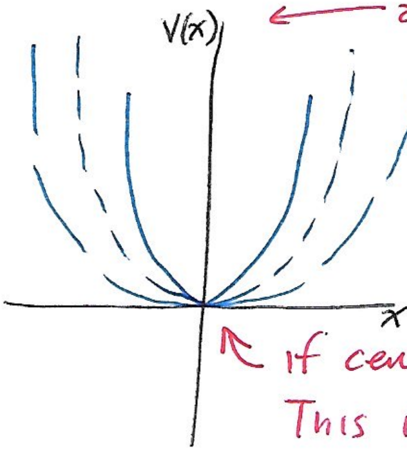
Oscillations

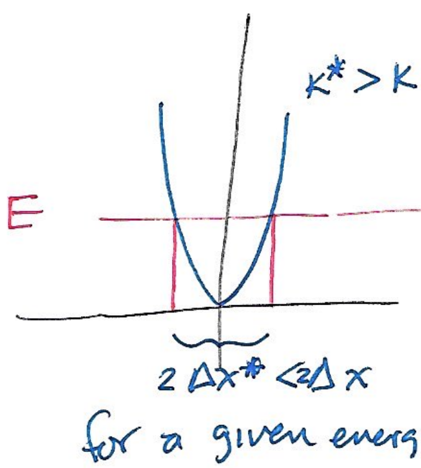
Finally something I know something about!

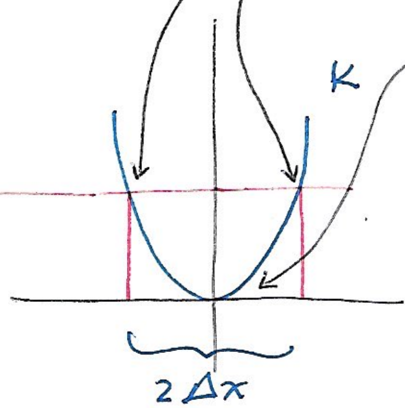
Consider the simplest potential that can produce oscillations, a parabola.



if centered at zero, then $V(x) = K' x^2 = \frac{1}{2} K x^2$

This is Hooke's law, K is the stiffness or force or spring constant. It describes how narrow or wide the parabola is.





All the energy is potential at the turning points

All the energy is kinetic at the equilibrium position

$$\cancel{\tfrac{1}{2}} m v^2 = \cancel{\tfrac{1}{2}} K(\Delta x)^2$$

$$\Rightarrow v = \sqrt{\frac{K(\Delta x)^2}{m}} = \Delta x \sqrt{\frac{K}{m}}$$

Approx.

$$\Rightarrow \frac{\Delta x}{\Delta t}\,\frac{1}{\Delta x} = \frac{1}{\Delta t} = \sqrt{\frac{K}{m}}$$

Average velocity, gives (angular) a frequency

More accurately, $v = \frac{dx}{dt} = x\sqrt{\frac{K}{m}}$

$$\Rightarrow \int \frac{dx}{x} = \sqrt{\frac{K}{m}} \int dt$$

$$\ln x = \sqrt{K/m}\; t$$

going back and forth $x + C = e^{i\sqrt{K/m}\,t} = \cos\left(\sqrt{K/m}\,\cancel{i}t\right) + i\sin\left(\sqrt{K/m}\,\cancel{i}t\right)$

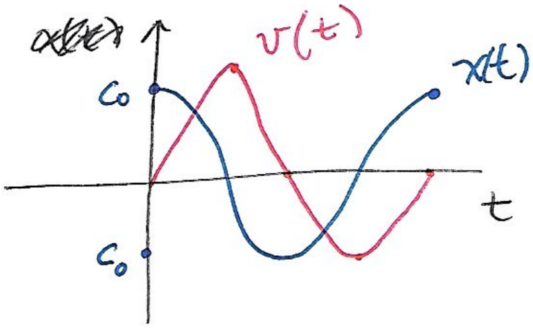
can be shifted

* shock absorber

The stiffer the parabola, the higher the frequency, the ~~la~~ larger the mass, the lower the frequency.

