

## Harmonic oscillator in several variables

### I. FORMULATION OF THE PROBLEM

We solve the Schrödinger equation in  $M$  variables

$$(T + V - E)\psi(q_1, q_2, \dots, q_M) = 0, \quad (1)$$

where  $T$  is a quadratic form of momenta  $p_i = \frac{\hbar}{i} \frac{\partial}{\partial q_i}$ ,

$$T = \frac{1}{2} \sum_{i,j=1}^M A_{i,j} p_i p_j \quad (2)$$

and  $V$  is a quadratic form of coordinates

$$V = \frac{1}{2} \sum_{i,j=1}^M B_{i,j} q_i q_j. \quad (3)$$

Alternatively, equations (2) and (3) could be written in matrix form as

$$T = \frac{1}{2} \mathbf{p}^T \mathbf{A} \mathbf{p}, \quad V = \frac{1}{2} \mathbf{q}^T \mathbf{B} \mathbf{q}, \quad (4)$$

where  $\mathbf{p}$  and  $\mathbf{q}$  are  $M$ -component vectors

$$\mathbf{p} \equiv (p_1, p_2, \dots, p_M), \quad \mathbf{q} \equiv (q_1, q_2, \dots, q_M), \quad (5)$$

and  $\mathbf{A}$  and  $\mathbf{B}$  are  $M \times M$  matrices with elements  $A_{i,j}$  and  $B_{i,j}$  respectively.

Here, we assume that  $\mathbf{A}$  and  $\mathbf{B}$  are positive definite real symmetric matrices.

We use units where  $\hbar = 1$ .

The problem reduces to simultaneous diagonalization of the matrices  $\mathbf{A}$  and  $\mathbf{B}$ . It is solved in three steps.

## II. STEP 1: DIAGONALIZATION OF A

Let  $\mathbf{y}^{(k)}$  ( $k = 1, 2, \dots, M$ ) is an eigenvector of the matrix  $\mathbf{A}$  corresponding to eigenvalue  $\lambda_k$ , i.e.

$$\sum_{j=1}^M A_{i,j} y_j^{(k)} = \lambda_k y_i^{(k)}, \quad (i = 1, 2, \dots, M). \quad (6)$$

For a symmetric real matrix, we could always assume that vectors  $\mathbf{y}^{(k)}$  are orthonormal, i.e.

$$\sum_{i=1}^M y_i^{(j)} y_i^{(k)} = \delta_{j,k}. \quad (7)$$

(see textbooks on linear algebra). For a positive definite matrix, all eigenvalues are positive.

If we introduce a matrix  $\mathbf{Q}$  with the eigenvectors in its columns,

$$Q_{i,j} \equiv y_i^{(j)}, \quad (8)$$

then equation (6) could be rewritten in matrix form as

$$\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{\Lambda}, \quad (9)$$

where  $\mathbf{\Lambda}$  is a diagonal matrix with the eigenvalues on its diagonal,  $\Lambda_{i,j} = \lambda_i \delta_{i,j}$ , and equation (7) as

$$\mathbf{Q}^T \mathbf{Q} = \mathbf{I}. \quad (10)$$

After multiplying equation (9) by  $\mathbf{Q}^{-1} = \mathbf{Q}^T$  from right, we obtain a “decomposition” [1]

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T, \quad (11)$$

Now, let us rewrite Schrödinger equation in terms of new variables

$$\mathbf{q} = \mathbf{Q}\mathbf{q}', \quad \mathbf{q}' = \mathbf{Q}^{-1}\mathbf{q} = \mathbf{Q}^T\mathbf{q}. \quad (12)$$

Since

$$q'_i = \sum_{j=1}^M Q_{j,i} q_j \quad (13)$$

and

$$\frac{\partial}{\partial q_j} = \sum_{i=1}^M \frac{\partial q'_i}{\partial q_j} \frac{\partial}{\partial q'_i} = \sum_{i=1}^M Q_{j,i} \frac{\partial}{\partial q'_i}, \quad (14)$$

or in matrix form

$$\mathbf{p} = \mathbf{Q}\mathbf{p}', \quad (15)$$

the kinetic energy transforms in new coordinates is

$$T \rightarrow T' = \frac{1}{2} \mathbf{p}'^T \mathbf{Q}^T \mathbf{A} \mathbf{Q} \mathbf{p}'. \quad (16)$$

Using equation (11), we obtain

$$T' = \frac{1}{2} \mathbf{p}'^T \mathbf{\Lambda} \mathbf{p}' = \frac{1}{2} \sum_{i=1}^M \lambda_i p_i'^2. \quad (17)$$

