Diagonalization of quasi-uniform tridiagonal matrices

Leonardo Banchi

*ISI Foundation, Via Alassio 11/c, I-10126 Torino (TO), Italy*

Ruggero Vaia

*Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, via Madonna del Piano 10, I-50019 Sesto Fiorentino (FI), Italy*

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The task of analytically diagonalizing a tridiagonal matrix can be considerably simplified when a part of the matrix is uniform. Such quasi-uniform matrices occur in several physical contexts, both classical and quantum, where one-dimensional interactions prevail. These include magnetic chains, 1D arrays of Josephson junctions or of quantum dots, boson and fermion hopping models, random walks, and so on. In such systems the bulk interactions are uniform, and differences may occur around the boundaries of the arrays. Since in the uniform case the spectrum consists of a band, we exploit the bulk uniformity of quasi-uniform tridiagonal matrices in order to express the spectral problem in terms of a variation of the distribution of eigenvalues in the band and of the corresponding eigenvectors. In the limit of large matrices this naturally leads to a deformation of the density of states which can be expressed analytically; a few out-of-band eigenvalues can show up and have to be accounted for separately. The general procedure is illustrated with some examples.

I. INTRODUCTION

The diagonalization of quasi-uniform tridiagonal matrices, namely tridiagonal matrices which are uniform except at the boundaries, appears in many branches of mathematics and physics [1–5]. In particular, tridiagonal matrices generally occur in the theory of one-dimensional lattices with nearest-neighbour interactions. In this context quasi-uniform tridiagonal matrices have been recently applied for achieving high quality quantum communication between distant parts [6–11], and for describing spin systems in a spin environment [12–14].

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. A small number of localized eigenstates could emerge from the band and have to be accounted for separately. Particular applications of this technique were made in Refs. [6, 15].

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 \( \ell \) eigenvectors of \( T \) with eigenvalues \( \lambda_k \), and \( \Lambda = \text{diag}\{\lambda_k\} \).

\( T \) 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 \[16\],

\[
O_{k,\ell+1-\mu} = (-)^{k+1} O_{k\mu} ;
\]

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,

\[
T_{\mu,\nu} = \begin{pmatrix}
  a_\mu & b_\mu & \cdots & b_{\mu+1} \\
  b_\mu & a_{\mu+1} & \cdots & \cdots \\
  \cdots & \cdots & \cdots & \cdots \\
  b_{\nu-1} & \cdots & b_{\nu-1} & a_\nu
\end{pmatrix},
\]
and for the corresponding characteristic polynomials,
\[ \chi_{\mu, \nu} (\lambda) = \det[\lambda - T_{\mu, \nu}] , \]
where \( \mu \leq \nu \); then \( T_{1,0} \equiv T \) and \( \chi_{1,0}(\lambda) \equiv \chi(\lambda) \); the eigenvalues are the \( \ell \) 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
\[
\begin{align*}
\chi_{\mu, \nu}(\lambda) &= (\lambda - a_\nu) \chi_{\mu, \nu-1}(\lambda) - b_{\nu-1}^2 \chi_{\mu, \nu-2}(\lambda), \\
\chi_{\mu, \nu}(\lambda) &= (\lambda - a_\mu) \chi_{\mu+1, \nu}(\lambda) - b_\mu^2 \chi_{\mu+2, \nu}(\lambda) .
\end{align*}
\]

