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Vibration of the Crystal Lattice and Euler-Lagrange Equations

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Contents

1	Introduction	3
2	Euler-Lagrange Equation	3
3	Euler-Lagrange Equation in Matrix Form	5
4	Vibration of the Crystal Lattice	6
4.1	1D Monatomic “Lattice” with Three Atoms	7
4.2	1D Monatomic Lattice and Lennard-Jones Potential	8
4.3	1D Diatomic Lattice	9
4.4	1D Monatomic Lattice With Two Different String Constants	10
4.5	2D Square Monatomic Lattice with Vibrations Perpendicular to the Lattice	10
5	Conclusion	11

1 Introduction

From the dispersion of frequencies ($\omega(\vec{k})$) it is possible to calculate the phase velocity, group velocity, sound speed, specific heat etc. At lectures we calculated simple monatomic and diatomic lattice with help of forces. Because this method “allows” mistakes concerning “signs”, I prefer using energies which have quadratic forms and signs don’t matter anymore. One way is calculating forces from the potential

$$\vec{F} = -\vec{\nabla}V, \quad (1)$$

where V is the potential, \vec{F} is the force in the second Newton’s law

$$\vec{F} = m\ddot{\vec{r}}, \quad (2)$$

where m is the mass of the particle, $\ddot{\vec{r}}$ is the acceleration. Another way is using Euler-Lagrange equations which represent the “craft” for solving many different physical problems.

In this seminar I am going to represent “handy tool” called Euler-Lagrange equations concerning lattice vibrations when having different lattices, when having basis and when having different potentials in 1D and 2D.

2 Euler-Lagrange Equation

For system of n particles deriving Euler-Lagrange equations starts from second Newton’s law

$$\vec{F}_i = m_i\ddot{\vec{r}}_i, \quad (3)$$

where $i = 1 : n$. For all particles equation 3 can be rewritten into matrix form

$$\begin{bmatrix} m_1\ddot{\vec{r}}_1 \\ m_2\ddot{\vec{r}}_2 \\ \vdots \\ m_n\ddot{\vec{r}}_n \end{bmatrix} = \begin{bmatrix} \vec{F}_1 \\ \vec{F}_2 \\ \vdots \\ \vec{F}_n \end{bmatrix} \quad (4)$$

which we multiply with transposed vector of

$$\begin{bmatrix} \frac{\partial \vec{r}_1}{\partial q_k} \\ \frac{\partial \vec{r}_2}{\partial q_k} \\ \vdots \\ \frac{\partial \vec{r}_n}{\partial q_k} \end{bmatrix}, \quad (5)$$

where q_k are parameters on which system depends. What we get is

$$m_1\ddot{\vec{r}}_1 \frac{\partial \vec{r}_1}{\partial q_k} + m_2\ddot{\vec{r}}_2 \frac{\partial \vec{r}_2}{\partial q_k} + \dots + m_n\ddot{\vec{r}}_n \frac{\partial \vec{r}_n}{\partial q_k} = \vec{F}_1 \frac{\partial \vec{r}_1}{\partial q_k} + \vec{F}_2 \frac{\partial \vec{r}_2}{\partial q_k} + \dots + \vec{F}_n \frac{\partial \vec{r}_n}{\partial q_k}, \quad (6)$$

where

$$\vec{r}_i = \vec{r}_i(q_1, q_2, \dots, q_N, t). \quad (7)$$

From expression 7 we can write

$$\dot{\vec{r}}_i = \sum_{j=1}^n \frac{\partial \vec{r}_i}{\partial q_j} \dot{q}_j + \frac{\partial \vec{r}_i}{\partial t}, \quad (8)$$

from which we can write the derivative with respect to \dot{q}_l

$$\frac{\partial \dot{\vec{r}}_i}{\partial \dot{q}_l} = \frac{\partial \vec{r}_i}{\partial q_l}. \quad (9)$$