Since  $\mathbf{q} = \mathbf{Q}\mathbf{q}'$ , the potential energy in new coordinates is

$$V \rightarrow V' = \frac{1}{2} \mathbf{q}'^T \mathbf{B}' \mathbf{q}', \quad (18)$$

where the matrix  $\mathbf{B}'$  is

$$\mathbf{B}' = \mathbf{Q}^T \mathbf{B} \mathbf{Q}. \quad (19)$$

### III. STEP 2: UNIFORM STRETCH/SHRINKAGE

Let us consider another coordinate system

$$q'_i = \lambda_i^{1/2} q''_i, \quad (20)$$

or in matrix form

$$\mathbf{q}' = \mathbf{\Lambda}^{1/2} \mathbf{q}''. \quad (21)$$

It is just a uniform stretch or a shrinkage along each coordinate.

Then, in a new coordinate system,

$$T' \rightarrow T'' = \frac{1}{2} \mathbf{q}''^T \mathbf{q}'', \quad V' \rightarrow V'' = \frac{1}{2} \mathbf{q}''^T \mathbf{B}'' \mathbf{q}'', \quad (22)$$

where

$$\mathbf{B}'' = \Lambda^{1/2} \mathbf{Q}^T \mathbf{B} \mathbf{Q} \Lambda^{1/2}. \quad (23)$$

#### IV. STEP 3: DIAGONALIZATION OF MATRIX B

Since  $\mathbf{B}''$  is a symmetric matrix ( $\mathbf{B}''^T = \mathbf{B}''$ ), we could decompose it in the same way as it was done for the matrix  $\mathbf{A}$  in Section II,

$$\mathbf{B}'' = \mathbf{S} \Omega^2 \mathbf{S}^T. \quad (24)$$

In equation (24), the matrix  $\mathbf{S}$  is formed from eigenvectors of  $\mathbf{B}''$  in its columns, and  $\Omega^2$  is a diagonal matrix with eigenvalues of  $\mathbf{B}''$  on its diagonal,  $\Omega^2_{i,j} = \omega_i^2 \delta_{i,j}$ .

Let us consider new variables

$$\mathbf{q}''' = \mathbf{S} \mathbf{q}'', \quad \mathbf{q}'' = \mathbf{S}^{-1} \mathbf{q}''' = \mathbf{S}^T \mathbf{q}'''. \quad (25)$$

Then, in a new coordinate system,

$$T'' \rightarrow T''' = \frac{1}{2} \mathbf{q}'''^T \mathbf{S}^T \mathbf{S} \mathbf{q}''' = \frac{1}{2} \mathbf{q}'''^T \mathbf{q}''', \quad V'' \rightarrow V''' = \frac{1}{2} \mathbf{q}'''^T \mathbf{B}''' \mathbf{q}''', \quad (26)$$

where the matrix  $\mathbf{B}'''$  is

$$\mathbf{B}''' = \mathbf{S}^T \mathbf{B}'' \mathbf{S} = \Omega^2. \quad (27)$$

In derivation of equation (27), we used the decomposition (24).

Collecting results for kinetic and potential energy given by equations (26) and (27), we rewrite Schrödinger equation as

$$\left( -\frac{1}{2} \sum_{i=1}^M \frac{\partial^2}{\partial q_i^{\prime\prime\prime 2}} + \frac{1}{2} \sum_{i=1}^M \omega_i^2 q_i^{\prime\prime\prime 2} - E \right) \psi^{\prime\prime\prime}(q_1^{\prime\prime\prime}, q_2^{\prime\prime\prime}, \dots, q_M^{\prime\prime\prime}) = 0. \quad (28)$$

It is a separable equation. It reduces to  $M$  one-dimensional harmonic oscillators. The energy is

$$E = \sum_{i=1}^M \left( n_i + \frac{1}{2} \right) \omega_i, \quad (29)$$

where  $n_1, n_2, \dots, n_M$  are some integer non-negative numbers.

In conclusion we notice that since from equation (11) it follows that

$$\Lambda^{1/2} = \mathbf{Q}^T \mathbf{A}^{1/2} \mathbf{Q}, \quad (30)$$

then, after substitution of equation (30) into equation (23) and then into equation (27) we obtain

$$\Omega^2 = \mathbf{S}^T \mathbf{Q}^T \mathbf{A}^{1/2} \mathbf{B} \mathbf{A}^{1/2} \mathbf{Q} \mathbf{S}, \quad (31)$$

i.e.  $\omega_i^2$  are eigenvalues of the matrix  $\mathbf{A}^{1/2} \mathbf{B} \mathbf{A}^{1/2}$ , with eigenvectors given by columns of the matrix  $\mathbf{Q} \mathbf{S}$ .

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[1] *Symmetric matrix*, Article in Wikipedia, on-line encyclopedia.