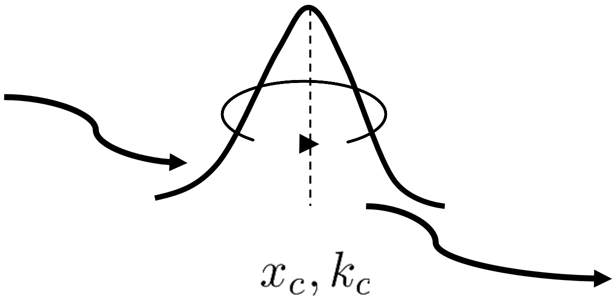
Lecture 7
Electrons in deformed crystals

- Semiclassical dynamics in perfect crystals
- Description of crystal deformation
- Geodynamics in deformed crystals
- Electromagnetic and mechanical properties
- Summary and outlook

Semiclassical dynamics in a perfect crystal

- Equations of motion

$$\dot{x}_c = \partial_{k_c}\varepsilon - \dot{k}_c \times \Omega$$
$$\dot{k}_c = -eE - e\dot{x}_c \times B$$



MC Chang, Phys. Rev. B，1999

- Berry curvature

$$\Omega_{mn} = i[\langle \partial_{k_m} u | \partial_{k_n} u\rangle - \langle \partial_{k_n} u | \partial_{k_m} u\rangle]$$

Under general perturbations slow in space and time

G. Sundaram and Q. Niu,
Phys. Rev. B, 1999

Equations of motion

$$\dot{x}_c = \partial_{k_c}\varepsilon - \Omega_{k_c k_c}\dot{k}_c - \Omega_{k_c x_c}\dot{x}_c - \Omega_{k_c t},$$
$$\dot{k}_c = -\partial_{x_c}\varepsilon + \Omega_{x_c x_c}\dot{x}_c + \Omega_{x_c k_c}\dot{k}_c + \Omega_{x_c t}.$$

Berry connections and Berry curvatures

$$A_{\xi_i} = i\langle u|\partial_{\xi_i} u\rangle \qquad \Omega_{\xi_i \xi_j} = \partial_{\xi_i} A_{\xi_j} - \partial_{\xi_j} A_{\xi_i}$$

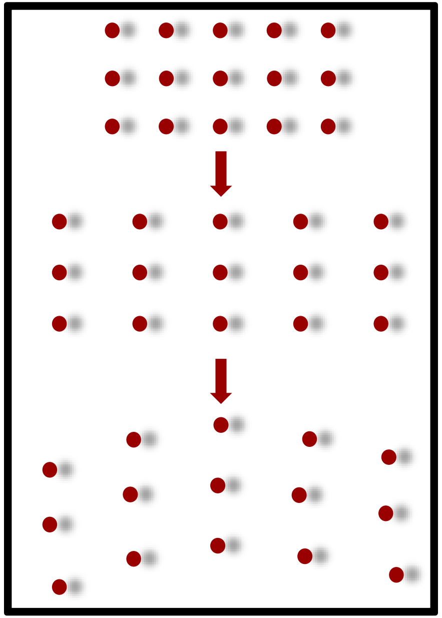
Crystal under deformation

Strain effect:

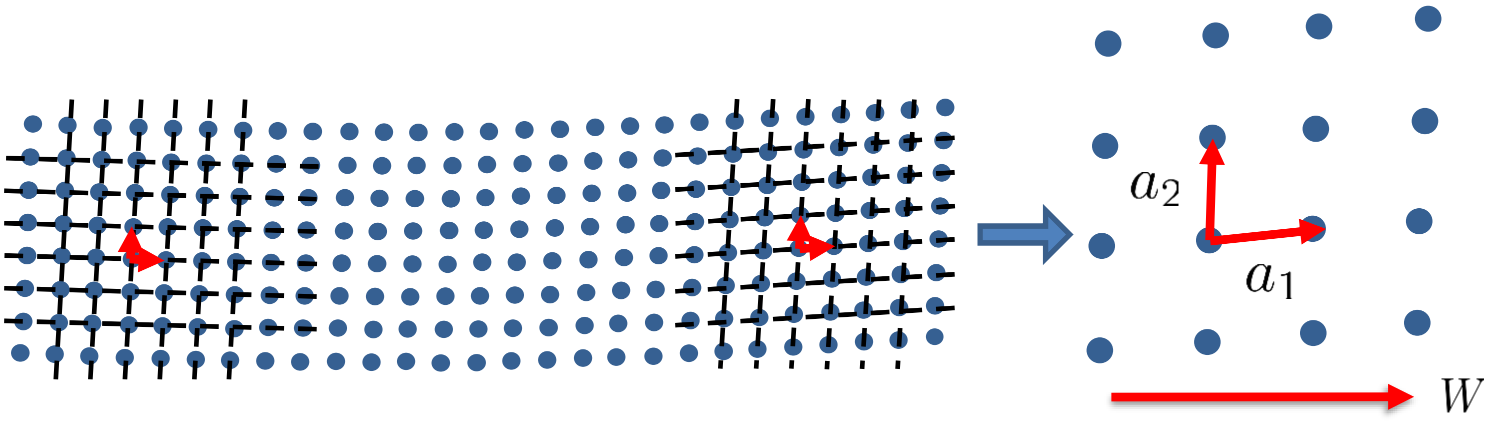
- Deformation potential, piezoelectricity, magnetostriction
- Still a periodic and static problem
  (not the focus of this work)