With expression 9 we can write the left side of equation 6

$$\begin{aligned} m_i \ddot{\vec{r}}_i \frac{\partial \vec{r}_i}{\partial q_k} &= m_i \ddot{\vec{r}}_i \frac{\partial \vec{r}_i}{\partial \dot{q}_k} = \\ &= \frac{d}{dt} (m_i \dot{\vec{r}}_i \frac{\partial \vec{r}_i}{\partial \dot{q}_k}) - m_i \dot{\vec{r}}_i \frac{d}{dt} \frac{\partial \vec{r}_i}{\partial \dot{q}_k} = \\ &= \frac{d}{dt} \left(\frac{1}{2} m_i \frac{\partial \dot{\vec{r}}_i^2}{\partial \dot{q}_k} \right) - m_i \dot{\vec{r}}_i \frac{d}{dt} \frac{\partial \vec{r}_i}{\partial q_k} = \\ &= \frac{d}{dt} \frac{\partial}{\partial \dot{q}_k} \left(\frac{1}{2} m_i \dot{\vec{r}}_i^2 \right) - m_i \dot{\vec{r}}_i \frac{\partial \vec{r}_i}{\partial q_k} = \\ &= \frac{d}{dt} \frac{\partial}{\partial \dot{q}_k} \left(\frac{1}{2} m_i \dot{\vec{r}}_i^2 \right) - \frac{\partial}{\partial q_k} \left(\frac{1}{2} m_i \dot{\vec{r}}_i^2 \right), \end{aligned} \quad (10)$$

where we have taken into account that $yy' = \frac{1}{2}(y^2)'$ and $\frac{\partial x^2}{\partial t} = 2x \frac{\partial x}{\partial t}$. If we say that kinetic energy is

$$T = \sum_i \frac{1}{2} m_i \dot{\vec{r}}_i^2, \quad (11)$$

equation 10 can be rewritten into

$$\frac{d}{dt} \frac{\partial T}{\partial \dot{q}_k} - \frac{\partial T}{\partial q_k}. \quad (12)$$

Right side of equation 6 can be with help of equation 1 written into

$$\sum_i \vec{F}_i \frac{\partial \vec{r}_i}{\partial q_k} = - \sum_i \frac{\partial V}{\partial \vec{r}_i} \frac{\partial \vec{r}_i}{\partial q_k} = - \frac{\partial V}{\partial q_k} = - \frac{\partial V}{\partial q_k} + \frac{d}{dt} \frac{\partial V}{\partial \dot{q}_k}, \quad (13)$$

where the last term, which equals 0, was added because of the symmetry with equation 12. We define Lagrangian¹

$$L = T - V. \quad (14)$$

With equations 6, 12, 13 and 14 we can write Euler-Lagrange equations

$$\frac{d}{dt} \frac{\partial \mathbf{L}}{\partial \dot{\mathbf{q}}_k} - \frac{\partial \mathbf{L}}{\partial \mathbf{q}_k} = \mathbf{0}. \quad (15)$$

¹Hamiltonian function equals $H = T + V$.

3 Euler-Lagrange Equation in Matrix Form

When system is oscillating around equilibrium P_0 , we can write for the system

$$P = P_0 + P' = P(q_1^0 + \eta_1, \dots, q_N^0 + \eta_N), \quad (16)$$

where η_i are small. Lagrangian can be written with matrices

$$L = \frac{1}{2} \dot{\eta}^k T_{kl} \dot{\eta}^l - \frac{1}{2} \eta^k V_{kl} \eta^l, \quad (17)$$

where

$$\eta = \begin{bmatrix} \eta_1 \\ \vdots \\ \eta_N \end{bmatrix}, \quad (18)$$

$$\underline{\underline{T}} = \begin{bmatrix} T_{11} & \dots & T_{1N} \\ \vdots & & \vdots \\ T_{N1} & \dots & T_{NN} \end{bmatrix}, \quad (19)$$

where $T_{ki} = T_{ik}$, $\underline{\underline{T}} = \underline{\underline{T}}^{Transponed}$,

$$\underline{\underline{V}} = \begin{bmatrix} V_{11} & \dots & V_{1N} \\ \vdots & & \vdots \\ V_{N1} & \dots & V_{NN} \end{bmatrix}, \quad (20)$$

where $V_{ki} = V_{ik}$, $\underline{\underline{V}} = \underline{\underline{V}}^{Transponed}$. Euler-Lagrange equation

