Phonon: Quantization of Elastic Waves (under construction)

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Let us consider a crystal made-up with N unit cells and having Born-von Karman boundary condition of macroscopic periodicity. Each unit cell is indexed by vector $\boldsymbol{R}$, a unit cell contains atoms indexed by I ($I = 1, \cdots, N_{\rm atom}$), and mass of each atom is M_I, as depicted in Fig. 1. Atomic displacements $q_{I\alpha}(\boldsymbol{R})$ from their equilibrium positions can have three independent Cartesian directions α, for instance $\alpha = x, y, z$.

The atomic displacements $q_{I\alpha}(\boldsymbol{R})$ are governed by the many-body potential Φ. This real function Φ can be expanded as

$$\Phi = \Phi_0 + \sum_{\boldsymbol{R}I\alpha} \Phi_{I\alpha}(\boldsymbol{R})\, q_{I\alpha}(\boldsymbol{R}) + \sum_{\boldsymbol{R}I\alpha} \sum_{\boldsymbol{R}'J\beta} q_{I\alpha}(\boldsymbol{R})\, \Phi_{I\alpha,J\beta}(\boldsymbol{R},\boldsymbol{R}')\, q_{J\beta}(\boldsymbol{R}') + \cdots \ , \tag{1}$$

where Φ_0 is the equilibrium value,

$$\Phi_{I\alpha}(\boldsymbol{R}) = \left(\frac{\partial \Phi}{\partial q_{I\alpha}(\boldsymbol{R})} \right)_0 \ , \tag{2}$$

and

$$\Phi_{I\alpha,J\beta}(\boldsymbol{R},\boldsymbol{R}') = \left(\frac{\partial^2 \Phi}{\partial q_{I\alpha}(\boldsymbol{R}) \partial q_{J\beta}(\boldsymbol{R}')} \right)_0 \ . \tag{3}$$

The subscript zero implies that the derivatives are evaluated at the equilibrium configuration. In the equilibrium position the second term on the right-hand side of (1) vanishes. $\Phi_{I\alpha,J\beta}(\boldsymbol{R},\boldsymbol{R}')$ is real and the condition of translational invariance applied to it yields the following results:

$$\Phi_{J\beta,I\alpha}(\boldsymbol{R}',\boldsymbol{R}) = \Phi_{I\alpha,J\beta}(\boldsymbol{R},\boldsymbol{R}') = \Phi_{I\alpha,J\beta}(\boldsymbol{R}-\boldsymbol{R}') \tag{4}$$

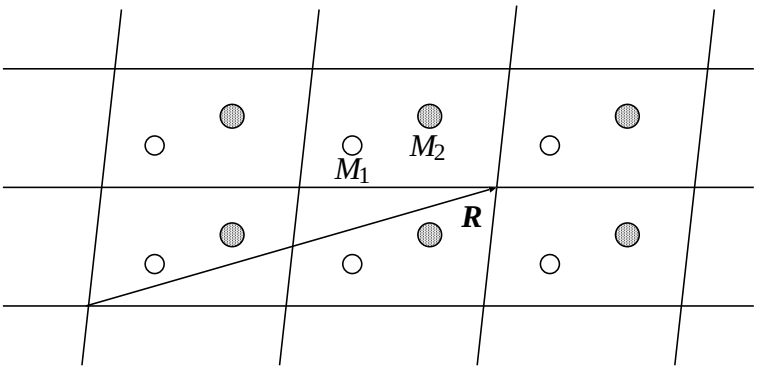

Figure 1: Crystal structure. Each unit cell is indexed by $\boldsymbol{R}$. Atoms in a unit cell is indexed by I.

and

$$\sum_{\boldsymbol{R}'J} \Phi_{I\alpha,J\beta}(\boldsymbol{R},\boldsymbol{R}') = 0 \ . \tag{5}$$

Equation (5) simply expresses the fact that the forces on any atom are zero if each atom is displaced from equilibrium by the same amount. [3]

