PARTICLE VIEW IN CRYSTALS

Qian Niu

University of Science and Technology of China

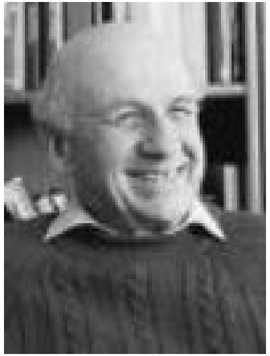
Outline

- Introduction
- Electron dynamics in crystals
- Crystal deformation and general covariance
- Summary

Condensed matter physics 101

- Structure and ordering
- Electronic bands
- Collective excitations
- Equilibrium and transport responses

- The role of theory in this field:
  - To develop useful models for experimental systems
  - To reveal mechanisms for observed phenomena
  - To develop accurate methods to predict properties
  - To establish a systematic world view of condensed matter



Walter Kohn, Nobel prize (1999)

力学

$$\vec{F} = m\vec{a}$$

$$F = -\frac{Gm_1m_2}{r^2}$$

$$\delta\int_{t_a}^{t_b}\mathcal{L}(\vec{q},\dot{\vec{q}},t)\,\mathrm{dt} = 0$$

$$\dot{\vec{q}} = \frac{\partial H}{\partial\vec{p}}$$

$$\dot{\vec{p}} = -\frac{\partial H}{\partial\vec{q}}$$

电动

$$\nabla\cdot\vec{E} = \frac{\rho}{\epsilon}$$

$$\nabla\cdot\vec{B} = 0$$

$$\nabla\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$

$$\nabla\times\vec{B} = \mu\vec{J} + \epsilon\mu\frac{\partial\vec{B}}{\partial t}$$

$$\vec{F} = q\vec{E} + \mathrm{q}\vec{v}\times\vec{B}$$

量子

$$E = \hbar\omega$$

$$\vec{p} = \hbar\vec{k}$$

$$i\hbar\frac{\partial}{\partial t}\psi = \widehat{H}\,\psi$$

$$\rho(\vec{r},t) = |\psi(\vec{r},t)|^2$$

$$[\hat{x},\hat{p}] = i\hbar$$

热统

$$\mathrm{d}U = \delta Q + \delta W$$

$$\oint\frac{\delta Q}{T} \geq 0$$

$$S = k_B\ln\Omega$$

$$Z = \sum e^{-\beta H}$$

$$f = \frac{1}{e^{\beta(\varepsilon-\mu)} \pm 1}$$

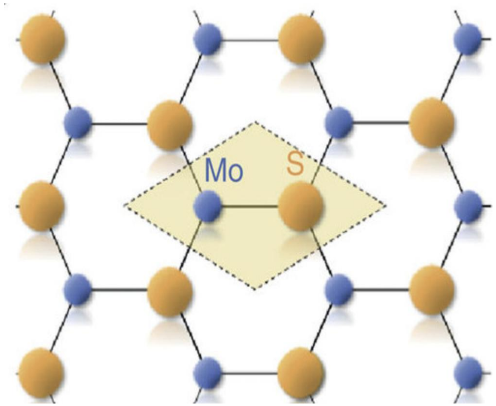
Newtonian Dynamics (1687)

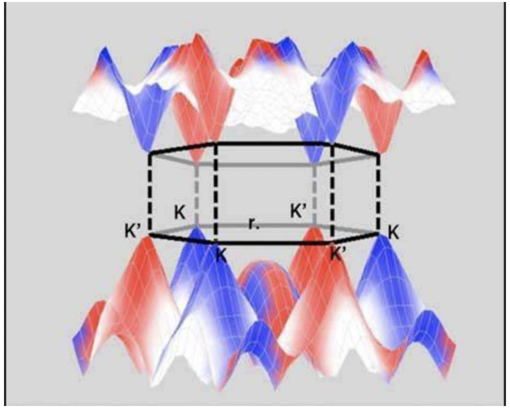
- Absolute space and time: continuous and flat
  - Gravity is just another force
  - Einstein (1916): gravity reflects space-time deformation
- Canonical phase space (1834)
  - Hamilton’s equations and Liouville’s theorem
  - Basis for statistical and quantum mechanics

$$\dot{\vec{q}} = \frac{\partial H}{\partial \vec{p}} \qquad \dot{\vec{p}} = -\frac{\partial H}{\partial \vec{q}}$$