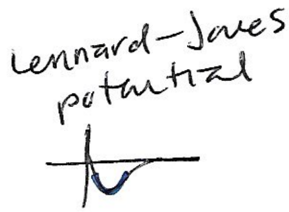
or better, $\ln x = \sqrt{k/m}\, t + c$

$$x = e^{i\sqrt{k/m}\,t + c} = e^{ic} \cdot e^{i\sqrt{k/m}\,t} = C_0 \cos\left(\sqrt{k/m} \cdot t\right) + iC_1 \sin\left(\sqrt{\tfrac{k}{m}}\, t\right)$$

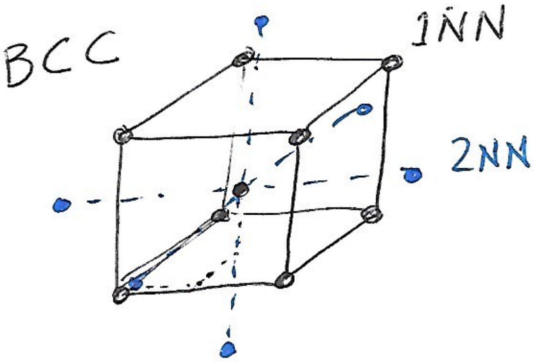


Notice $-\dfrac{d\,V(x)}{dx} = \vec{F} = \cancel{\tfrac{1}{2}} \cdot \cancel{2} k x$

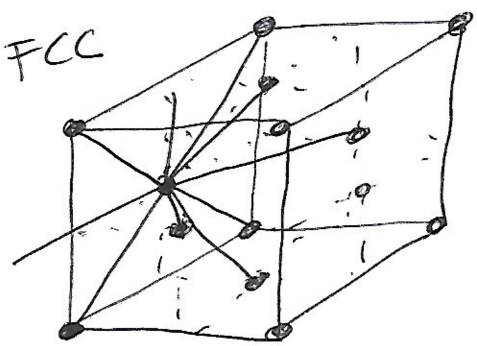
$\vec{F} = -kx$

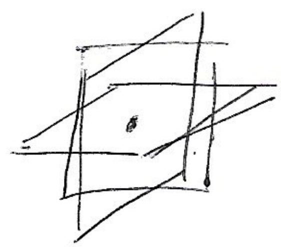


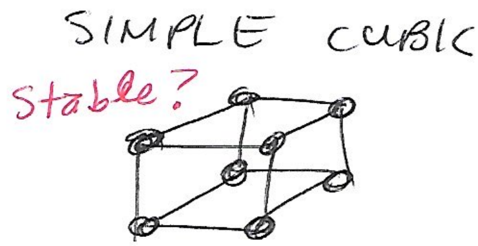
$-\dfrac{d\vec{F}}{dx} = -k \Rightarrow \dfrac{d^2V}{dx} = k$



The force constant is the second derivative of the potential, so at the equilibrium position it tells you, if the system is in stable or unstable equilibrium







★ What if we include friction? Then $\vec{F} = -kx + \lambda\dot{x} = m\ddot{x}$

★ What if we include higher terms? Above the harmonic?

★ The Lennard-Jones potential does not produce a perfect parabola at the bottom.

★ Since the effective potential of central force particles looked like the L-J, approximated by simple-H-Osc.

