Lecture 3
Pumping and Polarization

- Thouless adiabatic pumping
- Polarization as Zak's Berry phase
- Semiclassical theory
- Polarization due to inhomogeneity
- Phonon induced magnetization

Pumping in Insulating States

- Thouless (1983)
  - Ideal: filled bands in 1D periodic potential
  - Pumped charge in a cycle is a Chern number

$$C = \frac{i}{2\pi} \sum_{\lambda} f_{\lambda} \int_0^T dt \int_0^{2\pi/L} dk \Big[\Big\langle \frac{\partial \psi_{\lambda k}}{\partial t} \Big| \frac{\partial \psi_{\lambda k}}{\partial k} \Big\rangle - \Big\langle \frac{\partial \psi_{\lambda k}}{\partial k} \Big| \frac{\partial \psi_{\lambda k}}{\partial t} \Big\rangle \Big]$$

- Niu & Thouless (1984)

– General: disorder and many-body interaction.

– Quantization is as robust as the quantum Hall effect

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Towards a Quantum Pump of Electric Charges

Q. Niu

- **Gating a quantum wire**
- **Surface acoustic wave**

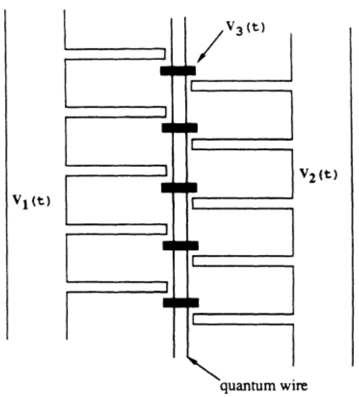
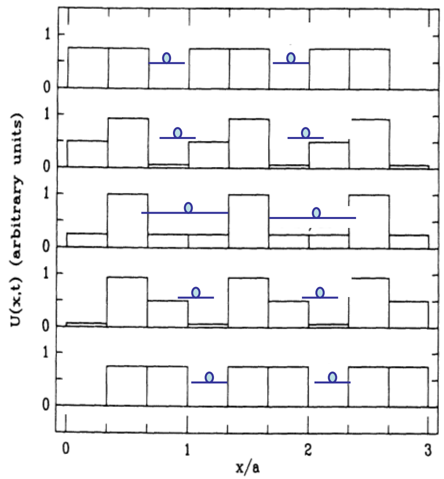
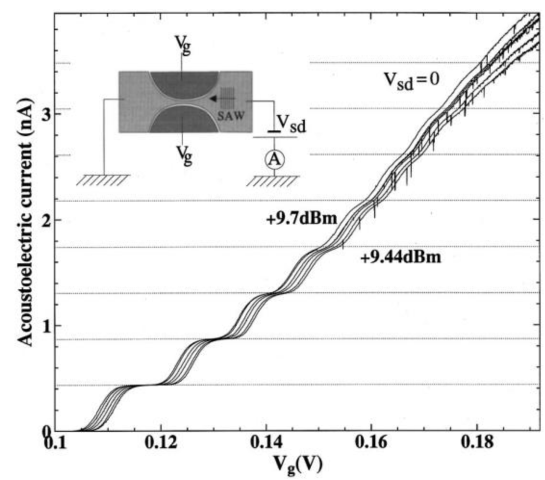


FIG. 2. The quantum wire and the voltage leads.





Patent: Quantum Wire CCD Charge Pump, Q. Niu and K. Ensslin, US paten No. 5,144,580. Sept. 1, 1992.

- **20 ppm achieved by**

J. Cunningham et al, PRB (1999)

Electric polarization

- A basic materials property of dielectrics
  - To keep track of bound charges
  - Order parameter of ferroelectricity
  - Characterization of piezoelectric effects, etc.
- Traditionally defined as density of electric dipoles, but
  - Problematic when such dipoles cannot be identified, e.g. covalant electrons
  - In a crystal, dipole moment of a unit cell depends on the choice of the cell.

Polarization: Modern Definition

To keep track of movement of bound charges in a slow process λ(t):

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{j} = 0$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{P} = -\rho$$

$$j = \partial_t P + \nabla \times M$$

$$\Rightarrow \quad \boldsymbol{P} = \int_0^T dt\, \boldsymbol{j}(\lambda, \dot{\lambda})$$

j is the transient current density during a process (characterized by change in the control parameters λ).

Experimentally, only the change in polarization is ever measured. So, polarization is defined only relative to a reference state (the initial state).

Polarization as a Berry Phase

- Thouless (1983):

$$Q = -e\int_0^T dt \int_0^{2\pi/a} \frac{dk}{2\pi} i\left[\left\langle \frac{\partial u}{\partial t}\middle|\frac{\partial u}{\partial k}\right\rangle - \left\langle \frac{\partial u}{\partial k}\middle|\frac{\partial u}{\partial t}\right\rangle\right]$$

- King-Smith and Vanderbilt (1993): Zak's Berry phase

$$\boldsymbol{P} = e\int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} i\left\langle u(\boldsymbol{k})\middle|\frac{\partial u(\boldsymbol{k})}{\partial \boldsymbol{k}}\right\rangle\Bigg|_{\mathrm{intial}}^{\mathrm{final}}$$

