Chapter 9
Eigenvalue Problems

Eigenvalue problems are omnipresent in physics. Important examples are the time independent Schrödinger equation in a finite orthogonal basis (Chap. 9)

$$\sum_{j=1}^{M} \langle \phi_{j'} | H | \phi_j \rangle C_j = E C_{j'} \tag{9.1}$$

or the harmonic motion of a molecule around its equilibrium structure (Sect. 14.4.1)

$$\omega^2 m_i \big(\xi_i - \xi_i^{eq} \big) = \sum_j \frac{\partial^2 U}{\partial \xi_i \partial \xi_j} \big(\xi_j - \xi_j^{eq} \big). \tag{9.2}$$

Most important are ordinary eigenvalue problems,[1] which involve the solution of a homogeneous system of linear equations

$$\sum_{j=1}^{N} a_{ij} x_j = \lambda x_i \tag{9.3}$$

with a Hermitian (or symmetric, if real) matrix [198]

$$a_{ji} = a_{ij}^{*}. \tag{9.4}$$

Matrices of small dimension can be diagonalized directly by determining the roots of the characteristic polynomial and solving a homogeneous system of linear equations. The Jacobi method uses successive rotations to diagonalize a matrix with a unitary transformation. A very popular method for not too large symmetric matrices reduces the matrix to tridiagonal form which can be diagonalized efficiently with the QL algorithm. Some special tridiagonal matrices can be diagonalized analytically. Special algorithms are available for matrices of very large dimension, for instance the famous Lanczos method.

[1] We do not consider general eigenvalue problems here.

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9.1 Direct Solution

For matrices of very small dimension (2, 3) the determinant

$$\det|a_{ij} - \lambda\delta_{ij}| = 0 \tag{9.5}$$

can be written explicitly as a polynomial of λ. The roots of this polynomial are the eigenvalues. The eigenvectors are given by the system of equations

$$\sum_j (a_{ij} - \lambda\delta_{ij})u_j = 0. \tag{9.6}$$

9.2 Jacobi Method

Any symmetric 2×2 matrix

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix} \tag{9.7}$$

can be diagonalized by a rotation of the coordinate system. Rotation by the angle φ corresponds to an orthogonal transformation with the rotation matrix

$$R_\varphi = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}. \tag{9.8}$$

In the following we use the abbreviations

$$c = \cos\varphi, \quad s = \sin\varphi, \quad t = \tan\varphi. \tag{9.9}$$

The transformed matrix is

$$\begin{aligned} RAR^{-1} &= \begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix} \begin{pmatrix} c & s \\ -s & c \end{pmatrix} \\ &= \begin{pmatrix} c^2 a_{11} + s^2 a_{22} - 2csa_{12} & cs(a_{11} - a_{22}) + (c^2 - s^2)a_{12} \\ cs(a_{11} - a_{22}) + (c^2 - s^2)a_{12} & s^2 a_{11} + c^2 a_{22} + 2csa_{12} \end{pmatrix}. \end{aligned} \tag{9.10}$$

It is diagonal if

$$0 = cs(a_{11} - a_{22}) + \left(c^2 - s^2\right)a_{12} = \frac{a_{11} - a_{22}}{2}\sin(2\varphi) + a_{12}\cos(2\varphi) \tag{9.11}$$

or

$$\tan(2\varphi) = \frac{2a_{12}}{a_{22} - a_{11}}. \tag{9.12}$$

Calculation of φ is not necessary since only its cosine and sine appear in (9.10). From [198]

$$\frac{1-t^2}{t} = \frac{c^2-s^2}{2cs} = \cot(2\varphi) = \frac{a_{22}-a_{11}}{2a_{12}} \tag{9.13}$$

we see that t is a root of

$$t^2 + \frac{a_{22}-a_{11}}{a_{12}} t - 1 = 0 \tag{9.14}$$

hence

$$t = -\frac{a_{22}-a_{11}}{2a_{12}} \pm \sqrt{1+\left(\frac{a_{22}-a_{11}}{2a_{12}}\right)^2} = \frac{1}{\frac{a_{22}-a_{11}}{2a_{12}} \pm \sqrt{1+(\frac{a_{22}-a_{11}}{2a_{12}})^2}}. \tag{9.15}$$