Electronic properties in a crystal

- Classical particle view fails at the atomic scale
- Need to solve for the quantum wave functions and energies
- Obtain macroscopic response properties from such knowledge





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  - Bloch dynamics
  - Berry curvature effects
- Crystal deformation and general covariance
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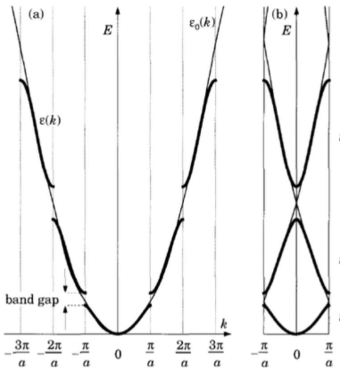
Bloch dynamics (1928)

- Real space becomes homogeneous beyond atomic scales: meta space
- Momentum space becomes a finite torus for each band



  - Band energy is periodic in k

$$\varepsilon(k+2\pi/a)=\varepsilon(k)$$

  - Particle dynamics in a band

$$\dot{x} = \partial_k \varepsilon,$$
$$\dot{k} = -eE - e\dot{x} \times B$$

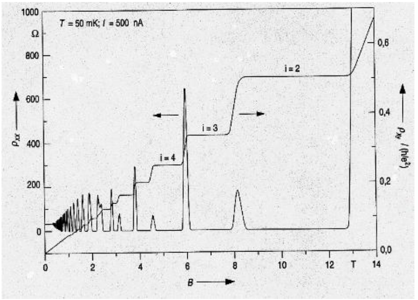
- Can be made canonical and quantized by the Peierles substitution (1933)

$k \to k + eA, \ \varepsilon \to \varepsilon - e\phi$

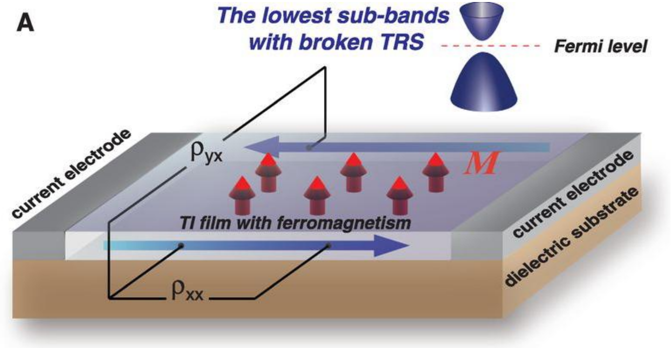
- Provide a basic theory for metals, semiconductors, and insulators (Luttinger &Kohn 1955).

Topological phases of matter

- Quantum Hall effects

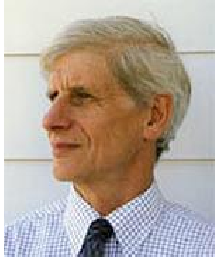


von Klitzing 1980



Q.K. Xue 2013

- Topological insulators and superconductors

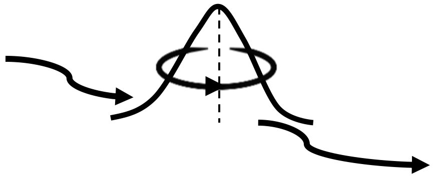


David Thouless
2016 Nobel prize

Berry curvature effect on Bloch dynamics

- Wave packet center motion

$$\dot{x} = \partial_k \varepsilon - \dot{k} \times \Omega,$$
$$\dot{k} = -eE - e\dot{x} \times B$$