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\eta}_i} - \frac{\partial L}{\partial \eta_i} = 0 \quad (21)$$

with equation 17 yields

$$T_{il} \ddot{\eta}^l + \ddot{\eta}^k T_{ki} + V_{il} \eta^l + \eta^k V_{ki} = 0. \quad (22)$$

There is no drawback for changing k to l in equation 22

$$T_{il} \ddot{\eta}^l + \ddot{\eta}^l T_{li} + V_{il} \eta^l + \eta^l V_{li} = 0. \quad (23)$$

Using $T_{ki} = T_{ik}$ and $V_{ki} = V_{ik}$ equation 23 turns to

$$T_{il} \ddot{\eta}^l + \ddot{\eta}^l T_{il} + V_{il} \eta^l + \eta^l V_{il} = 0. \quad (24)$$

When dealing with components of matrices and vectors, we can easily change the position of η^l and V_{il} or T_{il} . The equation 24 changes

$$T_{il} \ddot{\eta}^l + V_{il} \eta^l = 0. \quad (25)$$

Last equation can be rewritten into matrices and vector form

$$\underline{\underline{T}} \ddot{\eta} + \underline{\underline{V}} \eta = 0. \quad (26)$$

Ansatz for solving equation 26 is

$$\eta = \vec{E}e^{i\omega t}, \quad (27)$$

which gives

$$(-\omega^2 \underline{\underline{T}} + \underline{\underline{V}})\vec{E} = 0. \quad (28)$$

Equation 28 has nontrivial solution only when

$$\det(-\omega^2 \underline{\underline{T}} + \underline{\underline{V}}) = 0. \quad (29)$$

4 Vibration of the Crystal Lattice

Vibrations of the crystal lattice or so called phonons are usually calculated only concerning first neighbour interaction.

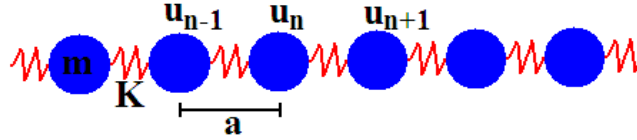


Figure 1: 1D monatomic lattice with N ions with mass m , string/potential coefficient K , displacement u_n .

From Figure 1 position of ions can be written as

$$x_n(t) = an + u_n(t). \quad (30)$$

Potential, when taking into account only nearest neighbour interactions, is

$$\begin{aligned} U &= \sum_n V(x_{n+1}(t) - x_n(t)) = \\ &\sim NV(a) + \frac{1}{1!} \sum_n (u_{n+1}(t) - u_n(t)) \frac{dV}{dx} \Big|_{x=a} + \frac{1}{2!} \sum_n (u_{n+1}(t) - u_n(t))^2 \frac{d^2V}{dx^2} \Big|_{x=a} + \dots = \\ &= NV(a) + \frac{1}{2} \sum_n (u_{n+1}(t) - u_n(t))^2 \frac{d^2V}{dx^2} \Big|_{x=a} + \dots, \end{aligned} \quad (31)$$

where we have expressed the sum in Taylor series and have taken into account that $\frac{dV}{dx} \Big|_{x=a} = 0$, because we are dealing with small oscillations i.e. we are always near equilibrium. Comparing equation 31 with potential energy of strings ($U = \frac{1}{2}Ku^2$) we get can write the string/potential coefficient as

$$K = \frac{d^2V}{dx^2} \Big|_{x=a}. \quad (32)$$

Kinetic energy is as usual

$$T = \frac{1}{2} \sum_n m \dot{u}_n^2. \quad (33)$$

Lagrangian is then

$$L = T - U = \frac{1}{2} \sum_n (m\dot{u}_n^2 - K(u_{n+1} - u_n)^2). \quad (34)$$