For reasons of convergence [198] the solution with smaller magnitude is chosen which can be written as

$$t = \frac{\operatorname{sign}(\frac{a_{22}-a_{11}}{2a_{12}})}{|\frac{a_{22}-a_{11}}{2a_{12}}| + \sqrt{1+(\frac{a_{22}-a_{11}}{2a_{12}})^2}} \tag{9.16}$$

again for reasons of convergence the smaller solution φ is preferred and therefore we take

$$c = \frac{1}{\sqrt{1+t^2}} \qquad s = \frac{t}{\sqrt{1+t^2}}. \tag{9.17}$$

The diagonal elements of the transformed matrix are

$$\tilde{a}_{11} = c^2 a_{11} + s^2 a_{22} - 2cs a_{12} \tag{9.18}$$

$$\tilde{a}_{22} = s^2 a_{11} + c^2 a_{22} + 2cs a_{12}. \tag{9.19}$$

The trace of the matrix is invariant

$$\tilde{a}_{11} + \tilde{a}_{22} = a_{11} + a_{22} \tag{9.20}$$

whereas the difference of the diagonal elements is

$$\begin{aligned}
\tilde{a}_{11} - \tilde{a}_{22} &= \left(c^2 - s^2\right)(a_{11} - a_{22}) - 4cs a_{12} \\
&= \frac{1-t^2}{1+t^2}(a_{11}-a_{22}) - 4\frac{a_{12}t}{1+t^2} \\
&= (a_{11}-a_{22}) + \left(-a_{12}\frac{1-t^2}{t}\right)\frac{-2t^2}{1+t^2} - 4\frac{a_{12}t}{1+t^2} \\
&= (a_{11}-a_{22}) - 2t a_{12}
\end{aligned} \tag{9.21}$$

and the transformed matrix has the simple form

$$\begin{pmatrix} a_{11} - a_{12}t & \\ & a_{22} + a_{12}t \end{pmatrix}. \tag{9.22}$$

For larger dimension $N > 2$ the Jacobi method uses the following algorithm:

(1) look for the dominant non-diagonal element $\max_{i \neq j} |a_{ij}|$
(2) perform a rotation in the (ij)-plane to cancel the element $\tilde{a}_{ij}$ of the transformed matrix $\tilde{A} = R^{(ij)} \cdot A \cdot R^{(ij)-1}$. The corresponding rotation matrix has the form

$$R^{(ij)} = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & c & & s & & \\ & & & \ddots & & & \\ & & -s & & c & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{pmatrix} \tag{9.23}$$

(3) repeat (1–2) until convergence (if possible).

The sequence of Jacobi rotations gives the over all transformation

$$RAR^{-1} = \cdots R_2 R_1 A R_1^{-1} R_2^{-1} \cdots = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{pmatrix}. \tag{9.24}$$

Hence

$$AR^{-1} = R^{-1} \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{pmatrix} \tag{9.25}$$

and the column vectors of $R^{-1} = (\mathbf{v}_1, \mathbf{v}_2 \cdots \mathbf{v}_N)$ are the eigenvectors of A:

$$A(\mathbf{v}_1, \mathbf{v}_2 \cdots \mathbf{v}_N) = (\lambda_1 \mathbf{v}_1, \lambda_2 \mathbf{v}_2 \cdots \lambda_N \mathbf{v}_N). \tag{9.26}$$

9.3 Tridiagonal Matrices

A tridiagonal matrix has nonzero elements only in the main diagonal and the first diagonal above and below. Many algorithms simplify significantly when applied to tridiagonal matrices.

9.3.1 Characteristic Polynomial of a Tridiagonal Matrix

The characteristic polynomial of a tridiagonal matrix

$$P_A(\lambda) = \det \begin{vmatrix} a_{11}-\lambda & a_{12} & & \\ a_{21} & a_{22}-\lambda & & \\ & & \ddots & a_{N-1N} \\ & & a_{NN-1} & a_{NN}-\lambda \end{vmatrix} \tag{9.27}$$

can be calculated recursively:

$$\begin{aligned} P_0 &= 1 \\ P_1(\lambda) &= a_{11}-\lambda \\ P_2(\lambda) &= (a_{22}-\lambda)P_1(\lambda) - a_{12}a_{21} \\ &\vdots \\ P_N(\lambda) &= (a_{NN}-\lambda)P_{N-1}(\lambda) - a_{N,N-1}a_{N-1,N}P_{N-2}(\lambda). \end{aligned} \tag{9.28}$$

9.3.2 Special Tridiagonal Matrices

Certain classes of tridiagonal matrices can be diagonalized exactly [55, 151, 281].

