Phonon modes in graphene and carbon nanotubes

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- Calculate the phonon modes in Graphene

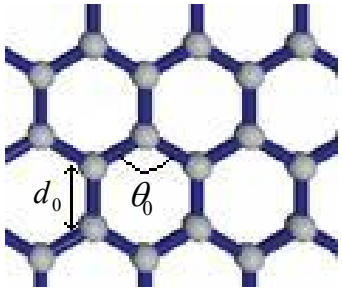
  → Methods: force constant models

- Calculate the phonon modes in carbon nanotubes

  → Method: force constant model with bond stretching and bond bending

  (**G.D.Mahan, G.S.Jeon, Phys. Rev. B** 70**, 075405 (2004)**)

Graphene



Keating/Hass

Bond stretching

$$V_s = \frac{k_s}{8d_0^2}\sum_{\langle ij\rangle}(\mathbf{x}_{ij}\cdot\mathbf{x}_{ij} - d_0^2)^2$$

Bond bending

$$V_s = \frac{k_b}{2d_0^2}\sum_{\langle ijk\rangle}(\mathbf{x}_{ji}\cdot\mathbf{x}_{jk} - d_0^2\cos\theta_0)^2$$

Saito/Dresselhaus

Direct parametrization of the diagonal force constants (up to 4th n.n.)

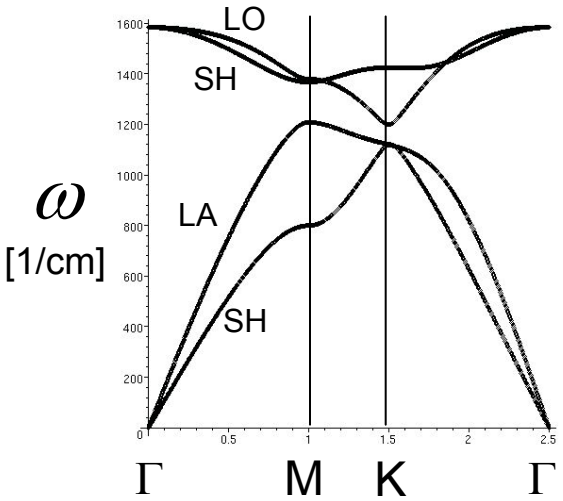
Mahan

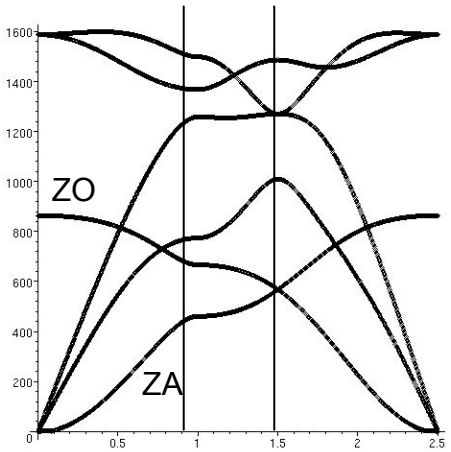
Bond stretching

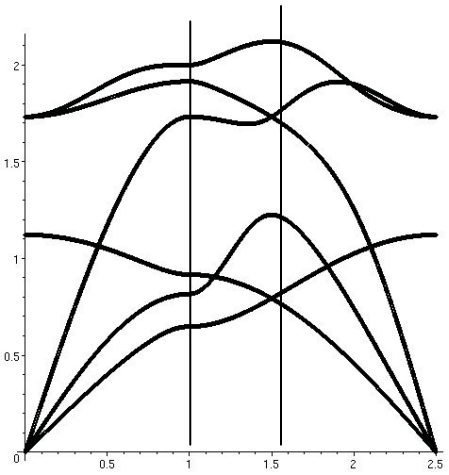
$$V_s = \frac{k_\alpha}{2}\sum_{\langle ij\rangle}\left|\hat{\boldsymbol{\delta}}_{ij}\cdot(\mathbf{u}_i - \mathbf{u}_j)\right|^2$$

Bond bending

$$V_b = \frac{k_b}{2}\sum_{j}\left|\sum_{i=1}^{3}\hat{\mathbf{n}}_{ij}\cdot(\mathbf{u}_i - \mathbf{u}_j)\right|^2$$