MC Chang and Q. Niu, Phys. Rev. B，1996

- Berry curvature

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

1) Quantum Hall Effect
2) Anomalous Hall Effect

$$j = -eE \times \int dk \Omega$$

Under general slow perturbations

$$\dot{x} = \partial_k \varepsilon - \Omega_{kk}\dot{k} - \Omega_{kx}\dot{x} - \Omega_{kt},$$
$$\dot{k} = -\partial_x \varepsilon + \Omega_{xk}\dot{k} + \Omega_{xx}\dot{x} + \Omega_{xt}$$

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

Berry connection and curvatures in phase space

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

Electromagnetic and artificial gauge fields,

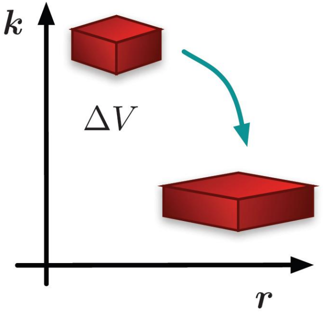
Adiabatic Thouless pumping and electric polarization,

Berry curvatures in kx planes: spin-orbit coupling, etc.

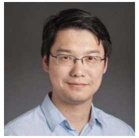
Non-canonical Hamiltonian dynamics: breakdown of Liouville theorem

Modified density of states and quantization rules

Evolution of Phase-Space Volume



Phase-space volume $\Delta V = \Delta \boldsymbol{r} \Delta \boldsymbol{k}$



Conservation of phase-space volume

$$\frac{1}{\Delta V}\frac{d\Delta V}{dt} = \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \dot{\boldsymbol{r}} + \boldsymbol{\nabla}_{\boldsymbol{k}} \cdot \dot{\boldsymbol{k}} = 0$$

With Berry curvatures

$$\frac{1}{\Delta V}\frac{d\Delta V}{dt} \neq 0$$

Liouville theorem breaks down! (unless the volume is redefined)

$$\Delta V = \frac{\text{const.}}{\sqrt{\det|\overleftrightarrow{\boldsymbol{\Omega}} - \overleftrightarrow{\mathbf{J}}|}}$$

$$\overleftrightarrow{\Omega} = \begin{pmatrix} \overleftrightarrow{\Omega}^{rr} & \overleftrightarrow{\Omega}^{rk} \\ \overleftrightarrow{\Omega}^{kr} & \overleftrightarrow{\Omega}^{kk} \end{pmatrix} \quad \overleftrightarrow{\mathbf{J}} = \begin{pmatrix} 0 & \overleftrightarrow{\mathrm{I}} \\ -\overleftrightarrow{\mathrm{I}} & 0 \end{pmatrix}$$

Modified Density of States

Density of states $D = \frac{1}{(2\pi)^d}$ → $D = \frac{1}{(2\pi)^d}\sqrt{\det|\overleftrightarrow{\mathbf{\Omega}} - \overleftrightarrow{\mathbf{J}}|}$

Special cases

$D = (2\pi)^{-d}\det(\overleftrightarrow{\mathrm{I}} - \overleftrightarrow{\Omega}^{rk})$ if $\boldsymbol{B} = 0, \overleftrightarrow{\mathbf{\Omega}}^{\boldsymbol{rk}} \neq 0$

$D = (2\pi)^{-d}(1 + \frac{e}{\hbar}\mathbf{\Omega}_{\boldsymbol{k}} \cdot \boldsymbol{B})$ if $\boldsymbol{B} \neq 0, \overleftrightarrow{\mathbf{\Omega}}^{\boldsymbol{rk}} = 0$

Physical quantity

$$\langle \mathcal{O} \rangle = \int d\boldsymbol{r} d\boldsymbol{k}\, D(\boldsymbol{r},\boldsymbol{k})\mathcal{O}(\boldsymbol{r},\boldsymbol{k})f(\boldsymbol{r},\boldsymbol{k})$$

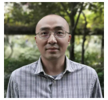
$f(\boldsymbol{r},\boldsymbol{k})$ - Distribution function