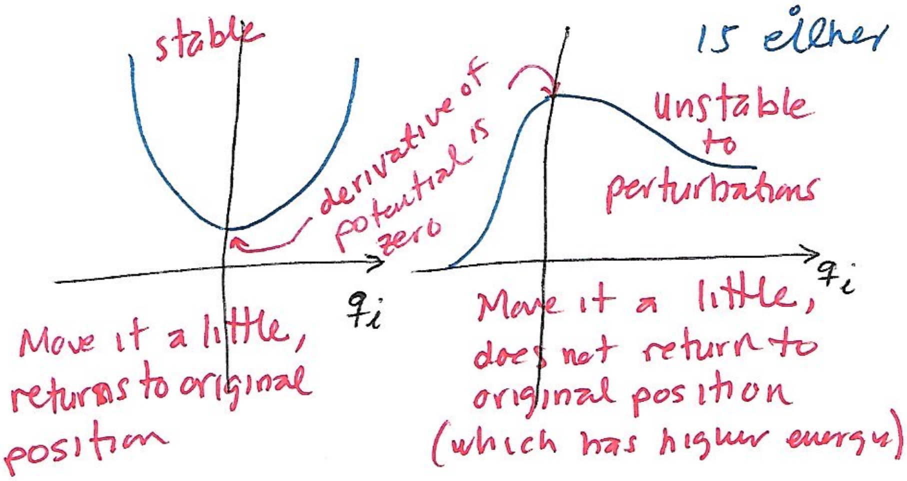
~~Assume~~ Consider a conservative system. Assume that ~~a~~ generalized coordinates transformations <u>do not</u> include time explicitly (so no time-dependent constraints). The system is in <u>equilibrium</u> if the forces vanish.

Eq. 6.1

$$Q_i = -\left(\frac{\partial V}{\partial q_i}\right)_0 = 0$$

★ Why? Otherwise there is an acceleration, thus there is a velocity, thus the system is moving.

★ Notice that if $\frac{\partial V}{\partial q_i} = 0$, the potential is either a maximum or minimum.



Consider a <u>small</u> perturbation, so $\boxed{q_i = q_{0i} + \eta_i}$ ~~q_i are~~

q_i are the new generalized coordinates. Expand about q_{0i}

multi-variable Taylor expansion

$$V(q_1, \ldots, q_n) = \underbrace{V(q_{01}, \cancel{q_0}, q_{0n})}_{\text{constant: can be shifted}} + \underbrace{\left(\frac{\partial V}{\partial q_i}\right)_0}_{\text{zero by definition}} \eta_i + \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_0 \eta_i \eta_j + \ldots$$

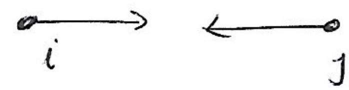
So to second order, which is the first non-vanishing approximation

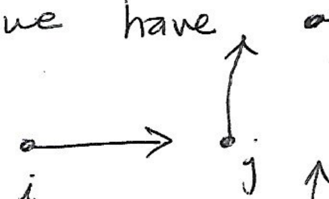
Eq. 6.4

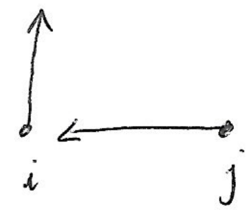
$$V = \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_0 \eta_i \eta_j = V_{ij} \eta_i \eta_j$$

Force constant

In the case of crystals, a solid with N particles will have 3N degrees of freedom, each one is a generalized coordinate. So η_i and η_j are the displacements from equilibrium of particles i and j, and V_{ij} is the force constant between them. In general the ~~the~~ particles can be displaced in 3 orthogonal directions, typically denoted by α, β for particle i and j respectively, so $V = \frac{1}{2} V_{i\alpha, j\beta} \eta_{i\alpha} \eta_{j\beta}$

if $\alpha = \beta$, we have  longitudinal force constant

otherwise  transverse force constant

which is the same as , so $V_{i\alpha, j\beta} = V_{i\beta, j\alpha}$

$$\Phi_{ij}^{\alpha\beta} = \begin{bmatrix} V_{i\alpha j\alpha} & V_{i\alpha j\beta} & V_{i\alpha j\gamma} \\ & V_{i\beta j\beta} & V_{i\beta j\gamma} \\ & & V_{i\gamma j\gamma} \end{bmatrix}$$

Force constant matrix
Due to the symmetry of the crystal, some of the elements are equal or zero. Rank-2 tensor

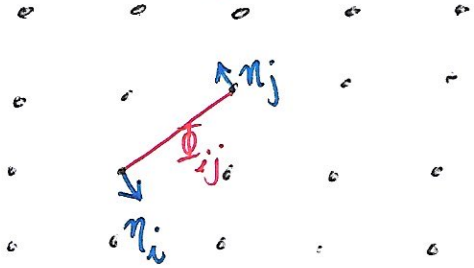
If we go to 3rd order, $V_{ijk}^{\alpha\beta\gamma} \eta_i^{\alpha} \eta_j^{\beta} \eta_k^{\gamma}$ Rank-3 tensor of force constants

4th order, $V_{ijkl}^{\alpha\beta\gamma\delta} \eta_i^{\alpha} \eta_j^{\beta} \eta_k^{\gamma} \eta_l^{\delta}$ Rank-4 tensor of force constants

And so on...