9.3.2.1 Discretized Second Derivatives

Discretization of a second derivative involves, under Dirichlet boundary conditions $f(x_0) = f(x_{N+1}) = 0$, the differentiation matrix (Sect. 18.2)

$$M = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}. \tag{9.29}$$

Its eigenvectors have the form

$$\mathbf{f} = \begin{pmatrix} f_1 \\ \vdots \\ f_n \\ \vdots \\ f_N \end{pmatrix} = \begin{pmatrix} \sin k \\ \vdots \\ \sin(nk) \\ \vdots \\ \sin(Nk) \end{pmatrix}. \tag{9.30}$$

This can be seen by inserting (9.30) into the n-th line of the eigenvalue equation (9.31)

$$M\mathbf{f} = \lambda\mathbf{f} \tag{9.31}$$

$$\begin{aligned}(M\mathbf{f})_n &= \big(\sin\big((n-1)k\big) + \sin\big((n+1)k\big) - 2\sin(nk)\big)\\ &= 2\sin(nk)\big(\cos(k) - 1\big) = \lambda(\mathbf{f})_n\end{aligned} \tag{9.32}$$

with the eigenvalue

$$\lambda = 2(\cos k - 1) = -4\sin^2\left(\frac{k}{2}\right). \tag{9.33}$$

The first line of the eigenvalue equation (9.31) reads

$$\begin{aligned}(M\mathbf{f})_1 &= \big(-2\sin(k) + \sin(2k)\big)\\ &= 2\sin(k)\big(\cos(k) - 1\big) = \lambda(\mathbf{f})_n\end{aligned} \tag{9.34}$$

and from the last line we have

$$\begin{aligned}(M\mathbf{f})_N &= \big(-2\sin(Nk) + \sin\big([N-1]k\big)\big)\\ &= \lambda(\mathbf{f})_N = 2\big(\cos(k) - 1\big)\sin(Nk)\end{aligned} \tag{9.35}$$

which holds if

$$\sin\big((N-1)k\big) = 2\sin(Nk)\cos(k). \tag{9.36}$$

This simplifies to

$$\begin{aligned}&\sin(Nk)\cos(k) - \cos(Nk)\sin(k) = 2\sin(Nk)\cos(k)\\ &\sin(Nk)\cos(k) + \cos(Nk)\sin(k) = 0\\ &\sin\big((N+1)k\big) = 0.\end{aligned} \tag{9.37}$$

Hence the possible values of k are

$$k = \frac{\pi}{(N+1)}l \quad \text{with } l = 1, 2 \cdots N \tag{9.38}$$

and the eigenvectors are explicitly (Fig. 9.1)

$$\mathbf{f} = \begin{pmatrix} \sin(\frac{\pi}{N+1}l) \\ \vdots \\ \sin(\frac{\pi}{N+1}l\,n) \\ \vdots \\ \sin(\frac{\pi}{N+1}l\,N) \end{pmatrix}. \tag{9.39}$$

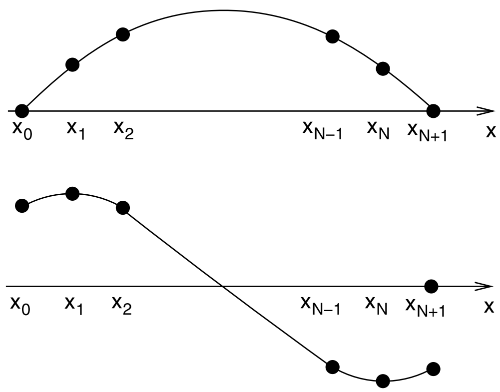

Fig. 9.1 (Lowest eigenvector for fixed and open boundaries) *Top*: for fixed boundaries $f_n = \sin(nk)$ which is zero at the additional points x_0, x_{N+1}. For open boundaries $f_n = \cos((n-1)k)$ with horizontal tangent at x_1, x_N due to the boundary conditions $f_2 = f_0$, $f_{N-1} = f_{N+1}$

