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DEAN´S ALGORITHM FOR CALCULATING EIGENVALUES OF THE DYNAMIC MATRIX WITH PERIODIC BOUNDARY CONDITIONS

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In many physical problems we are dealing with the standard equation

$$\mathbb{A}\,\vec{\mathbb{U}} = \Omega_i\,\vec{\mathbb{U}}\,, \qquad (1)$$

where Ω_i is an i-th eigenvalue of a matrix $\mathbb{A}$, $\vec{\mathbb{U}}$ denotes an eigenvector corresponding to Ω_i and $\mathbb{A}$ is given by

$$\mathbb{A} = \begin{pmatrix} a_1 & b_2 & c_3 & 0 & \cdots & \cdots & 0 & c_1 & b_1 \\ b_2 & a_2 & b_3 & c_4 & 0 & \cdots & \cdots & 0 & c_2 \\ c_3 & b_3 & a_3 & b_4 & c_5 & 0 & \cdots & \cdots & 0 \\ & c_4 & b_4 & a_4 & b_5 & c_6 & 0 & \cdots & 0 \\ & & & & \text{------} & & & & \\ & & & & & \text{------} & & & \\ c_1^{*} & 0 & \cdots & \cdots & 0 & c_{N-1} & b_{N-1} & a_{N-1} & b_N \\ b_1^{*} & c_2^{*} & 0 & \cdots & \cdots & 0 & c_N & b_N & a_N \end{pmatrix}, \qquad (2)$$

where a_i at $i= 1,2,\ldots,N$, b_i at $i= 2,3,\ldots,N$, c_i at $i= 3,4,\ldots,N$ are real numbers and c_1, c_2, b_1 mean complex numbers; stars indicate the complex conjugation.

In particular, if the periodic boundary conditions are used, then the equation for the stationary normal modes of the ideal, quasiperiodic or disorder chain of atoms takes the form given by Eqs. (1,2) with $\mathbb{A}$ being the dynamic matrix.

Our task is to present the algorithm for calculating the eigenvalues of $\mathbb{A}$, the matrix elements of which defines (2).

We shall applied the Dean's method of computing eigenvalues [1].

Let $\nu(\,\mathbb{B}\,)$ denote the number of real negative eigenvalues of matrix $\mathbb{B}$. Then, according to Ref. [1], $\nu(\mathbb{A}-x\mathbb{I})$, i.e., the number of Ω_i fulfilling the condition $\Omega_i \le x$ is given by

$$\nu\,\{\,\mathbb{A} - x\,\mathbb{I}\,\} = \sum_{i=1}^{N} \nu\,(\,y_i\,)\,, \qquad (3)$$

where (y_i) is the sequence of real numbers and $\mathbb{I}$ denotes the unit matrix.

We have derived (y_i) applying the partition procedure [1] to particular forms of $(\mathbb{A} - x \, \mathbb{I})$. Below we give (y_i) and auxiliary sequences (α_i), (β_i), (γ_i), (E_i), (P_i), (T_i), (Δ_i), (λ_i), (Υ_i), (μ_i) for specified cases. Notice that the greek capital letters denote the complex numbers.

Case I

If (2) defines the matrix elements of $\mathbb{A}$, then (y_i) and the elements of auxiliary sequences are as follows:

$i=1$

$$y_1=a_1-x \text{ and } \alpha_1=a_2-x, \quad \beta_1=b_2, \quad \gamma_1=c_3, \quad E_1=c_1, \quad P_1=b_1, \quad T_1=0,$$
$$\Delta_1=c_2, \quad \lambda_1=a_{N-1}-x, \quad \Upsilon_1=b_N, \quad \mu_1=a_N-x;$$

$i=2$

$$y_i=\alpha_1-\beta_1^2/y_1 \text{ and } \alpha_2=a_3-x-\gamma_1^2/y_1, \quad \beta_2=b_3-\beta_1\gamma_1/y_1, \quad \gamma_2=c_4,$$
$$E_2=\tau_1-\beta_1E_1/y_1, \quad P_2=\Delta_1-\beta_1P_1/y_1, \quad T_2=-\gamma_1E_1/y_1, \quad \Delta_2=-\gamma_1P_1/y_1,$$
$$\lambda_2=\lambda_1-E_1E_1^*/y_1, \quad \Upsilon_2=\Upsilon_1-E_1P_1/y_1, \quad \mu_2=\mu_1-P_1P_1^*/y_1;$$