The following important and useful formula (see, e.g., Ref. [17]) expresses the product of two components of the same eigenvector,
\[ \chi'(\lambda_k) O_{k\mu} O_{k\nu} = \chi_{1, \mu-1}(\lambda_k) \left( \prod_{\sigma = \mu}^{\nu-1} b_\sigma \right) \chi_{\nu+1, \ell}(\lambda_k) , \]
which holds for \( \mu \leq \nu \) if one defines \( \chi_{1, \ell}(\lambda_k) = \chi_{\nu+1, \ell}(\lambda_k) \equiv 1 \). One can assume \( b_\mu \neq 0 \) 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, \( \chi'(\lambda_k) \neq 0 \), and Eq. (6) can be solved for the eigenvector components, for example
\[
O_{k1}^2 = \frac{\chi_{\ell, \ell}(\lambda_k)}{\chi'(\lambda_k)} , \quad O_{k\ell}^2 = \frac{\chi_{1, \ell-1}(\lambda_k)}{\chi'(\lambda_k)} ,
\]
and from one of these (one can arbitrarily choose the positive root) the remaining elements of the \( k \)-th eigenvector follow by means of Eq. (5); for instance, taking \( \mu = 1 \),
\[ O_{k\nu} = O_{k1} b_1 \cdots b_{\nu-1} \frac{\chi_{\nu+1, \ell}(\lambda_k)}{\chi_{\ell, \ell}(\lambda_k)} = O_{k1} \prod_{\mu = 2}^{\nu} b_\mu^{-1} \frac{\chi_{\nu+1, \ell}(\lambda_k)}{\chi_{\nu, \ell}(\lambda_k)} . \]
This shows that the orthogonal matrix \( O \) can be fully expressed in terms of characteristic polynomials.

Note also that the recurrence equations (4) give
\[ O_{k, \nu+1} = \frac{\lambda_k - a_\nu}{b_\nu} O_{k\nu} - \frac{b_{\nu-1}}{b_\nu} O_{k, \nu-1} \quad (\nu = 1, \ldots, \ell-1) , \]
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. (5), 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 \( \ell \) 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 the forthcoming section 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 [18],
\[ U_n(\xi) = \frac{(\xi + \sqrt{\xi^2 - 1})^{n+1} - (\xi - \sqrt{\xi^2 - 1})^{n+1}}{2\sqrt{\xi^2 - 1}} , \]
(9)
the correspondence being \( \chi_{i,t}(\lambda) = U_0(\lambda/2) \). Setting \( \xi \equiv \cos k \) the Chebyshev polynomials of the second kind can be compactly written as

\[
U_n(\cos k) = \frac{\sin[(n+1)k]}{\sin k},
\]

so that the secular equation \( \chi(\lambda) = U_0(\lambda/2) = 0 \) defines the \( \ell \) eigenvalues \( \lambda \equiv 2 \cos k \) corresponding to

\[
k \equiv k_j = \frac{\pi j}{\ell + 1}, \quad (j = 1, \ldots, \ell).
\]

With no ambiguity we will use henceforth the index \( k \) as running over such a set of \( \ell \) discrete values, so we may keep the notations introduced for the spectral decomposition and, e.g., write the eigenvectors of the uniform case as \( O_{k,\ell} = \sqrt{2/((\ell+1) \sin(\mu k))} \).

**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 means 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 quasi-uniform tridiagonal (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 be expressed in terms of the Chebyshev polynomials \(^{18}\) of the first and second kind, \( T_{n+1}(\xi) \) and \( U_n(\xi) \),

\[
\chi(2\xi) \equiv \chi_{i,t}(2\xi) = u(\xi) U_n(\xi) + t(\xi) T_{n+1}(\xi),
\]

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. (11).

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. (11):

\[
\begin{align*}
\chi_{u,v}(2\xi) &= U_n(\xi), \\
\chi_{u,v+1}(2\xi) &= (2\xi - a_{v+1}) U_n(\xi) - b_{v+1}^2 U_{n-1}(\xi), \\
\chi_{u,v+2}(2\xi) &= (2\xi - a_{v+2}) \chi_{u,v+1}(2\xi) - b_{v+2}^2 U_n(\xi), \\
&\vdots \\
\chi_{u,t}(2\xi) &= \tilde{p}_0(\xi) U_n(\xi) + \tilde{p}_1(\xi) U_{n-1}(\xi); 
\end{align*}
\]

this holds for some polynomials \( \tilde{p}_0(\xi) = (2\xi)^{\ell-v} + \cdots \) and \( \tilde{p}_1(\xi) \), whose coefficients are products of the nonuniform matrix elements \( a_{v+1}, \ldots, a_{t} \) and \( b_v, \ldots, b_{\ell} \). By further enlarging the matrix \( T_{u,t} \) in the upper corner by means of Eq. (11) we first obtain

\[
\chi_{u-1,t}(2\xi) = (2\xi - a_{u-1}) \chi_{u,t}(2\xi) - b_{u-1}^2 \chi_{u+1,t}(2\xi),
\]