Hamiltonian for this system can be written

$$H = \sum_{\boldsymbol{R}I\alpha} \frac{p^2_{I\alpha}(\boldsymbol{R})}{2M_I} + \frac{1}{2}\sum_{\boldsymbol{R}I\alpha}\sum_{\boldsymbol{R}'J\beta} q_{I\alpha}(\boldsymbol{R})\Phi_{I\alpha,J\beta}(\boldsymbol{R}-\boldsymbol{R}')q_{J\beta}(\boldsymbol{R}') \ , \tag{6}$$

where $p_{I\alpha}(\boldsymbol{R})$ is the momentum of the atom. From now, we transform this Hamiltonian 6

Let us Fourier-transform this Hamiltonian into $\boldsymbol{k}$ representation. We expand mass-weighted atomic displacements $\sqrt{M_I}\, q_{I\alpha}(\boldsymbol{R})$ with Fourier coefficients $\tilde{q}_{I\alpha}(\boldsymbol{k})$,

$$\sqrt{M_I}\, q_{I\alpha}(\boldsymbol{R}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \tilde{q}_{I\alpha}(\boldsymbol{k}) \exp(i\boldsymbol{k}\cdot\boldsymbol{R}) \ , \tag{7}$$

consistent with the inverse transformation

$$\tilde{q}_{I\alpha}(\boldsymbol{k}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}} \sqrt{M_I}\, q_{I\alpha}(\boldsymbol{R}) \exp(-i\boldsymbol{k}\cdot\boldsymbol{R}) \ . \tag{8}$$

Here N of $\boldsymbol{k}$'s are defined in first Brillouin zone. We need the transformation from the momentum of the atom $p_{I\alpha}(\boldsymbol{R})$ to the momentum $\tilde{p}_{I\alpha}(\boldsymbol{k})$ that is canonically conjugate to the displacement $\tilde{q}_{I\alpha}(\boldsymbol{k})$. The transformation is

$$p_{I\alpha}(\boldsymbol{R}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \sqrt{M_I}\, \tilde{p}_{I\alpha}(\boldsymbol{k}) \exp(-i\boldsymbol{k}\cdot\boldsymbol{R}) \tag{9}$$

and

$$\tilde{p}_{I\alpha}(\boldsymbol{k}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}} \frac{1}{\sqrt{M_I}} p_{I\alpha}(\boldsymbol{R}) \exp(i\boldsymbol{k}\cdot\boldsymbol{R}) \ . \tag{10}$$

We verify that our choice of $\tilde{q}_{I\alpha}(\boldsymbol{k})$ and $\tilde{p}_{I\alpha}(\boldsymbol{k})$ satisfies the quantum commutation relation for canonical variables. We form the commutator

$$[\tilde{q}_{I\alpha}(\boldsymbol{k}), \tilde{p}_{J\beta}(\boldsymbol{k}')] = \frac{1}{N}..... \ . \tag{11}$$

Because the operators $q_{I\alpha}(\boldsymbol{R})$ and $p_{I\alpha}(\boldsymbol{R})$ are conjugate, they originally satisfy the commutation relation

$$[q_{I\alpha}(\boldsymbol{R}), p_{J\beta}(\boldsymbol{R}')] = i\hbar\, \delta(\boldsymbol{R},\boldsymbol{R}')\, \delta(I,J)\, \delta(\alpha,\beta) \ , \tag{12}$$

where $\delta(i,j)$ is the Kronecker delta symbol. Thus (11) becomes

$$[\tilde{q}_{I\alpha}(\boldsymbol{k}), \tilde{p}_{J\beta}(\boldsymbol{k}')] = \frac{1}{N} i\hbar ..... = i\hbar\, \delta(\boldsymbol{k},\boldsymbol{k}')\, \delta(I,J)\, \delta(\alpha,\beta) \ , \tag{13}$$

so that $\tilde{q}_{I\alpha}(\boldsymbol{k})$ and $\tilde{p}_{I\alpha}(\boldsymbol{k})$ are conjugate variables.

