12) by means of the properties (15), so with the notation of Sec. III we identify the coefficients of Eqs. (12) and (28) as

$$u(\xi) = \big[(2{-}y^2)\xi - x\big]^2 - y^4\,(1-\xi^2), \tag{46a}$$

$$t(\xi) = 2y^2\,\big[(2{-}y^2)\xi - x\big], \tag{46b}$$

$$u^{\ulcorner}(\xi) = u_{\lrcorner}(\xi) = (2{-}y^2)\xi - x, \tag{46c}$$

$$t^{\ulcorner}(\xi) = t_{\lrcorner}(\xi) = y^2. \tag{46d}$$

Of course, Eq. (45) can be obtained using straightforward trigonometric identities also from (24) and the above polynomials. As for the first components of the eigenvectors, they follow from Eq. (35):

$$O_{k1}^2 = O_{k\ell}^2 = \frac{2}{\ell{+}1{-}2\varphi_k'}\,\frac{y^2\sin^2\!k}{[(2{-}y^2)\cos k - x]^2 + y^4\sin^2\!k}. \tag{47}$$

Moreover, imposing to the generic solution (37) the conditions (8) at the corners, one finds

$$\alpha_k = \frac{1 - x\,e^{-ik} + (1{-}y^2)\,e^{-2ik}}{y\sin k}\,O_{k1}, \tag{48}$$

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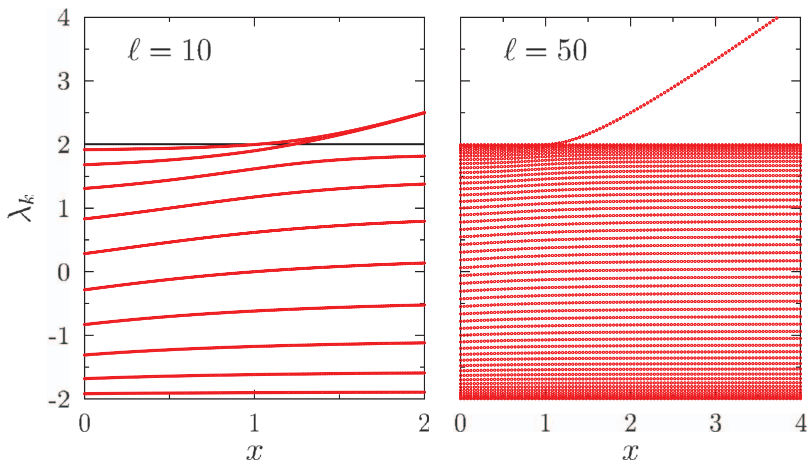

FIG. 1. Eigenvalues of the matrix (42) for $y = 1$ as a function of the corner element x, for matrix sizes $\ell = 10$ and 50. When $x > 1$ there can be two out-of-band eigenvalues.

so that all components of the eigenvectors have a fully analytical expression

$$O_{k\nu} = \frac{\sin \nu k - x \sin(\nu{-}1)k + (1{-}y^2)\sin(\nu{-}2)k}{y \sin k} O_{k1}$$
$$= \left(\frac{2}{\ell + 1 - 2\varphi_k'}\right)^{\frac{1}{2}} \sin(\nu k - \varphi_k), \tag{49}$$

for $\nu = 2, \ldots, \ell - 1$. Equations (49) and (47), together with (45) and (23), give a complete solution to the analytical diagonalization problem of matrix (42). Note that for $x = 0$ this expression is in agreement with Ref. 10.

We remark that as long as there are no out-of-band eigenvalues, Eq. (47) is exactly normalized, i.e., $\sum_k O_{k1}^2 = 1$; thanks to Eq. (27), in the large-ℓ limit the sum turns into the integral

$$\mathcal{I}(x, y) = \int_0^{\pi} \frac{dk}{\pi} \frac{2\, y^2 \sin^2 k}{[(2{-}y^2)\cos k - x]^2 + y^4 \sin^2 k} = 1. \tag{50}$$