Strain gradient, strain rate, lattice rotation and acceleration

- The goal of this work:
  a systematic theory valid in first order of these quantities
- Anticipated applications: flexoelectricity, viscosity …….



Lattice bundle picture



Locally, the crystal still looks periodic, but lattice periodicity varies in time and from one neighborhood to next.

$$\{a_\alpha(x,t), W(x,t)\}, \alpha = 1,2,3$$

Connection on a lattice bundle

How to describe the change of local lattices?

lattice connection Γ :

$$\partial_\mu a^i_\alpha = \Gamma^i_{j\mu} a^j_\alpha$$

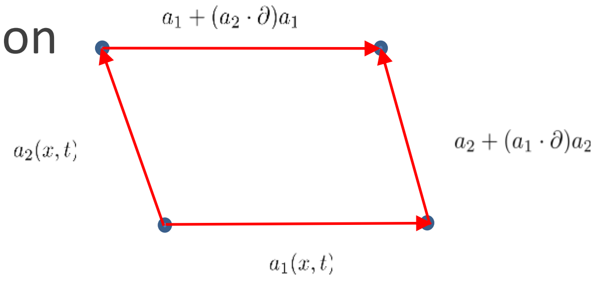
Physical meaning of Γ :

antisymmetric part $\Gamma^i_{j\mu} - \Gamma^j_{i\mu}$: rotation rate and gradient

symmetrical part $\Gamma^i_{j\mu} + \Gamma^j_{i\mu}$: strain rate and gradient

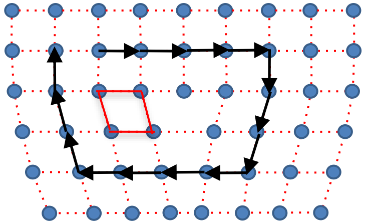
Elastic condition and topological defects

- Elastic condition



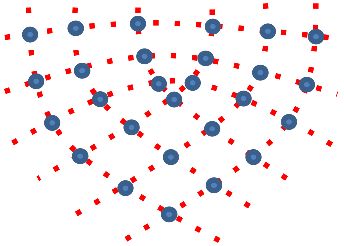
$$\Gamma^k_{ij} - \Gamma^k_{ji} = 0,$$
$$\Gamma^k_{i0} + \Gamma^k_{ji} W^j = \partial_i W^k.$$

- Dislocation:



$$\delta x^i = a^i_\alpha \delta l^\alpha \quad \Rightarrow \quad \oint_C b^\alpha_i(x) dx^i = Z^\alpha$$

- Disclination:



$$\partial_{x^\mu} a^i_\alpha = \Gamma^i_{j\mu} a^j_\alpha \quad \Rightarrow \quad a'_\alpha = \mathcal{T} exp(\oint dx^i \Gamma_i) a_\alpha$$

Phase space geometry

- ❑ Geometric change:

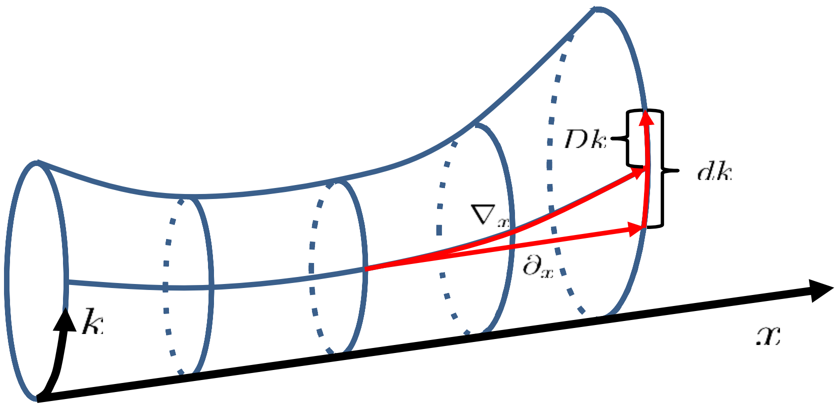
$$\delta k_i = -k_j \Gamma^j_{i\mu} dx^\mu$$