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

\[
\begin{align*}
\chi_{u-2,t}(2\xi) &= (2\xi - a_{u-2}) \chi_{u-1,t}(2\xi) - b_{u-2}^2 \chi_{u,t}(2\xi), \\
&\vdots \\
\chi_{t,t}(2\xi) &= p_0(\xi) U_n(\xi) + p_1(\xi) U_{n-1}(\xi) + p_2(\xi) U_{n-2}(\xi),
\end{align*}
\]
for some polynomials $p_0(\xi), p_1(\xi),$ and $p_2(\xi)$. This expression allows us to recover Eq. (12), using the identities

\begin{align}
U_{n-1}(\xi) &= \xi U_n(\xi) - T_{n+1}(\xi), \tag{15a} \\
U_{n-2}(\xi) &= 2\xi U_{n-1}(\xi) - U_n(\xi) = (2\xi^2 - 1)U_n(\xi) - 2\xi T_{n+1}(\xi), \tag{15b}
\end{align}

and identifying

\begin{align}
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}
\end{align}

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

$$T_n(\cos k) = \cos(nk),$$

which turns Eq. (12) into

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

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

$$\sin[(n+1)k - 2\phi_k] = 0,$$

with the angle $\phi_k$ defined by

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

Equivalently, the same form of the secular equation can be derived directly by simply rewriting Eq. (10) as $\sin kU_n(\cos k) = 3\{e^{i(n+1)k}\}$ and replacing it in Eq. (14), which turns indeed into

$$\Re\{e^{i(n+1)k-2\phi_k}\} = 0,$$

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

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

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

$$\sin[(\ell+1)k - 2\varphi_k] = 0,$$

with shifts $\varphi_k$ defined by

$$2\varphi_k = (\ell-n)k - \tan^{-1}\frac{t(\cos k) \sin k}{u(\cos k)}.$$ 

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

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

which determine the allowed values of $k$. Comparing with Eq. (11) it appears that the shifts $\varphi_k$ represent the deviation from the uniform case, where they vanish. Eq. (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, 15].

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

$$\rho_k^{-1} = \partial_k k = \frac{\pi}{\ell+1 - 2\varphi_k},$$

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

$$\sum_j (\cdots) \approx \int_0^\pi dk \rho_k (\cdots);$$

one can also observe that $\rho_k^{-1}$ 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 $\varphi_k$. 

C. 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. (25) has less than \( \ell \) 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 \( \pi \), i.e.,

\[
\lambda = \pm 2 \cosh p ,
\]

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,

\[
U_n(\pm \cosh p) = (\pm)^n \frac{\sinh (n+1)p}{\sinh p} .
\]

In the large-\( \ell \) 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. An example of how to deal with such eigenvalues is given in Section IV A.

D. Eigenvectors

The boundary elements of the eigenvectors given in Eq. (1) can be calculated using the same formalism. Indeed, following the construction of the previous subsection we can find the polynomials \( u'(\xi), t'(\xi), u_j(\xi), t_j(\xi) \) such that

\[
\chi_{c:2}(2\xi) = u'(\xi) U_n(\xi) + t'(\xi) T_{n+1}(\xi) , \quad \chi_{c:2}(2\xi) = u_j(\xi) U_n(\xi) + t_j(\xi) T_{n+1}(\xi) ,
\]

where the symbols \( c \) and \( j \) clearly refer to the submatrices \( T_{2:2} \) and \( T_{1:2} \), respectively. Accordingly, expressing \( \chi'_j(\lambda) \) as a function of \( U_n \) and \( T_{n+1} \) thanks to the relations

\[
T_{n+1}(\xi) = (n+1) U_n(\xi) , \quad (1-\xi^2) U_n'(\xi) = \xi U_n(\xi) - (n+1) T_{n+1}(\xi) ,
\]