In equation 36 we dropped out term $NV(a)$ because it is a constant and drops out when solving Euler-Lagrange equations

$$\begin{aligned} \frac{d}{dt} \frac{\partial L}{\partial \dot{u}_n} - \frac{\partial L}{\partial u_n} &= 0 \\ m\ddot{u}_n + K(2u_n - u_{n+1} - u_{n-1}) &= 0. \end{aligned} \quad (35)$$

At lectures we already solved this equation with ansatz $u_n = u_0 e^{i(\omega t - kna)}$ and we got for frequency dispersion

$$\omega = 2\sqrt{\frac{K}{m}} \left| \sin \frac{ka}{2} \right|. \quad (36)$$

4.1 1D Monatomic “Lattice” with Three Atoms

Lets say that we have 3 ions². This is the simplest example for using expressions from Chapter 3.

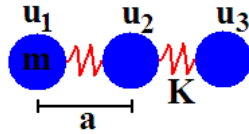


Figure 2: 1D monatomic “lattice” with 3 ions with mass m , string/potential coefficient K , displacement $u_{1,2,3}$.

Lagrangian in case of Figure 2 equals

$$L = \frac{1}{2}m(\dot{u}_1^2 + \dot{u}_2^2 + \dot{u}_3^2) - \frac{1}{2}K((u_2 - u_1)^2 + (u_3 - u_2)^2) = \frac{1}{2}\dot{\eta}^k T_{kl} \dot{\eta}^l - \frac{1}{2}\eta^k V_{kl} \eta^l, \quad (37)$$

where

$$\eta = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}, \quad (38)$$

$$\underline{\underline{T}} = m \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (39)$$

$$V = \frac{1}{2}K(u_1^2 + 2u_2^2 + u_3^2 - 2u_1u_2 - 2u_2u_3), \quad (40)$$

$$\underline{\underline{V}} = K \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}. \quad (41)$$

²Solutions of vibrations of 1D monatomic “lattice” with three atoms are eigenvectors of motion of 3-atomic molecule.

Using equation 28 we get

$$\begin{bmatrix} 1 - \frac{\omega^2 m}{K} & -1 & 0 \\ -1 & 2 - \frac{\omega^2 m}{K} & -1 \\ 0 & -1 & 1 - \frac{\omega^2 m}{K} \end{bmatrix} \vec{E} = 0. \quad (42)$$

Nontrivial solution we get from calculating the determinant of matrix in expression 42 which equals 0. We get 3 different values for frequency dispersions

$$\omega_1 = 0, \quad (43)$$

$$\omega_2 = \sqrt{\frac{K}{m}}, \quad (44)$$

$$\omega_3 = \sqrt{3\frac{K}{m}}, \quad (45)$$

with corresponding eigenvectors

$$\vec{E}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad (46)$$

$$\vec{E}_2 = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}, \quad (47)$$

$$\vec{E}_3 = \begin{bmatrix} -1 \\ 2 \\ -1 \end{bmatrix}. \quad (48)$$

4.2 1D Monatomic Lattice and Lennard-Jones Potential

Lets have N ions as in Figure 1 which feel Lennard-Jones potential and interaction between closest neighbours. Lennard-Jones potential (falls with distance x) yields

$$V = V_0 \left(\left(\frac{a}{x} \right)^{12} - 2 \left(\frac{a}{x} \right)^6 \right). \quad (49)$$

String coefficient is calculated using equation 32

$$K = 72 \frac{V_0}{a^2}. \quad (50)$$

Lagrangian is then

$$L = T - U = \sum_n \left(\frac{1}{2} m \dot{u}_n^2 - 36 \frac{V_0}{a^2} (u_{n+1} - u_n)^2 \right). \quad (51)$$

