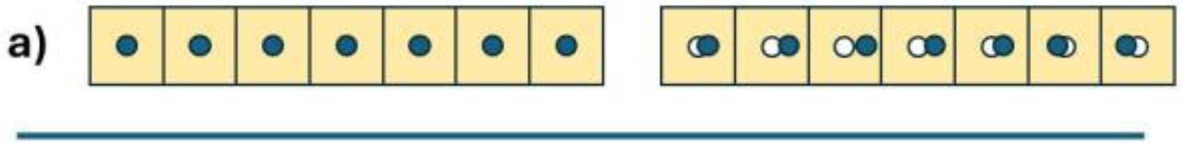
One-dimensional atomic chain



Hamiltonian

$$H = \frac{1}{2}\sum_q [\frac{1}{M}\Pi_q \Pi_q^\star + 2k(1-\cos q)\xi_q \xi_q^\star]$$

Eigenstates

$$|n_q\rangle \equiv |n_{q+2n\pi}\rangle$$

A one-dimensional phonon in real space with wave-vector q and frequency ω.

$$\langle x|\, n_q\rangle = e^{-i(qx-\omega t)}$$

What happens to the phase of the atomic wavefunction?

Recall equation 15 in the paper: $\exp\left\{[+i[\vec{k} - \frac{e}{2\hbar}(\vec{B} \times \sum_{l} \vec{r_l})] \cdot \vec{R_S}]\right\}$

$$\langle x | n_q \rangle = e^{-i[qx - \omega t + \varphi(x)]} \qquad \varphi(x) = \frac{x\,\delta u}{\ell_B^2}$$

δu is the distance between the nuclear and the electronic center of masses.

Berry connection in real space: $$i\langle n_q | \nabla n_q \rangle = \frac{\delta u}{\ell_B^2}$$

The Berry phase obtained by the integration of the Berry connection over a period

Berry connection $$A = \frac{\delta u}{\ell_B^2}$$

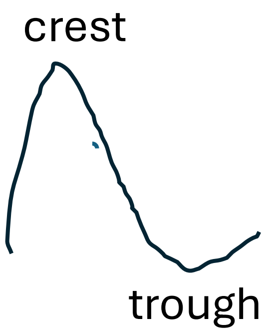
Berry phase $$\delta\phi_B = \lambda_{ph}\left\langle \frac{\delta u}{\ell_B^2} \right\rangle$$ Vanishes if δu averages to zero over a period.

This is what happens in a harmonic crystal.

In an anharmonic crystal

$$\langle \delta u \rangle = q_e \delta u_m$$

The average mismatch between the two center-of-masses is a fraction of the crest atomic displacement, δu_m.



The dimensionless q_e is the relative difference between atomic displacements at the crest and the trough.

$$q_e = (\delta u_{crest} - \delta u_{trough})/\delta u_{average}$$

Equation 16 in the paper:

$$\delta \phi_B \approx q_e \frac{\lambda_{ph} \delta u_m}{\ell_B^2}$$