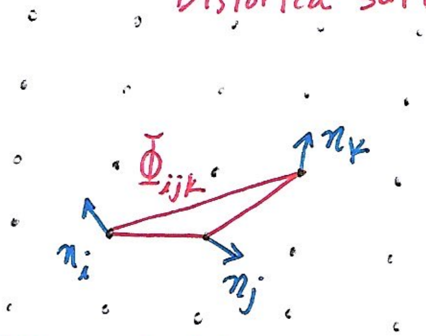
What does it mean?

2nd order — Distorted line



all possibilities in force constant matrix

3rd order — Distorted surface



All possibilities in rank-3 force constan tensor

4th order — Distorted Volume

All posibilities in rank-4 force constant tensor.

The Taylor expansion goes to infinite order, so this expansion accounts for many-body effects, but the number of force constants grows geometrically and it is infinite in principle

★ If the particles are in their ideal lattice equilibrium positions, they must obey symmetries, so by applying symmetry operations, the rotation matrices, you can eliminate many. Still, this explodes quickly and a rigurous description of the system when not in the ideal lattice state does not exist.

The kinetic energy can be similarly Taylor expanded, ~~But~~.

$$T = \frac{1}{2} m_{ij} \dot{q}_i \dot{q}_j = \frac{1}{2} m_{ij} (\cancel{\dot{q}_{0i}} + \dot{\eta}_i)(\cancel{\dot{q}_{0j}} + \dot{\eta}_j) = \frac{1}{2} m_{ij} \eta_i \eta_j$$

Notice that functionally, it looks like the potential energy if the mass is analogous to the force constant; but we can't

$$m_{ij}(q_1, \ldots, q_n) = m_{ij}(q_{0i}, \ldots, q_{0j}) + \overbrace{\left(\frac{\partial m_{ij}}{\partial q_k}\right)_0 \eta_k + \ldots}^{\text{take these terms}}$$

Denoting the values of m_{ij} at equilibrium by T_{ij},

$T = \frac{1}{2} T_{ij} \dot{\eta}_i \dot{\eta}_j$, so $\mathcal{L} = \frac{1}{2}\left(T_{ij} \dot{\eta}_i \dot{\eta}_j - V_{ij} \eta_i \eta_j \right)$

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_j}\right) - \frac{\partial \mathcal{L}}{\partial q_j} = 0$$

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\eta}_j}\right) - \frac{\partial \mathcal{L}}{\partial \eta_j} = \frac{d}{dt}\left[\frac{1}{2} T_{ij} \dot{\eta}_i\right] - \left[-\frac{1}{2} V_{ij} \eta_i\right]$$

Eq. 6.8

$$\frac{1}{2}\left[T_{ij} \ddot{\eta}_i + V_{ij} \eta_i\right] = 0 \Rightarrow T_{ij} \ddot{\eta}_i + V_{ij} \eta_i = 0$$

☆ What does it mean to have a mass that depends on the generalized coordinates??

We will focus on kinetic energies that have no cross-terms, so $T_{ij} = 0$ if $i \neq j$. In this case

$$\mathcal{L} = \frac{1}{2}\left(T_{ii} \dot{\eta}_i \dot{\eta}_i - V_{ij} \eta_i \eta_j\right) = \frac{1}{2}\left(T_i \dot{\eta}_i^2 - V_{ij} \eta_i \eta_j\right)$$

$$\frac{d}{dt}\left(\cancel{\tfrac{1}{2}} T_i \cdot \cancel{2} \dot{\eta}\right) - \left(-V_{ij} \eta_j\right) = 0$$

$$T_i \ddot{\eta}_i + V_{ij} \eta_j = 0$$

Eq. 6.10