- Dynamical change:

$$Dk_i = dk_i + k_j \Gamma^j_{i\mu} dx^\mu$$

- ❑ Lattice Covariant Derivative

$$\nabla_{x^\mu} = (\partial_{x^\mu} - k_l \Gamma^l_{j\mu} \partial_{k_j})$$



phase space

- ❑ Energy differential

deformation potential

group velocity

$$d\varepsilon = [dx^\mu \nabla_{x^\mu} + Dk_i \partial_{k_i}]\varepsilon = dx^\mu \Gamma^m_n D_{mn} + Dk_i \frac{\partial \varepsilon}{\partial k_i}$$

Semiclassical dynamics without Berry curvatures

Equations of motion relative to the local lattice:

$$D_t x = \partial_k \varepsilon,$$

$D_t x = \dot{x} - W$ is the velocity relative to lattice

$$D_t k = -\nabla_x \varepsilon + m_e D_t x \times 2\omega - m_e a.$$

$D_t k_i \equiv (\dot{k}_i + \Gamma^n_{it} k_n + \dot{x}^j \Gamma^n_{ij} k_n)$

dynamical change

$\nabla_{x^\mu} \varepsilon = D^n_m \Gamma^m_{n\mu}$

deformation force

$2\omega = \partial \times W$

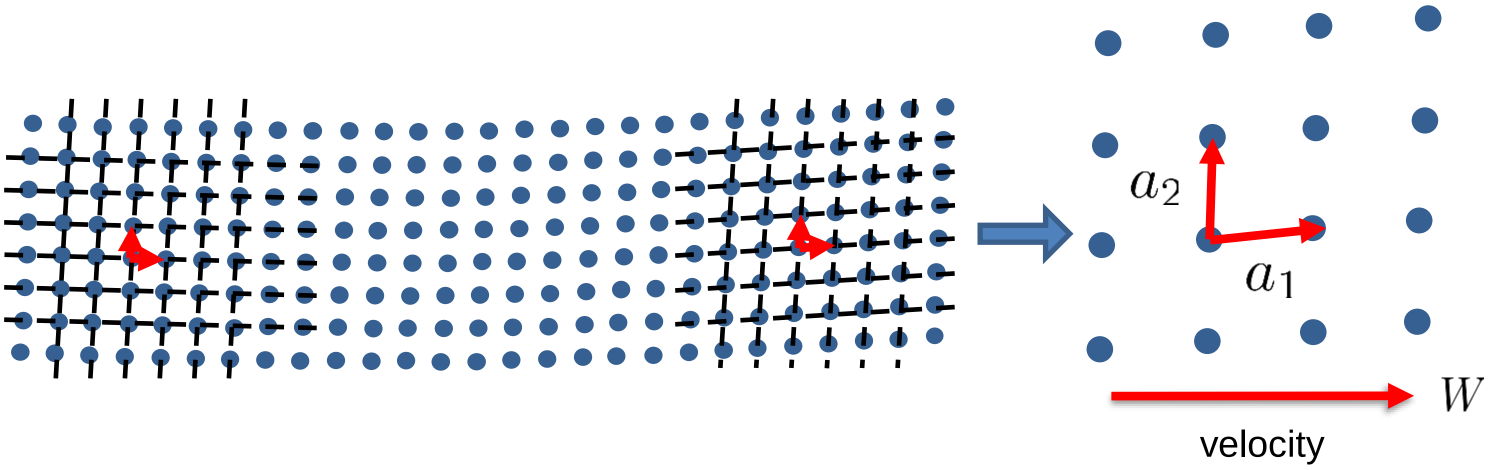
Vorticity

$a = \partial_t W + W \cdot \partial_x W$

lattice acceleration

Deformation effect is completely reflected in the lattice connection

A bundle of periodic Hamiltonians



Wave packet is constructed from local Bloch functions at each (x,t):

$$\hat{H}(k;x,t)u = \varepsilon(k;x,t)u$$

$$\hat{H}(k;x,t) = \frac{1}{2m_e}\left(\frac{1}{i}\frac{\partial}{\partial r} + k\right)^2 + V(\{l^\alpha a_\alpha(x,t) - r\})$$