$j=3,\dots,N-5$

$$y_j=\alpha_{j-1} - \beta_{j-1}^2/y_{j-1} \text{ and } \alpha_j = a_{j+1}-x-\gamma_{j-1}^2/y_{j-1}, \quad \gamma_j = c_{j+2},$$
$$\beta_j = b_{j+1} - \beta_{j-1}\gamma_{j-1} / y_{j-1}, \quad E_j = T_{j-1} - \beta_{j-1}E_{j-1} / y_{j-1},$$
$$P_j = \Delta_{j-1} - \beta_{j-1}P_{j-1} / y_{j-1}, \quad T_j = -\gamma_{j-1}E_{j-1} / y_{j-1},$$
$$\Delta_j = -\gamma_{j-1}P_{j-1} / y_{j-1}, \quad \lambda_j = \lambda_{j-1} - E_{j-1}E_{j-1}^* / y_{j-1},$$
$$\Upsilon_j = \Upsilon_{j-1} - E_{j-1}P_{j-1} / y_{j-1}, \quad \mu_j = \mu_{j-1} - P_{j-1}P_{j-1}^* / y_{j-1};$$

$i=N-4$

$$y_i=\alpha_{i-1}-\beta_{i-1}^2/y_{i-1} \text{ and } \alpha_i=a_{i+1} - x - \gamma_{i-1}^2 / y_{i-1}, \quad \gamma_i = c_{i+2},$$
$$\beta_i = b_{i+1} - \beta_{i-1}\gamma_{i-1} / y_{i-1}, \quad E_i = T_{i-1} - \beta_{i-1}E_{i-1} / y_{i-1},$$
$$P_i = \Delta_{i-1} - \beta_{i-1}P_{i-1} / y_{i-1}, \quad T_i = c_{i+3} - \gamma_{i-1}E_{i-1} / y_{i-1},$$
$$\Delta_i = - \gamma_{i-1}P_{i-1} / y_{i-1}, \quad \lambda_i = \lambda_{i-1} - E_{i-1}E_{i-1}^* / y_{i-1},$$
$$\Upsilon_i = \Upsilon_{i-1} - E_{i-1}P_{i-1} / y_{i-1}, \quad \mu_i = \mu_{i-1} - P_{i-1}P_{i-1}^* / y_{i-1};$$

$i=N-3$

$$y_i = \alpha_{i-1} - \beta_{i-1}^2 / y_{i-1} \text{ and } \alpha_i = a_{i+1} - x - \gamma_{i-1}^2 / y_{i-1},$$

$$\beta_i = b_{i+1} - \beta_{i-1}\gamma_{i-1} / y_{i-1}, \quad \Gamma_i = T_{i-1} - \beta_{i-1}E_{i-1} / y_{i-1},$$
$$E_i = \Delta_{i-1} - \beta_{i-1}P_{i-1} / y_{i-1}, \quad P_i = 0, \quad T_i = b_{i+2}-\gamma_{i-1}E_{i-1}/y_{i-1},$$
$$\Delta_i = c_{i+3} - \gamma_{i-1}P_{i-1} / y_{i-1}, \quad \lambda_i = \lambda_{i-1} - E_{i-1}E_{i-1}^* / y_{i-1},$$
$$\Upsilon_i = \Upsilon_{i-1} - E_{i-1}P_{i-1} / y_{i-1}, \quad \mu_i = \mu_{i-1} - P_{i-1}P_{i-1}^* / y_{i-1};$$

$i=N-2$

$$y_i = \alpha_{i-1} - \beta_{i-1}^2 / y_{i-1} \text{ and } \alpha_i = \lambda_{i-1} - \Gamma_{i-1}\Gamma_{i-1}^* / y_{i-1},$$
$$B_i = T_{i-1} - \beta_{i-1}\Gamma_{i-1} / y_{i-1}, \quad \Gamma_i = \Delta_{i-1} - \beta_{i-1}E_{i-1} / y_{i-1},$$
$$E_i = P_i = T_i = \Delta_i = \lambda_i = 0, \quad \Upsilon_i = \Upsilon_{i-1} - \Gamma_{i-1}E_{i-1} / y_{i-1},$$
$$\mu_i = \mu_{i-1} - E_{i-1}E_{i-1}^* / y_{i-1};$$