Xiao, Shi & Niu, PRL (2005)

Further Extensions

(Culcer 2005, Zhang 2006, Gao 2014, Dong 2018, Wang 2021, Gao 2021)

- Nonabelian: spin transport 

- Nonlinear: higher order in fields  

- Other particles: photons, quasiparticles,…

- Spatial deformation: strain gradients and rates

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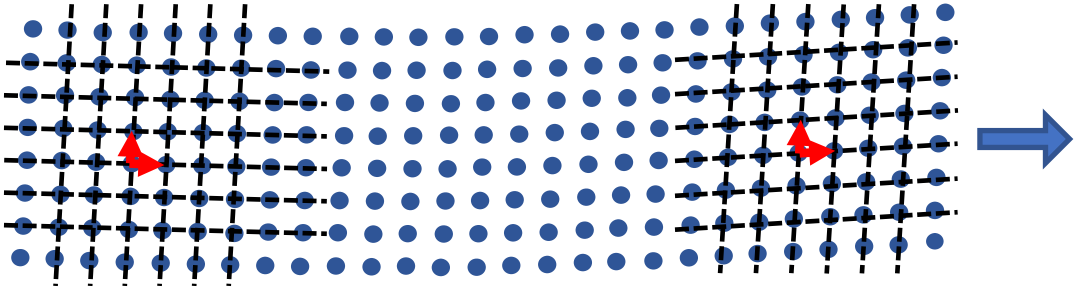
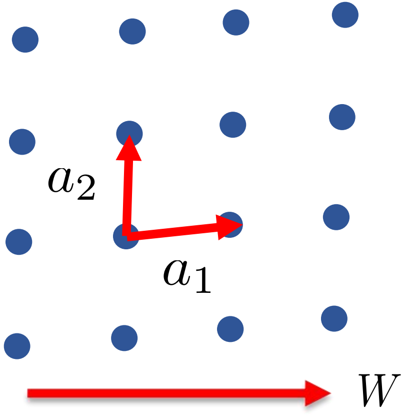
- Crystal deformation and general covariance
  - lattice bundle geometry and Berry curvatures
  - General relativity in the meta spacetime
- Summary

Crystal under deformation

L. Dong and Q. Niu, PRB 98,115162 2018





The crystal looks periodic locally,

a's and W change slowly in space and time

Connection on the lattice bundle

To count inhomogeneity and time dependence in local lattices

lattice connection:

$$\Gamma^i_{j\mu} = \frac{1}{2\pi} b^\alpha_j \partial_\mu a^i_\alpha$$

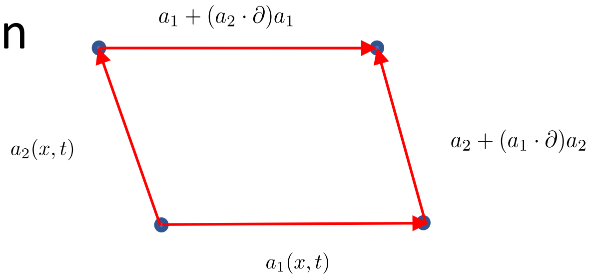
a_α local lattice vectors
b_α their reciprocals

Physical meaning of Γ:

1) strain rate: symmetric part in {i $\leftrightarrow$ j}
2) rotation rate： antisymmetric part in {i $\leftrightarrow$ j}

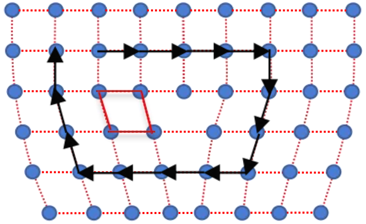
Elastic condition and topological defects

- Elastic condition



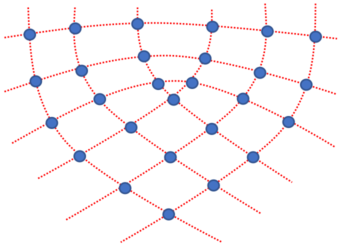
$$\Gamma^k_{ij} - \Gamma^k_{ji} = 0, \quad \Gamma^k_{i0} + \Gamma^k_{ji} W^j = \partial_i W^k.$$