Combine lattice connection with Berry connection

Lattice covariant Berry connection:

$$A_{x^\mu}(k,x,t) \equiv i\langle u(k;x,t)|\nabla_{x^\mu} u(k;x,t)\rangle,$$
$$A_k(k,x,t) \equiv i\langle u(k;x,t)|\partial_k u(k;x,t)\rangle.$$

Lattice covariant derivative of Bloch functions:

$$\nabla_{x^\mu} u(r,k;x,t) \equiv \partial_{x^\mu} u - \Gamma^n_{m\mu} k_n \frac{\partial u}{\partial k_m} + \Gamma^m_{n\mu} r^n \frac{\partial u}{\partial r^m}$$

Lattice covariant Berry curvatures:

$$\Omega_{k_i k_j} \equiv i[\langle \partial_{k_i} u|\partial_{k_j} u\rangle - \langle \partial_{k_j} u|\partial_{k_i} u\rangle],$$
$$\Omega_{k_i x^\mu} \equiv i[\langle \partial_{k_i} u|\nabla_{x^\mu} u\rangle - \langle \nabla_{x^\mu} u|\partial_{k_i} u\rangle].$$

Semiclassical dynamics with Berry curvatures

$$D_t x = \partial_k \varepsilon_{tot} - D_t k \times \Omega - \Omega_{kT},$$
$$D_t k = -\nabla_x \varepsilon_{tot} + m_e D_t x \times 2\omega - m_e a.$$

- $\varepsilon_{tot} = \varepsilon + 2\omega \cdot j + \Gamma^m_{nl} F^{nl}_m$

angular momentum of wave packet

flexopotential energy

- $\Omega_{kT} = \Omega_{kx} \cdot \dot{x} + \Omega_{kt}$

Applications

Insulator with filled bands of electrons

Electromagnetic property:

Adiabatic current, polarization induced by strain gradient (flexoelectricity), magnetization induced by strain rate.

Mechanical property: Stress tensor

deformation potential, gyroelasticity, piezoelectricity, and Hall viscosity.

Polarization and magnetization in deformed crystals

Adiabatic current See Xiao et al, PRL (2009) and lecture 3

$$j^i_{cs} = -e\int [\Omega_{k_ik_j}\Omega_{x_jt} + \Omega_{k_jx_j}\Omega_{k_it} + \Omega_{x_jk_i}\Omega_{k_jt}]$$

	magnetoelectricity	Flexso-electromagnetism
polarization	$P = \frac{1}{2}\theta B$	$P^i_{cs} = e\Gamma^n_{mj}\mu^{mij}_n$
magnetization	$M = -\frac{1}{2}\theta E$	$M^{ij}_{cs} = -e\partial_m W^n \mu^{mij}_n + (P^i_{cs}W^j - P^j_{cs}W^i)$
coefficient	$\theta = \int A_k \cdot \Omega$	$\mu^{mij}_n = \int A_{k_i}\nabla^m_n A_{k_j} + A_{k_j}\partial_{k_i}A^m_n + A^m_n\partial_{k_j}A_{k_i}$

Stress tensor to first order in time derivative

Variation of electron action with respect to lattice strain:

$$T_i^j = -\, a_\alpha^j \frac{\delta S}{\delta a_\alpha^i}$$

$$J = \frac{1}{2} m_e \,\mathrm{Im}\langle \partial_k u \mid \times(\varepsilon + \hat{H}) \mid \partial_k u \rangle$$

angular momentum

mass polarization

$$P_{m_e} = m_e \int dk A_k$$

Hall viscosity

$$\eta_{jn}^{im} = \int dk \Omega_{jn}^{im}$$

$$T_j^i = \int dk D_{ij} + 2\omega \cdot \nabla_j^i J + \nabla_j^i P \cdot a - \frac{1}{2}(\partial_l W^m + \partial_m W^l)\eta_{jm}^{il}$$

deformation potential

rotation rate

lattice acceleration

strain rate

Summary

Lattice covariant formulation of electrons in deforming crystals

Semi-classical equations of motion accurate to first order in strain rate, strain gradient, lattice acceleration and rotation

Polarization induced by strain gradient (flexoelectricity) and orbital magnetization induced by strain rate

Stress-energy tensor and its responses

Outlook

Lattice covariant electron transport

Lattice covariant phonon dynamics