$i=N-1$

$$y_i = \alpha_{i-1} - B_{i-1}B_{i-1}^* / y_{i-1} \text{ and } \alpha_i = \mu_{i-1} - \Gamma_{i-1}\Gamma_{i-1}^* / y_{i-1},$$
$$\Upsilon_i = \Upsilon_{i-1} - B_{i-1}\Gamma_{i-1} / y_{i-1}, \quad B_i=\Gamma_i=E_i=P_i=T_i=\Delta_i=\lambda_i=\mu_i=0;$$

$i=N$

$$y_i = \alpha_{i-1} - \Upsilon_{i-1}\Upsilon_{i-1}^* / y_{i-1}.$$

In particular, if $c_i=0$ at $1 \le i \le N$ then

$$y_1 = a_1 - x,$$
$$y_i = a_i - x - b_i^2/y_{i-1} \text{ at } i=2,\dots,N-1,$$
$$y_N = \alpha_N - x - B_NB_N^*/y_{N-1},$$

where

$$B_1 = b_1, \quad B_i = -b_i B_{i-1} / y_{i-1} \quad \text{at} \quad i = 2,\dots, N-1,$$
$$B_N = b_N + B_{N-1} \quad \text{and} \quad \alpha_N = a_N - \sum_{i=1}^{N-2} B_iB_i^*/y_i .$$

Case II

Let c_1, b_1, c_2 be real numbers. Then:

i=1

$y_1=a_1-x$ and $\alpha_1=a_2-x$, $\beta_1=b_2$, $\gamma_1=c_3$, $\varepsilon_1=c_1$, $\rho_1=b_1$, $\tau_1=0$, $\delta_1=c_2$, $\lambda_1=a_{N-1}-x$, $\varphi_1=b_N$, $\mu_1=a_N-x$;

i=2

$y_2=\alpha_1-\beta_1^2/y_1$ and $\alpha_2=a_3-x-\gamma_1^2/y_1$, $\beta_2=b_3-\beta_1\gamma_1/y_1$, $\gamma_2=c_4$, $\varepsilon_2=\tau_1-\beta_1\varepsilon_1/y_1$, $\rho_2=\delta_1-\beta_1\rho_1/y_1$, $\tau_2=-\gamma_1\varepsilon_1/y_1$, $\delta_2=-\gamma_1\rho_1/y_1$, $\lambda_2=\lambda_1-\varepsilon_1^2/y_1$, $\varphi_2=\varphi_1-\varepsilon_1\rho_1/y_1$, $\mu_2=\mu_1-\rho_1^2/y_1$;

j=3,...,N-5

$y_j=\alpha_{j-1}-\beta_{j-1}^2/y_{j-1}$ and $\alpha_j=a_{j+1}-x-\gamma_{j-1}^2/y_{j-1}$, $\gamma_j=c_{j+2}$,
$\beta_j=b_{j+1}-\beta_{j-1}\gamma_{j-1}/y_{j-1}$, $\varepsilon_j=\tau_{j-1}-\beta_{j-1}\varepsilon_{j-1}/y_{j-1}$,
$\rho_j=\delta_{j-1}-\beta_{j-1}\rho_{j-1}/y_{j-1}$, $\tau_j=-\gamma_{j-1}\varepsilon_{j-1}/y_{j-1}$,
$\delta_j=-\gamma_{j-1}\rho_{j-1}/y_{j-1}$, $\lambda_j=\lambda_{j-1}-\varepsilon_{j-1}^2/y_{j-1}$, $\varphi_j=\varphi_{j-1}-\varepsilon_{j-1}\rho_{j-1}/y_{j-1}$,
$\mu_j=\mu_{j-1}-\rho_{j-1}^2/y_{j-1}$;

i=N-4

$y_i=\alpha_{i-1}-\beta_{i-1}^2/y_{i-1}$ and $\alpha_i=a_{i+1}-x-\gamma_{i-1}^2/y_{i-1}$, $\gamma_i=c_{i+2}$,
$\beta_i=b_{i+1}-\beta_{i-1}\gamma_{i-1}/y_{i-1}$, $\varepsilon_i=\tau_{i-1}-\beta_{i-1}\varepsilon_{i-1}/y_{i-1}$,
$\rho_i=\delta_{i-1}-\beta_{i-1}\rho_{i-1}/y_{i-1}$, $\tau_i=c_{i+3}-\gamma_{i-1}\varepsilon_{i-1}/y_{i-1}$,
$\delta_i=-\gamma_{i-1}\rho_{i-1}/y_{i-1}$, $\lambda_i=\lambda_{i-1}-\varepsilon_{i-1}^2/y_{i-1}$, $\varphi_i=\varphi_{i-1}-\varepsilon_{i-1}\rho_{i-1}/y_{i-1}$,
$\mu_i=\mu_{i-1}-\rho_{i-1}^2/y_{i-1}$;