(3,3) Carbon Nanotube

Mahan model for CNT

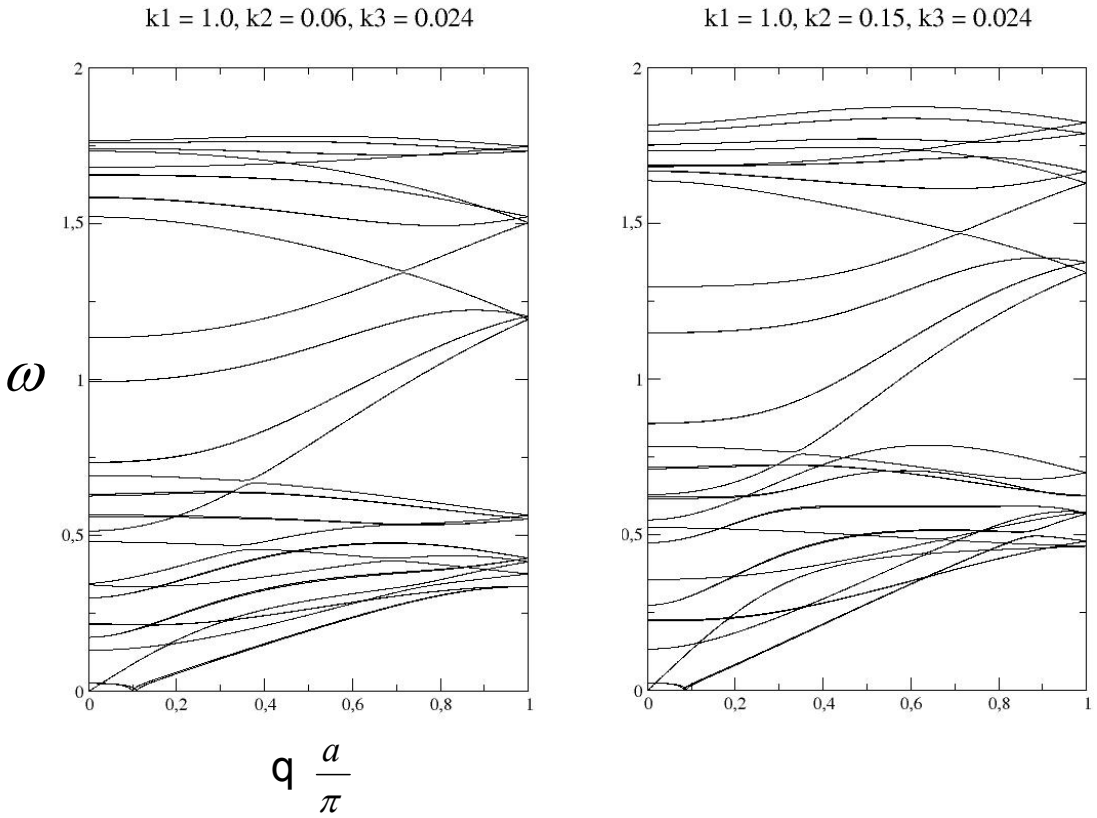
k1 → bond stretching 1st nearest neighb.

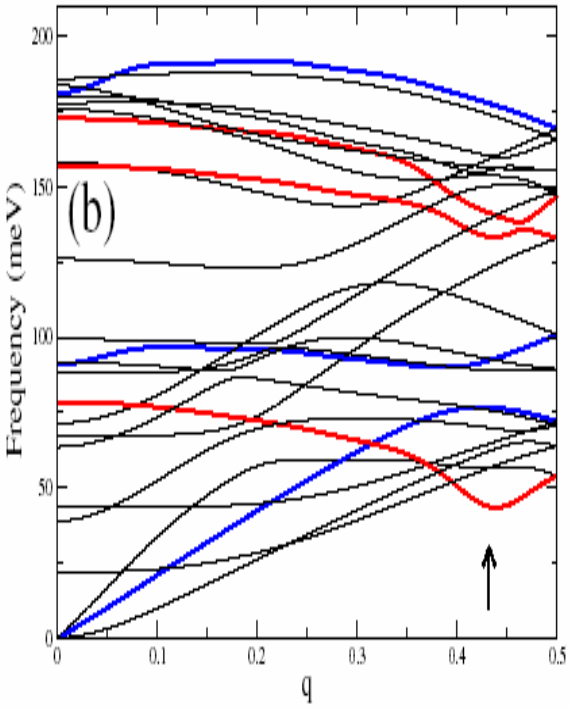
k2 → bond stretching 2nd nearest neighb.

k3 → bond bending

Comparison:

(3,3) CNT *ab initio* calculation
(Bohnen, Heid *et al*.)





Perspectives

- The Mahan model is optimized for a (10,10) CNT

  → calculate and verify the phonon dispersion relation for a (10,10) CNT

- Electron-phonon coupling