- Dislocation:



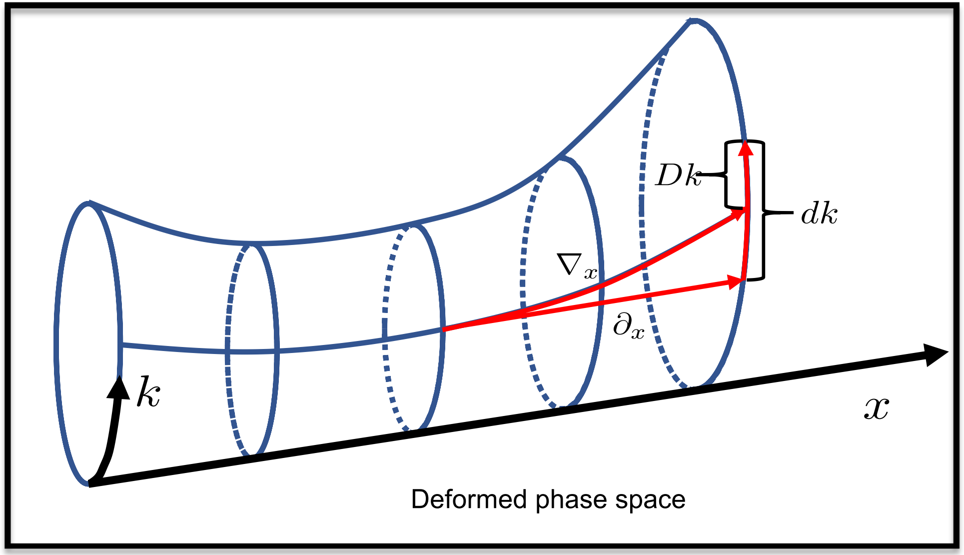
$$\delta x^i = a^i_\alpha \delta l^\alpha \quad \Rightarrow \quad \oint_C b^\alpha_i(x) dx^i = Z^\alpha$$

- 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

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

Energy differential

deformation potential

group velocity

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

Geodynamics in deformed crystal

Equations of motion

velocity relative to ions:

Lattice covariant Berry curvatures:

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

dynamical change rate

deformation potential force

Coriolis force

Inertial force

Flexso- electricity and magnetism

Chern-Simons polarization/magnetization

$$j^i_{cs} = -e \int [\Omega_{k_i k_j}\Omega_{x_j t} + \Omega_{k_j x_j}\Omega_{k_i t} + \Omega_{x_j k_i}\Omega_{k_j t}]$$

Xiao et al, PRL (2009)

	magnetoelectrical	electromechanical
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	$\theta = \int A_k \cdot \Omega$	$\mu^{mij}_n = \int A_{k_i}\nabla^m_n A_{k_j} + A_{k_j}\partial_{k_i}A^m_n + A^m_n\partial_{k_j}A_{k_i}$

Implication on lattice dynamics

Stress tensor for a band insulator: $$T_i^j = -\, a_\alpha^j \frac{\delta S}{\delta a_\alpha^i}$$

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

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

Lattice rotation

lattice acceleration

strain rate

Deformation of a spacetime crystal: general relativity in meta spacetime

Lattice 4-vectors and lattice 4-connection

$\{\boldsymbol{a}_\alpha\}$ with $\alpha = 0, 1, 2, 3$

$$\Gamma^{\xi}_{\nu\mu} = \frac{1}{2\pi} b^{\alpha}_{\nu} \partial_\mu a^{\xi}_{\alpha}$$

Equations of motion

$$\dot{x}^\mu = \frac{\partial \lambda}{\partial k_\mu} - \Omega_{k_\mu T},$$

$$D_\tau k_\mu = -\nabla_{x^\mu} \lambda + \Omega_{x^\mu T}.$$

where $D_\tau k_\mu \equiv \dot{k}_\mu + \Gamma^{\alpha}_{\nu\mu} k_\alpha \dot{x}^\mu$