For Neumann boundary conditions $\frac{\partial f}{\partial x}(x_1) = \frac{\partial f}{\partial x}(x_N) = 0$ the matrix is slightly different (Sect. 18.2)

$$M = \begin{pmatrix} -2 & 2 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 2 & -2 \end{pmatrix}. \tag{9.40}$$

Its eigenvalues are also given by the expression (9.33). To obtain the eigenvectors, we try a more general ansatz with a phase shift

$$\mathbf{f} = \begin{pmatrix} \sin \Phi_1 \\ \vdots \\ \sin(\Phi_1 + (n-1)k) \\ \vdots \\ \sin(\Phi_1 + (N-1)k) \end{pmatrix}. \tag{9.41}$$

Obviously

$$\begin{aligned} &\sin\big(\Phi_1 + (n-1)k - k\big) + \sin\big(\Phi_1 + (n-1)k + k\big) - 2\sin\big(\Phi_1 + (n-1)k\big) \\ &\quad = 2(\cos k - 1)\sin\big(\Phi_1 + (n-1)k\big). \end{aligned} \tag{9.42}$$

The first and last lines of the eigenvalue equation give

$$\begin{aligned} 0 &= -2\sin(\Phi_1) + 2\sin(\Phi_1 + k) - 2(\cos k - 1)\sin(\Phi_1) \\ &= 2\cos \Phi_1 \sin k \end{aligned} \tag{9.43}$$

and

$$\begin{aligned}0 &= -2\sin\big(\Phi_1 + (N-1)k\big) + 2\sin\big(\Phi_1 + (N-1)k - k\big)\\ &\quad - 2(\cos k - 1)\sin\big(\Phi_1 + (N-1)k\big)\\ &= 2\cos\big(\Phi_1 + (N-1)k\big)\sin k \end{aligned} \tag{9.44}$$

which is solved by

$$\Phi_1 = \frac{\pi}{2} \quad k = \frac{\pi}{N-1}l, \quad l = 1, 2 \cdots N \tag{9.45}$$

hence finally the eigenvector is (Fig. 9.1)

$$\mathbf{f} = \begin{pmatrix} 1 \\ \vdots \\ \cos(\frac{n-1}{N-1}\pi l) \\ \vdots \\ (-1)^l \end{pmatrix}. \tag{9.46}$$

Even simpler is the case of the corresponding cyclic tridiagonal matrix

$$M = \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 1 & & & 1 & -2 \end{pmatrix} \tag{9.47}$$

which has eigenvectors

$$\mathbf{f} = \begin{pmatrix} e^{ik} \\ \vdots \\ e^{ink} \\ \vdots \\ e^{iNk} \end{pmatrix} \tag{9.48}$$

and eigenvalues

$$\lambda = -2 + e^{-ik} + e^{ik} = 2\big(\cos(k) - 1\big) = -\sin^2\left(\frac{k}{2}\right) \tag{9.49}$$

where the possible $k-$values again follow from the first and last line

$$-2e^{ik} + e^{i2k} + e^{iNk} = \big(-2 + e^{-ik} + e^{ik}\big)e^{ik} \tag{9.50}$$

$$e^{ik} + e^{i(N-1)k} - 2e^{iNk} = \big(-2 + e^{-ik} + e^{ik}\big)e^{iNk} \tag{9.51}$$

which both lead to

$$e^{iNk} = 1 \tag{9.52}$$

$$k = \frac{2\pi}{N} l, \quad l = 0, 1 \cdots N-1. \tag{9.53}$$

9.3.2.2 Discretized First Derivatives

Using symmetric differences to discretize a first derivative in one dimension leads to the matrix[2]

$$D = \begin{pmatrix} & 1 & & & & \\ -1 & & 1 & & & \\ & \ddots & & \ddots & & \\ & & \ddots & & \ddots & \\ & & & -1 & & 1 \\ & & & & -1 & \end{pmatrix}. \tag{9.54}$$

The characteristic polynomial of the Hermitian matrix iD is given by the recursion (9.3.1)

$$\begin{aligned} P_0 &= 1 \\ P_1 &= -\lambda \\ &\vdots \\ P_N &= -\lambda P_{N-1} - P_{N-2} \end{aligned} \tag{9.55}$$

which after the substitution $x = -\lambda/2$ is exactly the recursion for the Chebyshev polynomial of the second kind $U_N(x)$. Hence the eigenvalues of D are given by the roots x_k of $U_N(x)$ as

$$\lambda_D = 2ix_k = 2i\cos\left(\frac{k\pi}{N+1}\right) \quad k = 1, 2 \cdots N. \tag{9.56}$$