Inserting expression 51 into

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{u}_n} - \frac{\partial L}{\partial u_n} = 0, \quad (52)$$

we get

$$M\ddot{u}_n + 72\frac{V_0}{a^2}(2u_n - u_{n+1} - u_{n-1}) = 0, \quad (53)$$

which can be solved using ansatz $u_n = u_0 e^{i(\omega t - kx_n)}$

$$\omega = 2\sqrt{\frac{72V_0}{a^2}} \sin \frac{ka}{2}. \quad (54)$$

If we would have to take into account also second closest neighbours interaction, we would have to add extra term in potential energy

$$U = \frac{1}{2} \sum_n (u_{n+1} - u_n)^2 \frac{d^2V}{dx^2} \Big|_{x=a} + \frac{1}{2} \sum_n (u_{n+2} - u_n)^2 \frac{d^2V}{dx^2} \Big|_{x=2a}. \quad (55)$$

4.3 1D Diatomic Lattice

At lectures we already solved example of vibration of lattice with two different atoms (see Figure 3)

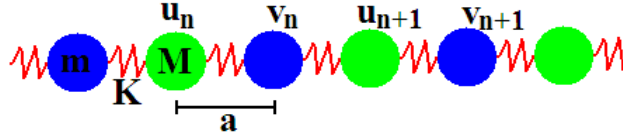


Figure 3: 1D diatomic lattice with N ions with mass m, and N ions with mass M, string/potential coefficient K, displacement u_n, v_n .

Once again we can write Lagrangian

$$L = \frac{1}{2} \sum_n (m\dot{v}_n^2 + M\dot{u}_n^2) - \frac{1}{2} K \sum_n ((v_n - u_n)^2 + (u_{n+1} - v_n)^2). \quad (56)$$

In this case we have two parameters i.e. u_n and v_n i.e. two Euler-Lagrange equations

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{u}_n} - \frac{\partial L}{\partial u_n} = 0, \quad (57)$$

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{v}_n} - \frac{\partial L}{\partial v_n} = 0 \quad (58)$$

$$(59)$$

from which we get

$$M\ddot{u}_n = -K(2u_n - v_n - v_{n-1}), \quad (60)$$

$$m\ddot{v}_n = -K(2v_n - u_n - u_{n+1}). \quad (61)$$

$$(62)$$

Using two ansatzes ($u_n = u_0 e^{i(\omega t - kna)}$ and $v_n = v_0 e^{i(\omega t - kna)}$) in equations 61 and 62 we get two independent equations from which we get two solutions (acoustic and optical branch)

$$\omega_{1,2}^2 = K \left(\frac{1}{m} + \frac{1}{M} \right) \pm \sqrt{K^2 \left(\frac{1}{m} + \frac{1}{M} \right)^2 - \frac{4K^2}{mM} \sin^2 \frac{ka}{2}}. \quad (63)$$

4.4 1D Monatomic Lattice With Two Different String Constants

Instead of having two different atoms in the lattice, we can have two different strings between ions (see Figure 4).

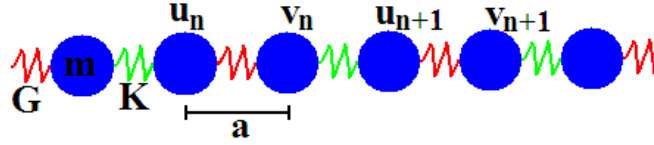


Figure 4: 1D monatomic lattice with $2N$ ions with mass m , N string coefficients K , N string coefficients G , displacement u_n, v_n .