Using $q_{I\alpha}(\boldsymbol{R})$ and $p_{I\alpha}(\boldsymbol{R})$ are real, i.e., $q_{I\alpha}(\boldsymbol{R}) = q^*_{I\alpha}(\boldsymbol{R})$ and $p_{I\alpha}(\boldsymbol{R}) = p^*_{I\alpha}(\boldsymbol{R})$, relation between -k and k, ... it can be evidently shown that

$$\tilde{q}_{I\alpha}(-\boldsymbol{k}) = \tilde{q}^*_{I\alpha}(\boldsymbol{k}) \tag{14}$$

and

$$\tilde{p}_{I\alpha}(-\boldsymbol{k}) = \tilde{p}^*_{I\alpha}(\boldsymbol{k}) \ . \tag{15}$$

Furthermore, we introduce the Fourier expansion of the second derivative of many-body potential $\Phi_{I\alpha,J\beta}(\boldsymbol{R})$,

$$\Phi_{I\alpha,J\beta}(\boldsymbol{R}) = \frac{1}{N}\sum_{\boldsymbol{k}} \sqrt{M_I M_J}\, \tilde{\Phi}_{I\alpha,J\beta}(\boldsymbol{k}) \exp(i\boldsymbol{k}\cdot\boldsymbol{R}) \ , \tag{16}$$

and, consequently, inverse transformation becomes

$$\tilde{\Phi}_{I\alpha,J\beta}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} \frac{\Phi_{I\alpha,J\beta}(\boldsymbol{R})}{\sqrt{M_I M_J}} \exp(-i\boldsymbol{k}\cdot\boldsymbol{R}) \ . \tag{17}$$

Using symmetricity of the real function $\Phi_{I\alpha,J\beta}(\boldsymbol{R})$, it can be evidently shown that $\tilde{\Phi}_{I\alpha,J\beta}(\boldsymbol{k})$ is an Hermitian matrix

$$\tilde{\Phi}_{J\beta,I\alpha}(\boldsymbol{k}) = \tilde{\Phi}^*_{I\alpha,J\beta}(\boldsymbol{k}) \tag{18}$$

and

$$\tilde{\Phi}_{I\alpha,J\beta}(-\boldsymbol{k}) = \tilde{\Phi}^*_{I\alpha,J\beta}(\boldsymbol{k}) \ . \tag{19}$$

Substituting Fourier expantions of (7), (9) and (16) into the Hamiltonian (6), we get ...

It may be a good approximation[4, 1, 2] to assume that the true ion-ion interaction in a crystal is consisting of shor-range interaction somewhat described in ... and long-range interaction exactly described in ....

$$\tilde{\Phi}_{I\alpha,J\beta}(\boldsymbol{k}) = \tag{20}$$

(To be continued.)

References

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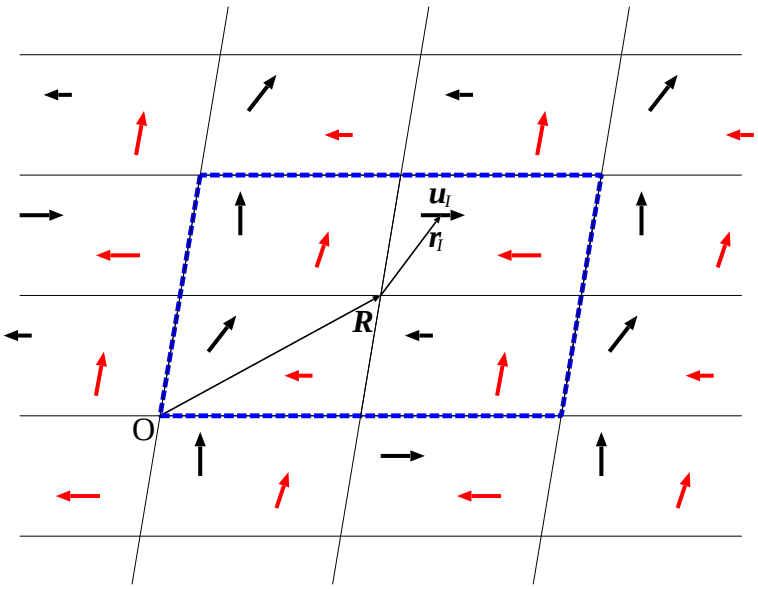

Figure 2: Dipole Crystal