The eigenvalues of the corresponding cyclic tridiagonal matrix

$$D = \begin{pmatrix} & 1 & & & & -1 \\ -1 & & 1 & & & \\ & \ddots & & \ddots & & \\ & & \ddots & & \ddots & \\ & & & -1 & & 1 \\ 1 & & & & -1 & \end{pmatrix} \tag{9.57}$$

[2]This matrix is skew symmetric, hence iT is Hermitian and has real eigenvalues iλ.

are easy to find. Inserting the ansatz for the eigenvector

$$\begin{pmatrix} \exp \mathrm{i}k \\ \vdots \\ \exp \mathrm{i}Nk \end{pmatrix} \tag{9.58}$$

we find the eigenvalues

$$e^{\mathrm{i}(m+1)k} - e^{\mathrm{i}(m-1)k} = \lambda e^{\mathrm{i}mk} \tag{9.59}$$

$$\lambda = 2\mathrm{i} \sin k \tag{9.60}$$

and from the first and last equation

$$1 = e^{\mathrm{i}Nk} \tag{9.61}$$

$$e^{\mathrm{i}k} = e^{\mathrm{i}(N+1)k} \tag{9.62}$$

the possible k-values

$$k = \frac{2\pi}{N} l, \quad l = 0, 1 \cdots N-1. \tag{9.63}$$

9.3.3 The QL Algorithm

Any real matrix A can be decomposed into the product of a lower triangular matrix L and an orthogonal matrix $Q^T = Q^{-1}$ (this is quite similar to the QR factorization with an upper triangular matrix which is discussed in Sect. 5.2)

$$A = QL. \tag{9.64}$$

For symmetric tridiagonal matrices this factorization can be efficiently realized by multiplication with a sequence of rotation matrices which eliminate the off-diagonal elements in the lower part

$$Q = R^{(N-1,N)} \cdots R^{(2,3)} R^{(1,2)}. \tag{9.65}$$

An orthogonal transformation of A is given by

$$Q^T A Q = Q^T Q L Q = L Q. \tag{9.66}$$

The QL algorithm is an iterative algorithm. It uses the transformation

$$\begin{aligned} A_{n+1} &= Q_n^T A_n Q_n = Q_n^T (A_n - \sigma_n) Q_n + \sigma_n = Q_n^T Q_n L_n Q_n + \sigma_n \\ &= L_n Q_n + \sigma_n \end{aligned} \tag{9.67}$$

where the shift parameter σ_n was introduced to improve convergence and the QL factorization is applied to $A_n - \sigma_n$. This transformation conserves symmetry and tridiagonal form. Repeated transformation gives a sequence of tridiagonal matrices, which converge to a diagonal matrix if the shifts σ_n are properly chosen. A very popular choice [198] is Wilkinson's shift

$$\sigma = a_{11} - \mathrm{sign}(\delta)\frac{a_{12}^2}{|\delta| + \sqrt{\delta^2 + a_{12}^2}} \quad \delta = \frac{a_{22} - a_{11}}{2} \tag{9.68}$$

which is that eigenvalue of the matrix $\begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix}$ which is closer to a_{11} (the smaller one if $a_{11} = a_{22}$).

9.4 Reduction to a Tridiagonal Matrix

Any symmetric matrix can be transformed to a tridiagonal matrix by a series of Householder transformations (5.53)

$$A' = PAP \quad \text{with } P = P^T = 1 - 2\frac{\mathbf{u}\mathbf{u}^T}{|\mathbf{u}|^2}. \tag{9.69}$$

The following orthogonal transformation P_1 brings the first row and column to tridiagonal form. We divide the matrix A according to

$$A = \begin{pmatrix} a_{11} & \boldsymbol{\alpha}^T \\ \boldsymbol{\alpha} & A_{rest} \end{pmatrix} \tag{9.70}$$

with the $(N-1)$-dimensional vector

$$\boldsymbol{\alpha} = \begin{pmatrix} a_{12} \\ \vdots \\ a_{1n} \end{pmatrix}.$$