Eqs. (24) take the form

\[
O_{jk}^2 = 2 \frac{u'(\xi_k) U_n(\xi_k) + t'(\xi_k) T_{n+1}(\xi_k)}{u_n(\xi_k) U_n(\xi_k) + t_n(\xi_k) T_{n+1}(\xi_k)} , \quad O_{jk}^2 = 2 \frac{u_j(\xi_k) U_n(\xi_k) + t_j(\xi_k) T_{n+1}(\xi_k)}{u_n(\xi_k) U_n(\xi_k) + t_n(\xi_k) T_{n+1}(\xi_k)} ,
\]

where \( \xi_k \equiv \lambda_k/2 \equiv \cos k \) and

\[
u_n(\xi) = u'(\xi) + \frac{\xi}{1-\xi^2} u(\xi) + (n+1) t(\xi) , \quad t'_n(\xi) = t'(\xi) - \frac{n+1}{1-\xi^2} u(\xi) .
\]

As the eigenvalues are the solutions of the secular equation,

\[
0 = u(\xi_k) U_n(\xi_k) + t(\xi_k) T_{n+1}(\xi_k) ,
\]

the high-degree polynomials \( U_n(\xi_k) \) and \( T_{n+1}(\xi_k) \) can be removed from (32) and accordingly

\[
O_{jk}^2 = 2 \frac{u'(\xi_k) t(\xi_k) - t'(\xi_k) u(\xi_k)}{u_n(\xi_k) t(\xi_k) - t_n(\xi_k) u(\xi_k)} , \quad O_{jk}^2 = 2 \frac{u_j(\xi_k) t(\xi_k) - t_j(\xi_k) u(\xi_k)}{u_n(\xi_k) t(\xi_k) - t_n(\xi_k) u(\xi_k)} .
\]
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)

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

(36)

where the argument $\xi_k$ of $u$ and $t$ is understood, so that the eigenvector elements [35] read

$$O_{1k}^2 = \frac{2 \sin^2 k}{\ell + 1 - 2\varphi_k'} \frac{u_{\xi_k}(\xi_k) t(\xi_k) - l_{\xi_k}(\xi_k) u(\xi_k)}{u^2(\xi_k) + t^2(\xi_k) \sin^2 k}.$$  

(37a)

$$O_{2k}^2 = \frac{2 \sin^2 k}{\ell + 1 - 2\varphi_k'} \frac{u_{\xi_k}(\xi_k) t(\xi_k) - l_{\xi_k}(\xi_k) u(\xi_k)}{u^2(\xi_k) + t^2(\xi_k) \sin^2 k}.$$  

(37b)

These expressions generalize what was found in Refs. [6, 13].

As for the remaining elements, note that the recurrence relation [38] in the bulk, i.e., for $u < \nu < v$, reads

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

(38)

whose generic solution is

$$O_{k\nu} = 3 \{ e^{ik\nu} \alpha_k \},$$

(39)

for any complex number $\alpha_k$ independent of $\nu$, which has to be determined by requiring that the ‘boundary’ relations [38], i.e., for $\nu = 2, \ldots, u$ and $\nu = v, \ldots, \ell - 1$ be satisfied.

IV. EXAMPLES

A. Persymmetric 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 $a = 0$,

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

(40)

and, with the notations of the previous section, $u = 2$ and $v = \ell - 1$.