i=N-3

$y_i=\alpha_{i-1}-\beta_{i-1}^2/y_{i-1}$ and $\alpha_i=a_{i+1}-x-\gamma_{i-1}^2/y_{i-1}$,
$\beta_i=b_{i+1}-\beta_{i-1}\gamma_{i-1}/y_{i-1}$, $\gamma_i=\tau_{i-1}-\beta_{i-1}\varepsilon_{i-1}/y_{i-1}$,
$\varepsilon_i=\delta_{i-1}-\beta_{i-1}\rho_{i-1}/y_{i-1}$, $\rho_i=0$, $\tau_i=b_{i+2}-\gamma_{i-1}\varepsilon_{i-1}/y_{i-1}$,
$\delta_i=c_{i+3}-\gamma_{i-1}\rho_{i-1}/y_{i-1}$, $\lambda_i=\lambda_{i-1}-\varepsilon_{i-1}^2/y_{i-1}$,
$\varphi_i=\varphi_{i-1}-\varepsilon_{i-1}\rho_{i-1}/y_{i-1}$, $\mu_i=\mu_{i-1}-\rho_{i-1}^2/y_{i-1}$;

i=N-2

$y_i=\alpha_{i-1}-\beta_{i-1}^2/y_{i-1}$ and $\alpha_i=\lambda_{i-1}-x-\gamma_{i-1}^2/y_{i-1}$,

$\beta_i=\tau_{i-1}-\beta_{i-1}\gamma_{i-1}/y_{i-1}$, $\gamma_i=\delta_{i-1}-\beta_{i-1}\varepsilon_{i-1}/y_{i-1}$,
$\varepsilon_i=\rho_i=\tau_i=\delta_i=\lambda_i=0$, $\varphi_i=\varphi_{i-1}-\gamma_{i-1}\varepsilon_{i-1}/y_{i-1}$, $\mu_i=\mu_{i-1}-\varepsilon_{i-1}^2/y_{i-1}$;

i=N-1

$y_i=\alpha_{i-1}-\beta_{i-1}^2/y_{i-1}$ and $\alpha_i=\mu_{i-1}-\gamma_{i-1}^2/y_{i-1}$,
$\varphi_i=\varphi_{i-1}-\beta_{i-1}\gamma_{i-1}/y_{i-1}$, $\beta_i=\gamma_i=\varepsilon_i=\rho_i=\tau_i=\delta_i=\lambda_i=\mu_i=0$;

i=N

$y_i=\alpha_{i-1}-\varphi_{i-1}^2/y_{i-1}$.

In particular case, if $c_i=0$ at $1\le i\le N$, then:

$y_1=a_1-x$,
$y_i=a_i-x-b_i^2/y_{i-1}$ at $i=2,\dots,N-1$,
$y_N=\alpha_N-x-\beta_N\beta_N/y_{N-1}$,

where

$\beta_1=b_1$, $\beta_i=-b_i\,\beta_{i-1}/y_{i-1}$ at $i=2,\dots,N-1$,

$$\beta_N=b_N+\beta_{N-1} \quad \text{and} \quad \alpha_N=a_N-\sum_{i=1}^{N-2}\beta_i^2/y_i.$$

Case III

Let $c_1=c_2=b_1=0$. In this case the free or fixed ends boundary conditions are imposed on the system and:

$y_1=a_1-x$, $\beta_1=b_2$;

$y_2=a_2-x-\beta_1^2/y_1$, $\beta_2=b_3-\beta_1c_3/y_1$;

$y_j=a_j-x-c_j^2/y_{j-2}-\beta_{j-1}^2/y_{j-1}$,

$\beta_j=b_{j+1}-\beta_{j-1}c_{j+1}/y_{j-1}$ at $j=3,\dots,N$.

Finally, let us notice that the eigenvalue Ω_i of A in I - III cases can be calculate numerically from (3) on the basis of the above given (y_i) using a simple bisection method [1].

References

1. P.Dean, Rev. Mod. Phys. 44, 127 (1972)

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