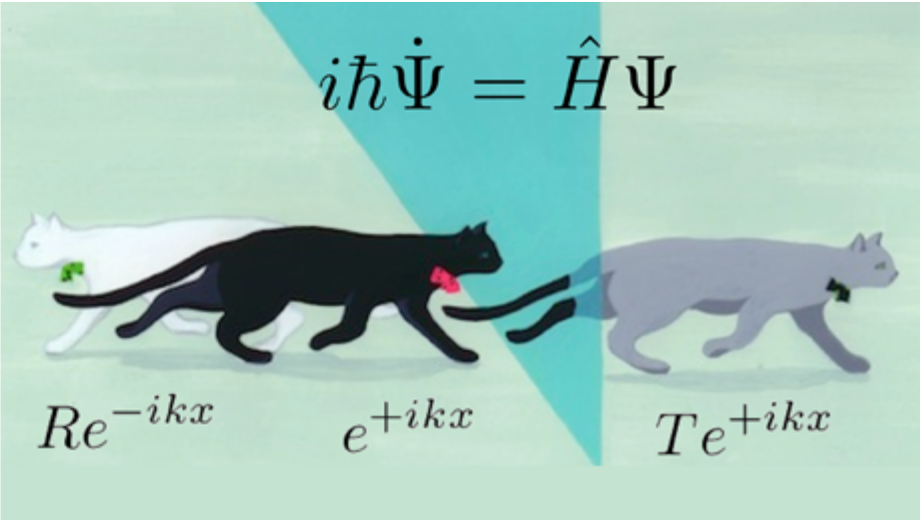
Exploring Quantum Physics

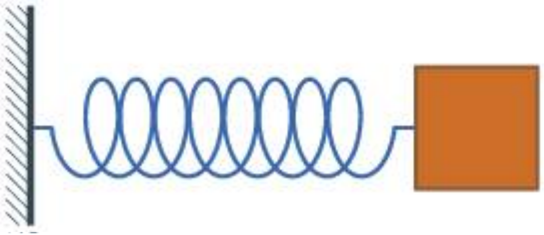
Coursera, Spring 2013 Instructors: Charles W. Clark and Victor Galitski