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

$$\chi_{u}(2\xi) = (2\xi - x)U_u(\xi) - y^2 U_{u-1}(\xi)$$

$$\chi_{o}(2\xi) = (2\xi - x)U_{u-1}(\xi) - y^2 U_{u-2}(\xi)$$

$$\chi_{o}(2\xi) = (2\xi - x)\chi_{o}(2\xi) - y^2 \chi_{o},$$

$$= (2\xi - x)^2 U_u(\xi) - 2(2\xi - x)y^2 U_{u-1}(\xi) + y^4 U_{u-2}(\xi).$$

(41)

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,

$$w_k = (2\xi - x - y^2 e^{-ik})^2 = \left[(2 - y^2) \cos k - x + iy^2 \sin k\right]^2,$$

(42)
FIG. 1: Eigenvalues of the matrix (40) for $y = 1$ as a function of the corner element $x$, for matrix sizes $ℓ = 10$ and 50. When $x > 1$ there can be two out-of-band eigenvalues.

so that

$$\varphi_k = k - \tan^{-1} \frac{y^2 \sin k}{(2-y^2) \cos k - x}.$$  (43)

The expression (41) can be rewritten in the form (12) by means of the properties (15), so with the notation of the previous section we identify the coefficients of Eqs. (12) and (30) as

$$u(\xi) = \left[(2-y^2)\xi - x\right]^2 - y^4 (1 - \xi^2),$$  (44a)

$$t(\xi) = 2y^2 \left[(2-y^2)\xi - x\right],$$  (44b)

$$u'(\xi) = u_\downarrow(\xi) = (2-y^2)\xi - x,$$  (44c)

$$t'(\xi) = t_\downarrow(\xi) = y^2.$$  (44d)

Of course, Eq. (43) can be obtained using straightforward trigonometric identities also from (24) and the above polynomials. As for the first components of the eigenvectors, the follow from Eq. (37):

$$O_{k1} = \frac{2}{\ell+1-2\varphi_k} \frac{y^2 \sin^2 k}{[(2-y^2) \cos k - x]^2 + y^4 \sin^2 k}. $$  (45)

Moreover, imposing to the generic solution (39) the conditions (8) at the corners, one finds

$$\alpha_k = \frac{1 - x e^{-ik} + (1-y^2) e^{-2ik}}{y \sin k} O_{k1}, $$  (46)

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

$$O_{k\nu} = \frac{\sin \nu k - x \sin(\nu-1)k + (1-y^2) \sin(\nu-2)k}{y \sin k} O_{k1}, $$  (47)

for $\nu = 2, \ldots, \ell - 1$. Eqs. (47) and (45), together with (43) and (23), give a complete solution to the analytical diagonalization problem of the matrix (40). Note that for $x = 0$ this expression is in agreement with Ref. [10] and that the term with $\varphi_k'$ becomes irrelevant for large $n$.

We remark that as long as there are no out-of-band eigenvalues Eq. (43) is exactly normalized, i.e., $\sum_k O_{k1}^2 = 1$, a sum that in the large-$\ell$ limit turns into the integral

$$I(x, y) = \int_0^\pi \frac{dk}{\pi} \frac{y^2 \sin^2 k}{[(2-y^2) \cos k - x]^2 + y^4 \sin^2 k} = 1.$$  (48)

Eigenvalues $\lambda \notin [-2, 2]$ can exist for large $x$ or $y$. Let us consider the simpler case $y = 1$, with $x > 0$, for which numerical results are shown in Fig. 1: it appears that when $x$ is raised above 1 two eigenvalues can leave the band. Indeed, from Eq. (41) one finds the secular equation

$$U_\ell - 2x U_{\ell-1} + x^2 U_{\ell-2} = 0.$$
FIG. 2: Eigenvalues of the matrix (40) 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.

that by means of the representation (29) is easily shown to imply

$$x = \cosh p + \sinh p \left[ \tanh \left( \frac{\ell - 1}{2} p \right) \right]^{\pm 1} \geq 1,$$

and two out-of-band eigenvalues can indeed exist if $x > 1$: in the large-$\ell$ limit they converge to the same value $\lambda = x + x^{-1}$. On the other hand, for $x < 1$ all eigenvalues belong to the band. This fact is reflected in the integral (48), because $I(x, 1) = 1$ for $x \leq 1$, while $I(x, 1) = x^{-2} < 1$ for $x > 1$: indeed, the full normalization requires the contribution from the out-of-band components.