Eigenvalues $\lambda \notin [-2, 2]$ can exist for large x or y. Let us consider the simpler case $y = 1$, with $x > 0$, which is reported in Fig. 1. From Eq. (43) one finds the secular equation

$$U_\ell - 2xU_{\ell-1} + x^2 U_{\ell-2} = 0, \tag{51}$$

that, by means of the representation (39), gives rise to two implicit solutions,

$$x = \begin{cases} \dfrac{\cosh \frac{\ell+1}{2} p}{\cosh \frac{\ell-1}{2} p} \geq 1 \\[2ex] \dfrac{\sinh \frac{\ell+1}{2} p}{\sinh \frac{\ell-1}{2} p} \geq \dfrac{\ell+1}{\ell-1} \end{cases}, \tag{52}$$

hence, two eigenvalues $\lambda = 2\cosh p$ can emerge from the band, one for $x > 1$ and the second for $x > \frac{\ell+1}{\ell-1}$, which correspond to a mirror-symmetric and a mirror-antisymmetric eigenvector; in the large-ℓ limit both equations tend to $x = e^p$ so the two eigenvalues converge to the value $\lambda = x + x^{-1}$. The existence of out-of-band eigenvalues for $x > 1$ is reflected in the integral (50), because $\mathcal{I}(x, 1) = \theta(1{-}x) + \theta(x{-}1)x^{-2}$: indeed, the full normalization requires the contribution from the out-of-band components.

The above application, besides the in-band state density, has immediately given the exact out-of-band eigenvalues. The comparison with the approach of Ref. 20, where the same task is accomplished by perturbation theory and by an ansatz for the eigenvectors, illustrates how effective and general is our technique. In particular, the ansatz is nothing but the bulk solution (41).

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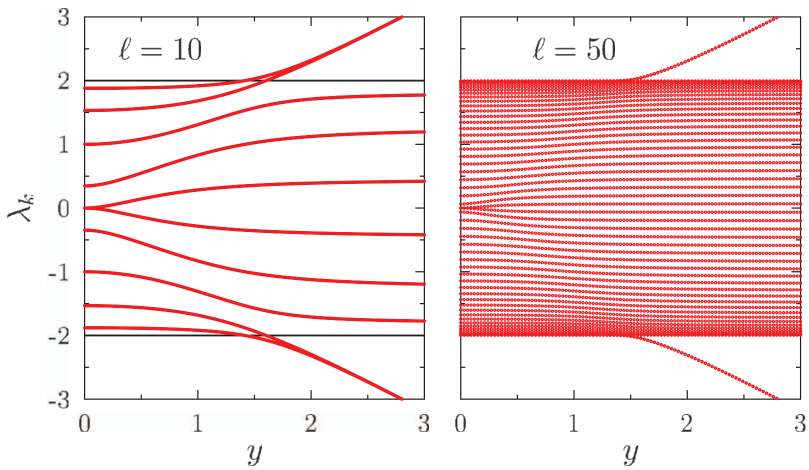

FIG. 2. Eigenvalues of the matrix (42) for $x = 0$ as a function of y, for matrix sizes $\ell = 10$ and 50. When $y > \sqrt{2}$ there can be two pairs of opposite out-of-band eigenvalues.

A similar reasoning applies when y is left to vary while $x = 0$, reported in Fig. 2, though in this case the out-of-band eigenvalues occur as two pairs of opposite sign. We find indeed $\mathcal{I}(0, y) = \theta(2 - y^2) + \theta(y^2 - 2)(y^2{-}1)^{-1}$, which is smaller than 1 for $y > \sqrt{2}$.

To establish, the existence of out-of-band states becomes difficult in complex scenarios (e.g., with more elements on the boundaries): still, verifying the continuum-limit normalization of the in-band eigenvectors allows one to immediately detect whether out-of-band states exist or not.

For instance, let us consider the general case with both x and y varying: although calculating the integral (50) is not trivial, we know that it must evaluate to 1 as long as all eigenvalues belong to the band $[-2, 2]$. This can be shown to be the case whenever $y < \sqrt{2 - x}$. The appearance of out-of-band states occurs when crossing the line $y^2 + x = 2$, as for $\sqrt{2{-}x} < y < \sqrt{2{+}x}$ one has

$$\mathcal{I}(x, y) = \frac{2y^2}{x^2{+}4y^2{-}4 + x\sqrt{x^2{+}4y^2{-}4}}, \tag{53}$$

eventually, for $y > \sqrt{2{+}x}$ the result is even independent of x, namely $\mathcal{I}(x, y) = (y^2{-}1)^{-1}$.