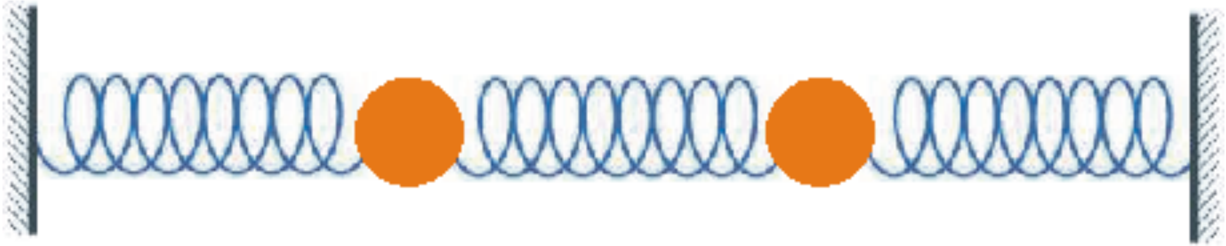
Phonons in crystals

Part I: Preliminary discussion

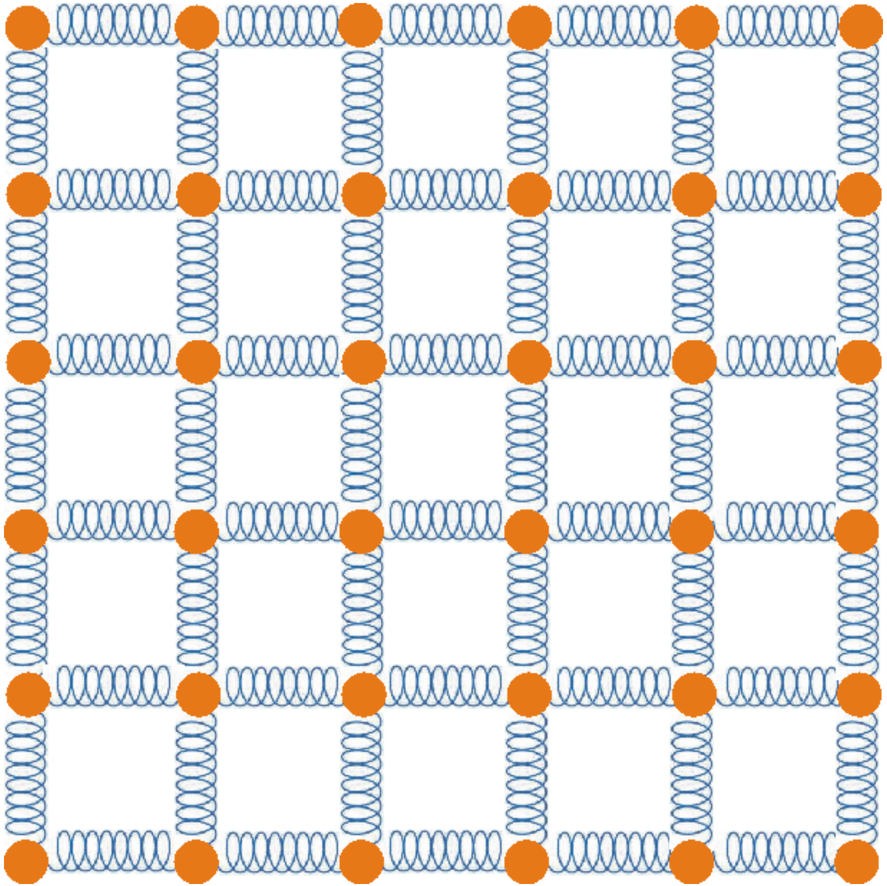


Normal modes





“Spherical cow” model of a crystal



Symmetries and broken symmetries

Poor man's version of the Goldstone theorem

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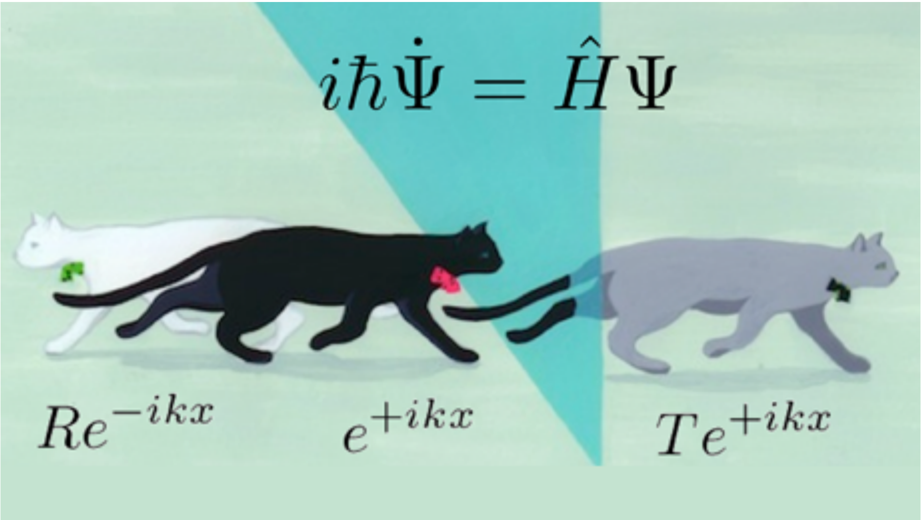
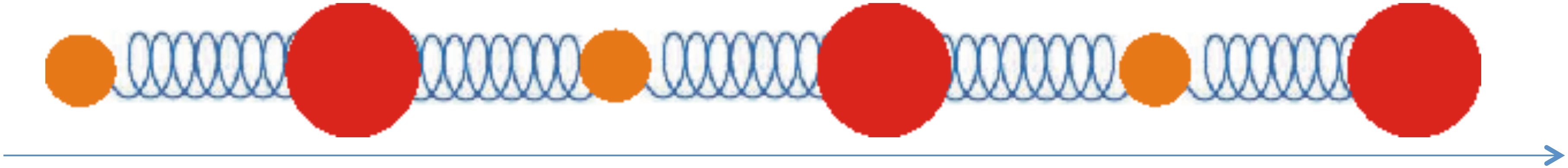
Part I: Classical oscillator chain



The model



- Classical energy (classical Hamiltonian):

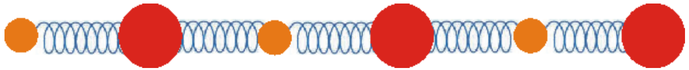
$$H = \sum_n \Big[\underbrace{\frac{p_n^2}{2m} + \frac{P_n^2}{2M}}_{\text{kinetic energy}} + \underbrace{\frac{k}{2}(x_n - Y_n)^2 + \frac{k}{2}\left(x_{n+1} - Y_n\right)^2}_{\text{potential energy}, V} \Big]$$

- Eqs. of motion (Newton's Eqs.) follow from $\dot{p}_n = -\frac{\partial V}{\partial x_n}$ and $\dot{P}_n = -\frac{\partial V}{\partial Y_n}$

$$\dot{p}_n = k(Y_n - x_n) + k(Y_{n-1} - x_n)$$

$$\dot{P}_n = k(x_n - Y_n) + k(x_{n+1} - Y_n)$$

Wave solutions to Newton's Eqs.

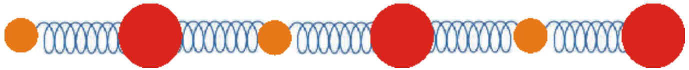


$$\begin{cases} m\ddot{x}_n = k\left[Y_n + Y_{n-1} - 2x_n\right] \\ M\ddot{Y}_n = k\left[x_n + x_{n+1} - 2Y_n\right] \end{cases}$$

$$x_n(t) = \int \frac{dq}{2\pi} x_q e^{iqn - i\omega t}$$

$$Y_n(t) = \int \frac{dq}{2\pi} Y_q e^{iq(n+1/2) - i\omega t}$$

Wave solutions to Newton's Eqs.



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$$\begin{cases} -\omega^2 m x_q = 2k\cos(q/2) Y_q - 2k x_q \\ -\omega^2 M Y_q = 2k\cos(q/2) x_q - 2k Y_q \end{cases}$$

The wave dispersion; acoustic and optical phonons

$$\begin{pmatrix} m\omega^2 - 2k & 2k\cos(q/2) \\ 2k\cos(q/2) & M\omega^2 - 2k \end{pmatrix} \begin{pmatrix} x_q \\ Y_q \end{pmatrix} = 0$$

- Self-consistency condition:

$$\det \begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \end{pmatrix} = \omega^4 - 2k(m+M)\omega^2 + 4k^2\left[1 - \cos^2(q/2)\right] = 0$$

$$\omega_{\pm}^2(q) = \frac{k}{\mu}\left[1 \pm \sqrt{1 - \frac{4\mu^2}{mM}\sin^2(qa)}\right]$$

$$\mu = \frac{mM}{m+M}$$

Speed of sound