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 $I(0, y) = 1$ for $y \leq \sqrt{2}$, while $I(0, y) = (y^2 - 1)^{-1} < 1$ for $y > \sqrt{2}$. It is to be noted that calculating the integral (48) in the general case is not trivial; nevertheless, we can say that it evaluates to 1 as long as all eigenvalues belong to the band $[-2, 2]$.

B. More mirror symmetric elements

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

$$
\begin{pmatrix}
0 & x & x & x & x & \ldots & x & x & 1 \\
x & 0 & y & y & y & \ldots & y & y & 0 \\
y & y & 0 & 1 & 0 & \ldots & y & y & 0 \\
1 & 0 & 1 & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
1 & 0 & y & y & y & \ldots & y & y & 0 \\
1 & 0 & x & x & x & \ldots & x & x & 0 \\
x & 0 & x & x & x & \ldots & x & x & 1 \\
0 & x & x & x & x & \ldots & x & x & 1 \\
\end{pmatrix}_{\ell \times \ell}
$$

(49)

Using straightforward algebra we find

$$w_k = \left[ 2 - y^2 - x^2 + (2 - y^2) \cos 2k + iy^2 \sin 2k \right]^2,$$

$$u(\xi) = \left[ 2\xi^2(2 - y^2) - x^2 \right]^2 - (1 - \xi^2) 4\xi^2 y^4,$$

$$t(\xi) = 4\xi y^2 \left[ 2\xi^2(2 - y^2) - x^2 \right],$$

$$u^r(\xi) = u(\xi) = \xi \left[ -2y^4 + x^2(-2 + y^2) + 4(2 - 2y^2 + y^4)\xi^2 \right],$$

$$t^r(\xi) = t(\xi) = y^2 \left[ 4(2 - y^2)\xi^2 - x^2 \right].$$
and accordingly
\[
\phi_k = 2k - \tan^{-1}\left[\frac{y^2 \sin 2k}{z^2 + (2 - y^2) \cos 2k}\right],
\]  
(50)

\[
O_{1k}^2 = O_{k\ell}^2 = \frac{2}{\ell + 1 - 2\phi'_k} \frac{x^2 y^2 \sin^2 k}{z^2 + (2 - y^2) \cos 2k} + y^4 \sin^2 2k
\]  
(51)
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

\[
\begin{pmatrix}
  x & y \\
  y & 0 & 1 \\
  1 & 0 & 1 \\
  & & \ddots \\
  1 & 0 & 1 \\
  & & & 1 & z
\end{pmatrix}_{\ell \times \ell}
\]  
(52)

where \(\ell = n + 2\). We find

\[
\begin{align*}
  t'(\xi) &= 1, \\
  l_\ell(\xi) &= y^2, \\
  t(\xi) &= 2\xi - x - y^2 z, \\
  u_\ell(\xi) &= (2 - y^2)\xi - x, \\
  u(\xi) &= (x - 2\xi)(z - \xi) + y^2(z\xi - 1),
\end{align*}
\]

and in particular

\[
\tan 2\phi_k = \frac{(x + y^2z - 2\cos k) \sin k}{(x - 2\cos k)(z - \cos k) + y^2(z\cos k - 1)},
\]  
(53)

from which the spectral decomposition follows. In fact, it can be shown that, once \(O_{k1}\) is calculated with Eq. (37), the remaining eigenvectors are given by (47), except for the \(\ell\)th one that follows from Eq. (8). Eq. (53) 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

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

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 quasi-uniform tridiagonal (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 \(\phi_k\), 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 (37) 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. (39), all components can be expressed as \(O_{k1}\) times a combination of Chebyshev polynomials, as shown in a particular example by Eq. (7).

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 section III C and exemplified in section IV A.
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