Now let

$$\mathbf{u} = \begin{pmatrix} 0 \\ a_{12} + \lambda \\ \vdots \\ a_{1N} \end{pmatrix} = \begin{pmatrix} 0 \\ \boldsymbol{\alpha} \end{pmatrix} + \lambda \mathbf{e}^{(2)} \quad \text{with } \mathbf{e}^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{9.71}$$

Then

$$|\mathbf{u}|^2 = |\boldsymbol{\alpha}|^2 + \lambda^2 + 2\lambda a_{12} \tag{9.72}$$

and

$$\mathbf{u}^T \begin{pmatrix} a_{11} \\ \boldsymbol{\alpha} \end{pmatrix} = |\alpha|^2 + \lambda a_{12}. \tag{9.73}$$

The first row of A is transformed by multiplication with P_1 according to

$$P_1 \begin{pmatrix} a_{11} \\ \boldsymbol{\alpha} \end{pmatrix} = \begin{pmatrix} a_{11} \\ \boldsymbol{\alpha} \end{pmatrix} - 2\frac{|\alpha|^2 + \lambda a_{12}}{|\boldsymbol{\alpha}|^2 + \lambda^2 + 2\lambda a_{12}} \left[\begin{pmatrix} 0 \\ \boldsymbol{\alpha} \end{pmatrix} + \lambda \mathbf{e}^{(2)} \right]. \tag{9.74}$$

The elements number $3 \cdots N$ are eliminated if we choose[3]

$$\lambda = \pm|\alpha| \tag{9.75}$$

because then

$$2\frac{|\alpha|^2 + \lambda a_{12}}{|\boldsymbol{\alpha}|^2 + \lambda^2 + 2\lambda a_{12}} = 2\frac{|\alpha|^2 \pm |\alpha| a_{12}}{|\alpha|^2 + |\alpha|^2 \pm 2|\alpha| a_{12}} = 1 \tag{9.76}$$

and

$$P_1 \begin{pmatrix} a_{11} \\ \boldsymbol{\alpha} \end{pmatrix} = \begin{pmatrix} a_{11} \\ \boldsymbol{\alpha} \end{pmatrix} - \begin{pmatrix} 0 \\ \boldsymbol{\alpha} \end{pmatrix} - \lambda \mathbf{e}^{(2)} = \begin{pmatrix} a_{11} \\ \mp|\alpha| \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{9.77}$$

Finally we have

$$A^{(2)} = P_1 A P_1 = \begin{pmatrix} a_{11} & a_{12}^{(2)} & 0 & \cdots & 0 \\ a_{12}^{(2)} & a_{22}^{(2)} & a_{23}^{(2)} & \cdots & a_{2N}^{(2)} \\ 0 & a_{23}^{(2)} & \ddots & & a_{3N}^{(2)} \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & a_{2N}^{(2)} & a_{3N}^{(2)} & \cdots & a_{NN}^{(2)} \end{pmatrix} \tag{9.78}$$

as desired.

For the next step we choose

$$\boldsymbol{\alpha} = \begin{pmatrix} a_{22}^{(2)} \\ \vdots \\ a_{2N}^{(2)} \end{pmatrix}, \qquad \mathbf{u} = \begin{pmatrix} 0 \\ 0 \\ \alpha \end{pmatrix} \pm |\alpha| \mathbf{e}^{(3)} \tag{9.79}$$

[3]To avoid numerical extinction we choose the sign to be that of A_{12}.

to eliminate the elements $a_{24}\cdots a_{2N}$. Note that P_2 does not change the first row and column of $A^{(2)}$ and therefore

$$A^{(3)} = P_2 A^{(2)} P_2 = \begin{pmatrix} a_{11} & a_{12}^{(2)} & 0 & \cdots & \cdots & 0 \\ a_{12}^{(2)} & a_{22}^{(2)} & a_{23}^{(3)} & 0 & \cdots & 0 \\ 0 & a_{23}^{(3)} & a_{33}^{(3)} & \cdots & \cdots & a_{3N}^{(3)} \\ \vdots & 0 & \vdots & & & \vdots \\ \vdots & \vdots & \vdots & & & \vdots \\ 0 & 0 & a_{3N}^{(3)} & \cdots & \cdots & a_{NN}^{(3)} \end{pmatrix}. \tag{9.80}$$

After $N-1$ transformations finally a tridiagonal matrix is obtained.