Geodesic equation

Anzhuoer Li

Free fall:

$$\nabla_{x_c^\mu} \lambda(k_c, x_c) = 0$$

Geodesic:

$$\ddot{x}^\rho + (\nabla_{x^\sigma} \Omega_{k_\rho x^\nu} - \Gamma^\rho_{\nu\sigma}) \dot{x}^\sigma \dot{x}^\nu = (\Omega_{x^l x^\alpha} \partial_{k_\alpha} \partial_{k_\rho} \lambda + \Omega_{k_\rho k_\nu} \nabla_{x^l} \nabla_{x^\nu} \lambda) \dot{x}^l$$

Berry curvature effects:

Lorentz forces

Spacetime connection

Summary

- Electron dynamics in crystals
  - from Newtonian to Bloch dynamics
  - Berry curvature effects
- Crystal deformation and general relativity
  - Lattice connection and Berry curvatures
  - General relativity in meta spacetime

Take home message

Our world view of solid state has been greatly shaped by quantum mechanics:

- Classical particle view fails on the atomic scale
- Energy momentum structure is modified into Bloch bands in crystals
- Particle view re-emerges beyond atomic scales
- Berry curvature effects further modifies the dynamics with dramatic effects

- Spacetime crystals open up an new scope

Example: atomic chain with a sound wave

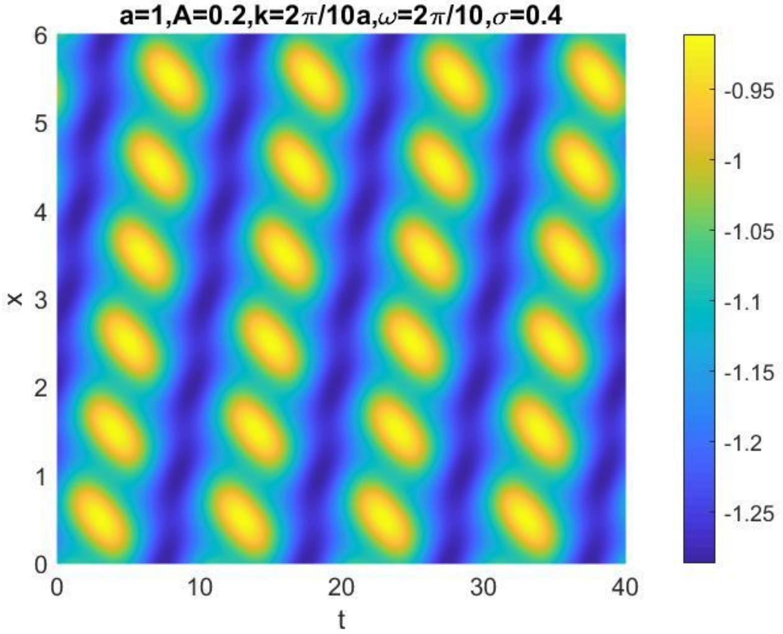
Atomic positions in a sound wave

$$x_l(t) = la - A\cos(kla - \omega t)$$

Potential energy for electron

$$V(x,t) = \sum_{l=-\infty}^{+\infty} f(x - x_l(t))$$

Where: $f(x) = -e^{-\frac{x^2}{\sigma}}$

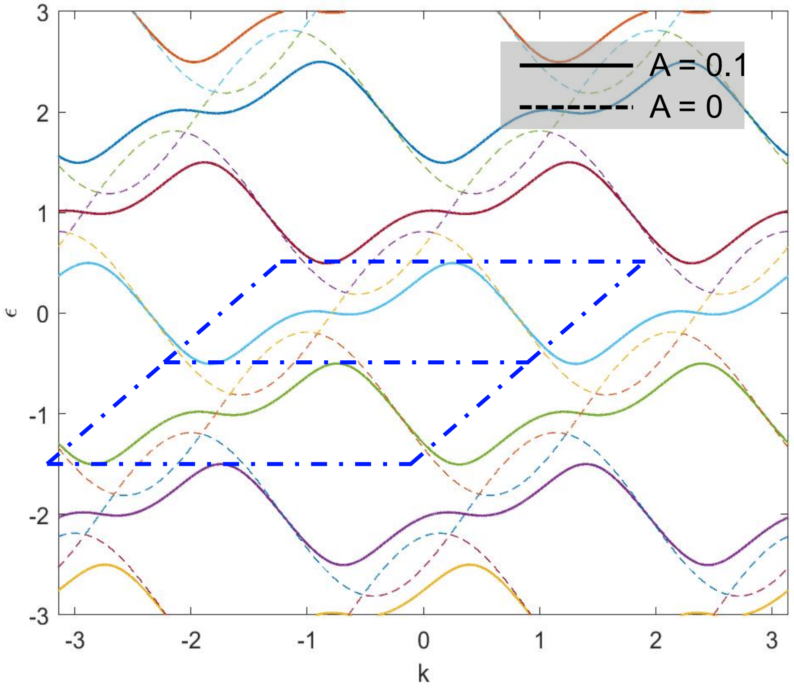