Lagrangian for the case of two different strings yields

$$L = \frac{1}{2}m \sum_n (\dot{u}_n^2 + \dot{v}_n^2) - \frac{1}{2} \sum_n (K(u_{n+1} - v_n)^2 + G(v_n - u_n)^2). \quad (64)$$

With Euler-Lagrange equations 58 and 59 we get

$$m\ddot{u}_n - ((K - G)u_n - Kv_{n-1} - Gv_n) = 0, \quad (65)$$

$$m\ddot{v}_n - ((K + G)v_n - Ku_{n+1} - Gu_n) = 0. \quad (66)$$

$$(67)$$

Using ansatzes $u_n = u_0 e^{i(\omega t - kna)}$ and $v_n = v_0 e^{i(\omega t - kna)}$ the frequency dispersion yields

$$\omega_{1,2}^2 = \frac{K + G}{m} \pm \frac{1}{m} \sqrt{K^2 + G^2 + 2KG \cos ka}. \quad (68)$$

4.5 2D Square Monatomic Lattice with Vibrations Perpendicular to the Lattice

Simplest example of monatomic 2D lattice is square lattice (see Figure 5).

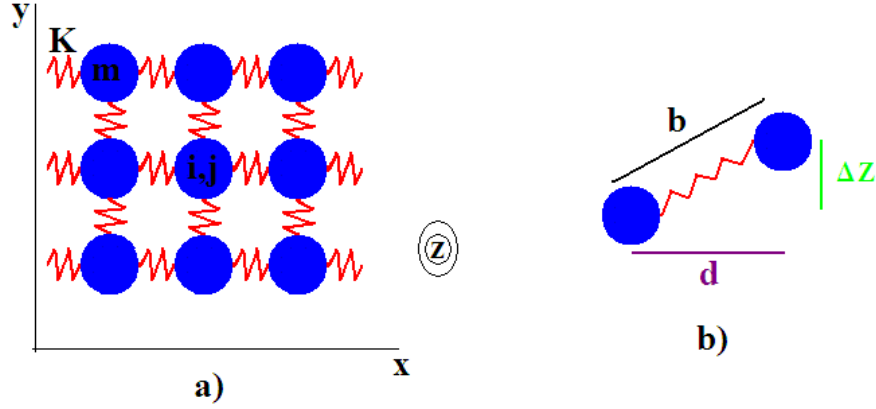


Figure 5: 2D monatomic lattice with N^2 ions with mass m , string coefficients K , displacement z_n perpendicular to the lattice plane.

From Figure 5 we can write

$$b = \sqrt{d^2 + \Delta z^2} = d \sqrt{1 + \left(\frac{\Delta z}{d}\right)^2} \sim d + \frac{1}{2} \frac{\Delta z^2}{d} + \dots, \quad (69)$$

where $d = l + \Delta l$, $\Delta z \ll d$, so we could introduce Taylor series into equation 69. Lagrangian for square lattice can be written as

$$\begin{aligned} L &= \frac{1}{2} \sum_{i,j} m \dot{z}_{i,j}^2 - \frac{1}{2} \sum_{i,j} K (b - l)^2 = \\ &= \frac{1}{2} \sum_{i,j} m \dot{z}_{i,j}^2 - \frac{1}{2} \sum_{i,j} K \left((d - l) + \frac{1}{2} \frac{\Delta z^2}{d} \right)^2 \sim \\ &\sim \frac{1}{2} \sum_{i,j} m \dot{z}_{i,j}^2 - \frac{1}{2} \sum_{i,j} K_{eff} \Delta z^2. \end{aligned} \quad (70)$$

$$(71)$$

From Euler-Lagrange equations

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{z}_{i,j}} - \frac{\partial L}{\partial z_{i,j}} = 0 \quad (72)$$

we get

$$m \ddot{z}_{i,j} = K_{eff} (z_{i+1,j} + z_{i-1,j} + z_{i,j+1} + z_{i,j-1} - 4z_{i,j}). \quad (73)$$

Using ansatz $z_{i,j} = u_0 e^{i(\omega t - \vec{k} \cdot \vec{r})}$ we calculated the frequency dispersion

$$\omega = \sqrt{\frac{K_{eff}}{m}} \sqrt{\sin^2 \frac{k_x d}{2} + \sin^2 \frac{k_y d}{2}}. \quad (74)$$

5 Conclusion

We have shown that solving problems of vibration in crystal lattices is a completely routine work when using Euler-Lagrange equations.