9.5 Large Matrices

Special algorithms are available for matrices of very large dimension to calculate only some eigenvalues and eigenvectors. The famous Lanczos method [153] diagonalizes the matrix in a subspace which is constructed from the vectors

$$\mathbf{x}_0, A\mathbf{x}_0, A^2\mathbf{x}_0 \cdots A^N\mathbf{x}_0 \tag{9.81}$$

which, starting from an initial normalized guess vector $\mathbf{x}_0$ are orthonormalized to obtain a tridiagonal matrix,

$$\begin{aligned} \mathbf{x}_1 &= \frac{A\mathbf{x}_0 - (\mathbf{x}_0 A\mathbf{x}_0)\mathbf{x}_0}{|A\mathbf{x}_0 - (\mathbf{x}_0 A\mathbf{x}_0)\mathbf{x}_0|} = \frac{A\mathbf{x}_0 - a_0\mathbf{x}_0}{b_0} \\ \mathbf{x}_2 &= \frac{A\mathbf{x}_1 - b_0\mathbf{x}_0 - (\mathbf{x}_1 A\mathbf{x}_1)\mathbf{x}_1}{|A\mathbf{x}_1 - b_0\mathbf{x}_0 - (\mathbf{x}_1 A\mathbf{x}_1)\mathbf{x}_1|} = \frac{A\mathbf{x}_1 - b_0\mathbf{x}_\mathbf{0} - a_1\mathbf{x}_1}{b_1} \\ &\vdots \\ \mathbf{x}_N &= \frac{A\mathbf{x}_{N-1} - b_{N-2}\mathbf{x}_{N-2} - (\mathbf{x}_{N-1} A\mathbf{x}_{N-1})\mathbf{x}_{N-1}}{|A\mathbf{x}_{N-1} - b_{N-2}\mathbf{x}_{N-2} - (\mathbf{x}_{N-1} A\mathbf{x}_{N-1})\mathbf{x}_{N-1}|} \\ &= \frac{A\mathbf{x}_{N-1} - b_{N-2}\mathbf{x}_{N-2} - a_{N-1}\mathbf{x}_{N-1}}{b_{N-1}} = \frac{\mathbf{r}_{N-1}}{b_{N-1}}. \end{aligned} \tag{9.82}$$

This series is truncated by setting

$$a_N = (\mathbf{x}_N A\mathbf{x}_N) \tag{9.83}$$

and neglecting

$$\mathbf{r}_N = A\mathbf{x}_N - b_{N-1}\mathbf{x}_{N-1} - a_N\mathbf{x}_N. \tag{9.84}$$

Within the subspace of the $\mathbf{x}_1 \cdots \mathbf{x}_N$ the matrix A is represented by the tridiagonal matrix

$$T = \begin{pmatrix} a_0 & b_0 & & & \\ b_0 & a_1 & b_1 & & \\ & & \ddots & \ddots & \\ & & \ddots & a_{N-1} & b_{N-1} \\ & & & b_{N-1} & a_N \end{pmatrix} \tag{9.85}$$

which can be diagonalized with standard methods. The whole method can be iterated using an eigenvector of T as the new starting vector and increasing N until the desired accuracy is achieved. The main advantage of the Lanczos method is that the matrix A will not be stored in memory. It is sufficient to calculate scalar products with A.

9.6 Problems

Problem 9.1 (Computer experiment: disorder in a tight-binding model) We consider a two-dimensional lattice of interacting particles. Pairs of nearest neighbors have an interaction V and the diagonal energies are chosen from a Gaussian distribution

$$P(E) = \frac{1}{\Delta\sqrt{2\pi}} e^{-E^2/2\Delta^2}. \tag{9.86}$$

The wave function of the system is given by a linear combination

$$\psi = \sum_{ij} C_{ij}\psi_{ij} \tag{9.87}$$

where on each particle (i, j) one basis function ψ_{ij} is located. The nonzero elements of the interaction matrix are given by

$$H(ij|ij) = E_{ij} \tag{9.88}$$

$$H(ij|i \pm 1, j) = H(ij|i, j \pm 1) = V. \tag{9.89}$$

The matrix H is numerically diagonalized and the amplitudes C_{ij} of the lowest state are shown as circles located at the grid points. As a measure of the degree of localization the quantity

$$\sum_{ij} |C_{ij}|^4 \tag{9.90}$$

is evaluated. Explore the influence of coupling V and disorder Δ.