spacetime crystal → meta spacetime

Floquet Bloch bands — semiclassical dynamics

Qiang Gao and QN

PHYSICAL REVIEW LETTERS **127,** 036401 (2021)



Band crossing and change of topology

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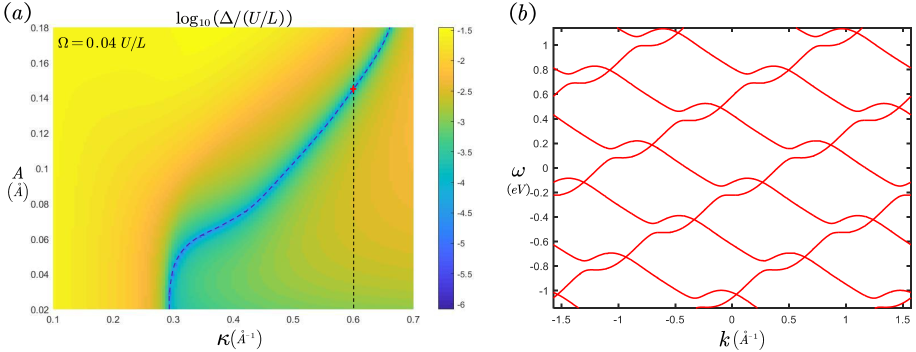

FIG. S1: (a) The color map of the logarithm of the bandgap Δ ($\log_{10}\Delta/(U/L)$) as a function of the oscillating amplitude A and the phonon wavelength κ, where we have fixed the phonon frequency to be $\Omega = 0.04U/L$. The blue dashed line emphasizes the parameters which give gapless band structures. $U/L = 7.62$eV. (b) The band structure corresponding to the parameters labeled by the red star in panel (a), which is gapless.

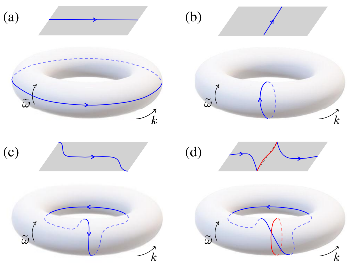

FIG. 2. The topology of band dispersions (blue curves) as seen in the Brillouin zone and on the torus after shearing it and wrapping around along the reciprocal lattice vectors: $\tilde{\boldsymbol{\omega}} = (\kappa, \Omega)$ and $\boldsymbol{k} = (G, 0)$. (a) Corresponds to the class shown in Fig. 1. (b) Is a class that has yet to be seen and is only possible in oblique spacetime crystals [25]. (c) Corresponds to typical edge states of topological Floquet insulator in a higher dimension [3]. (d) Shows to a unique gapless band structure that combines the topologies in both (b),(c).

Intraband Zener tunneling