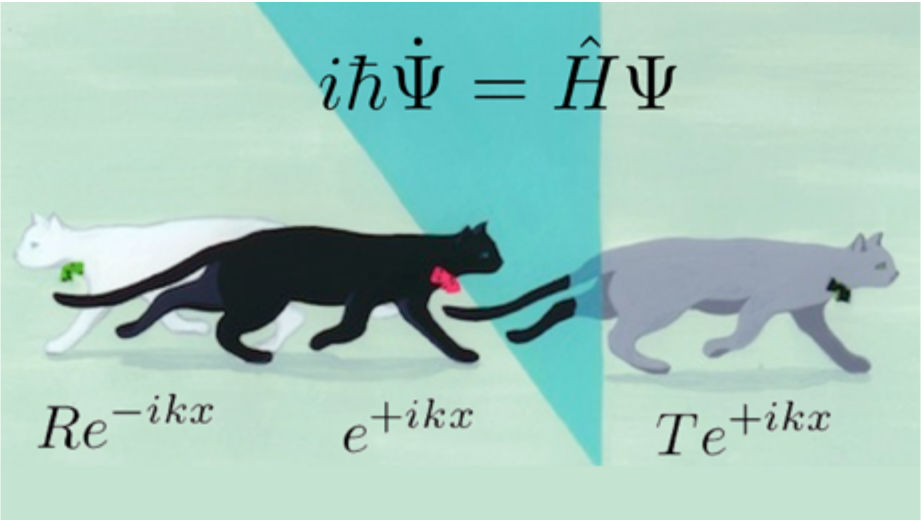
Exploring Quantum Physics

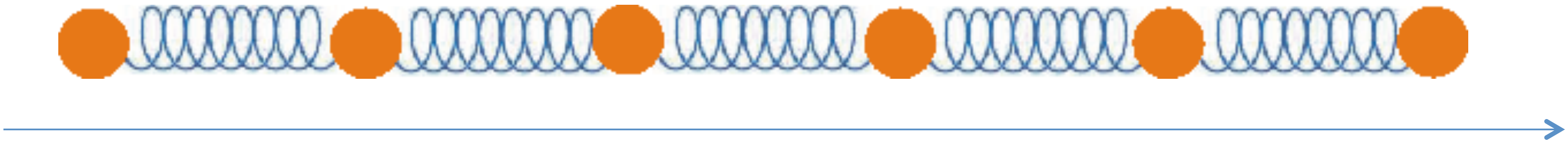
Coursera, Spring 2013 Instructors: Charles W. Clark and Victor Galitski

Phonons in crystals

Part III: Quantum oscillator chain



Quantizing the classical model



- Classical Hamiltonian

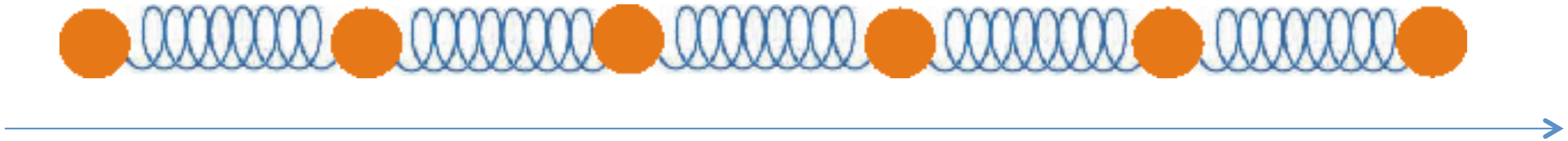
$$H = \sum_n \left[\frac{p_n^2}{2m} + \frac{k}{2} \left(x_n - x_{n+1} \right)^2 \right]$$

- Introduce creation/annihilation operators for each oscillator:

$$\hat{x}_n = \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a}_n^\dagger + \hat{a}_n \right) \text{ and } \hat{p}_n = i\sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a}_n^\dagger - \hat{a}_n \right)$$

- They satisfy the canonical commutation relations, $\left[\hat{a}_n, \hat{a}_m^\dagger \right] = \delta_{nm}$

Quantum oscillator chain in terms of creation/annihilation operators



- Hamiltonian

$$\hat{H} = \frac{\hbar\omega}{4}\sum_n \left[-\left(\hat{a}_n^\dagger - \hat{a}_n\right)^2 + \left(\hat{a}_n^\dagger + \hat{a}_n - \hat{a}_{n+1}^\dagger - \hat{a}_{n+1}\right)^2 \right]$$

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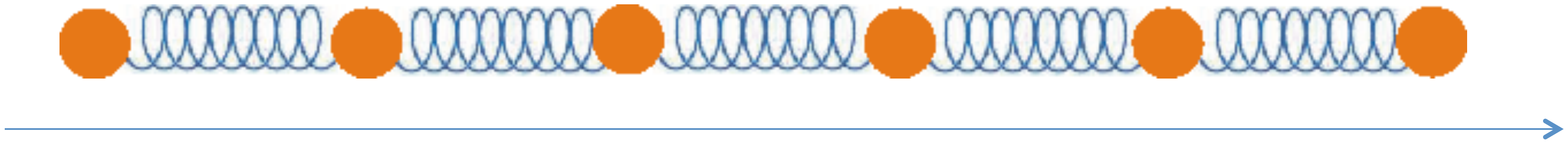

- Hamiltonian

$$\hat{H} = \frac{\hbar\omega}{4}\sum_n \left[-\left(\hat{a}_n^\dagger - \hat{a}_n\right)^2 + \left(\hat{a}_n^\dagger + \hat{a}_n - \hat{a}_{n+1}^\dagger - \hat{a}_{n+1}\right)^2\right]$$

$$= \frac{\hbar\omega}{4}\sum_n \left[\hat{a}_n^\dagger \hat{a}_n - \hat{a}_n^2 + \left(\hat{a}_n - \hat{a}_{n+1}\right)^2 + \left(\hat{a}_n - \hat{a}_{n+1}\right)\left(\hat{a}_n^\dagger - \hat{a}_{n+1}^\dagger\right) + \text{H.c.}\right]$$

Creation/annihilation operators in the q-space

- Lets Fourier-transform the operators:

$$\hat{a}_n = \underbrace{\int_{-\pi}^{\pi} \frac{dq}{2\pi}}_{\int_q} \hat{a}_q e^{iqn} \text{ and } \hat{a}_n^\dagger = \int_q \hat{a}_q^\dagger e^{-iqn}$$

- Important identities: $\sum_n e^{iqn} = 2\pi\delta(q)$ and $\int_q e^{iqn} = \delta_{n,0}$

Hamiltonian in the q-space

$$\hat{H} = \int_q \left[A(q)\hat{a}^\dagger\hat{a} + B(q)\hat{a}_q\hat{a}_{-q} + \text{H.c.} \right]$$

- The coefficients:

$$A(q) = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{2}(1 - \cos q)$$

$$B(q) = -\frac{\hbar\omega}{4} + \frac{\hbar\omega}{2}(1 - \cos q)$$