B. More mirror symmetric elements

As a second example we consider a mirror-symmetric matrix with more nonuniform elements on the edges,

$$\begin{pmatrix} 0 & x & & & & & & & \\ x & 0 & y & & & & & & \\ & y & 0 & 1 & & & & & \\ & & 1 & 0 & 1 & & & & \\ & & & \ddots & \ddots & \ddots & & & \\ & & & & 1 & 0 & 1 & & \\ & & & & & 1 & 0 & y & \\ & & & & & & y & 0 & x \\ & & & & & & & x & 0 \end{pmatrix}_{\ell\times\ell} . \tag{54}$$

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Using straightforward algebra we find

$$\begin{aligned}
w_k &= \big[2-y^2-x^2+(2-y^2)\cos 2k+i\,y^2\sin 2k\big]^2,\\
u(\xi) &= \big[2\xi^2(2-y^2)-x^2\big]^2-(1-\xi^2)\,4\xi^2y^4,\\
t(\xi) &= 4\xi\,y^2\big[2\xi^2(2-y^2)-x^2\big],\\
u^{\ulcorner}(\xi) &= u_{\lrcorner}(\xi)=\xi\big[-2y^4-x^2(2-y^2)+4(2-2y^2+y^4)\xi^2\big],\\
t^{\ulcorner}(\xi) &= t_{\lrcorner}(\xi)=y^2\big[4(2-y^2)\xi^2-x^2\big],
\end{aligned}$$

and accordingly

$$\varphi_k = 2k-\tan^{-1}\left[\frac{y^2\sin 2k}{z^2+(2-y^2)\cos 2k}\right], \qquad (55)$$

$$O_{1k}^2 = O_{k\ell}^2 = \frac{2}{\ell+1-2\varphi'_k}\,\frac{x^2y^2\sin^2 k}{\big[z^2+(2-y^2)\cos 2k\big]^2+y^4\sin^2 2k}, \qquad (56)$$

where $z^2\equiv 2-x^2-y^2$.

C. Non-mirror-symmetric matrix

In order to connect our formalism with the results of Ref. 1, let us consider the following non-mirror-symmetric matrix

$$\begin{pmatrix}
x & y & & & & & & \\
y & 0 & 1 & & & & & \\
 & 1 & 0 & 1 & & & & \\
 & & 1 & 0 & 1 & & & \\
 & & & 1 & \ddots & \ddots & & \\
 & & & & \ddots & & 1 & \\
 & & & & & 1 & 0 & 1\\
 & & & & & & 1 & z
\end{pmatrix}_{\ell\times\ell}, \qquad (57)$$

where $\ell = n+2$. We find

$$\begin{aligned}
t^{\ulcorner}(\xi) &= 1, & u^{\ulcorner}(\xi) &= \xi-z,\\
t_{\lrcorner}(\xi) &= y^2, & u_{\lrcorner}(\xi) &= (2-y^2)\xi-x,\\
t(\xi) &= 2\xi-x-y^2z, & u(\xi) &= (x-2\xi)(z-\xi)+y^2(z\xi-1),
\end{aligned}$$

and in particular

$$\tan 2\phi_k = \frac{(x+y^2z-2\cos k)\sin k}{(x-2\cos k)(z-\cos k)+y^2(z\cos k-1)}, \qquad (58)$$

from which the spectral decomposition follows. In fact, it can be shown that, once O_{k1} is calculated with Eq. (35), the remaining eigenvectors are given by (49), except for the ℓth one that follows from Eq. (8). Equation (58) extends the results of Ref. 1: for example when $x=0$, $y=1$, and $z=-1$ we find $2\phi_k = -\frac{3}{2}k$ and

$$k_j = \frac{2\pi j}{2\ell+1},$$

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recovering Theorem 1 of Ref. 1. With the proper parametrization it can be shown that the other theorems of Ref. 1 concerning symmetric tridiagonal matrices follow as well.

V. CONCLUSIONS

We have introduced a technique for the analytical diagonalization of large QUT matrices. The quasi-uniformity has been exploited to show that almost all eigenvalues belong to the same band of those of the fully uniform matrix, $\lambda = 2\cos k$, with $k \in [0, \pi]$, and that their distribution is a deformation of the equally spaced k's of the uniform case, characterized by *shifts* φ_k, as Eqs. (24) and (25) show. The first components O_{k1} of the normalized eigenvectors are written in terms of ratios of low-degree polynomials (35) that can be easily calculated from the non-uniform part of the QUT matrix, while the other components are constructed recursively from O_{k1} using Eq. (8); exploiting the uniform-bulk property, i.e., using Eq. (37), all components can be expressed as O_{k1} times a combination of Chebyshev polynomials, as shown in a particular example by Eq. (49).

In the case of a large QUT matrix, the eigenvalues can be described in terms of a modified density of states within the band of the corresponding uniform matrix. A limited number of out-of-band eigenvalues can exist and have to be accounted for separately as discussed in Sec. III D and exemplified in Sec. IV A.

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