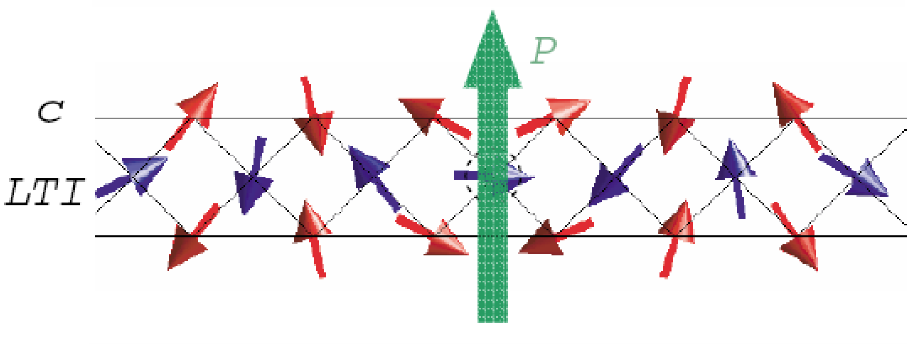
Under periodic gauge of Bloch function

- Led to great success in first principles calculations

Polarization in Inhomogeneous Systems?

- **A multiferroic problem:** electric polarization induced by inhomogeneous magnetic ordering

G. Lawes et al, PRL (2005)



- **Soliton charge:** it can be obtained from polarization due to an inhomogeneous parametric field

$$\rho(\boldsymbol{r}) = -\boldsymbol{\nabla} \cdot \boldsymbol{P}$$

- **Theoretical difficulty:** translational symmetry is broken, no well-defined Bloch basis

- **Solution:** semiclassical formalism
  - polarization as a Chern-Simons field!

- **Bonas:** theta vacuum constant in topological insulators

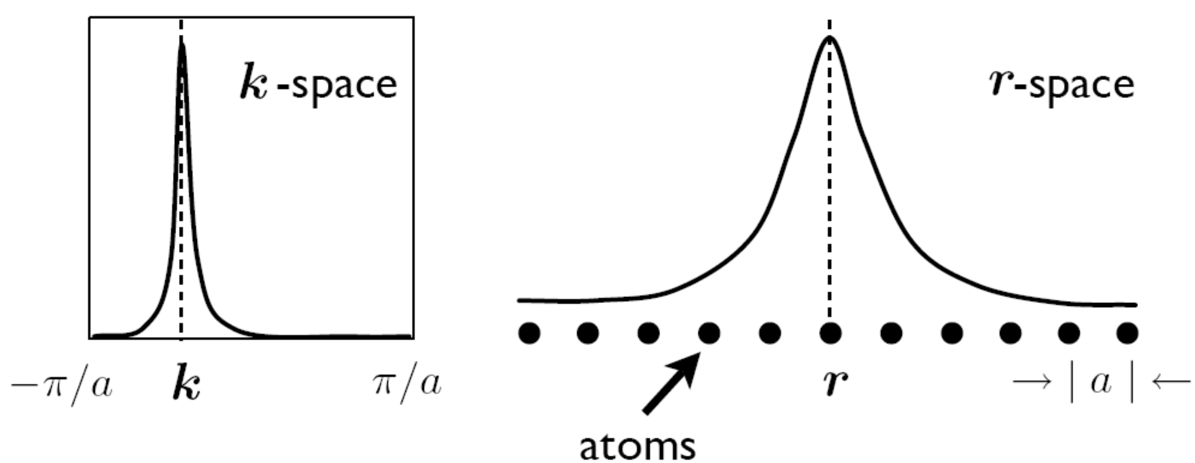
Semiclassical Approach

Hamiltonian $H(\hat{\boldsymbol{r}}, \hat{\boldsymbol{k}}; \beta(\hat{\boldsymbol{r}}, t))$

Fast and periodic

Slowly varying parameters

Classical particle described by a wave packet centered at k and r.



Equations of Motion

Sundaram & Niu, PRB (1999)

$$\dot{\boldsymbol{x}} = \frac{\partial \varepsilon}{\partial \boldsymbol{k}} - (\overleftrightarrow{\Omega}_{\boldsymbol{kx}} \cdot \dot{\boldsymbol{x}} + \overleftrightarrow{\Omega}_{\boldsymbol{kk}} \cdot \dot{\boldsymbol{k}}) + \boldsymbol{\Omega}_{t\boldsymbol{k}}$$

$$\dot{\boldsymbol{k}} = -\frac{\partial \varepsilon}{\partial \boldsymbol{x}} + (\overleftrightarrow{\Omega}_{\boldsymbol{xx}} \cdot \dot{\boldsymbol{x}} + \overleftrightarrow{\Omega}_{\boldsymbol{xk}} \cdot \dot{\boldsymbol{q}}) - \boldsymbol{\Omega}_{t\boldsymbol{x}}$$

Local basis

Berry curvatures:

$$(\overleftrightarrow{\Omega}_{\boldsymbol{kk}})_{\alpha\beta} \equiv \Omega_{k_\alpha k_\beta} \equiv i\left[\left\langle \frac{\partial u}{\partial k_\alpha}\middle|\frac{\partial u}{\partial k_\beta}\right\rangle - \left\langle \frac{\partial u}{\partial k_\beta}\middle|\frac{\partial u}{\partial k_\alpha}\right\rangle\right]$$

$$(\boldsymbol{\Omega}_{t\boldsymbol{x}})_\alpha \equiv \Omega_{t x_\alpha} \equiv i\left[\left\langle \frac{\partial u}{\partial t}\middle|\frac{\partial u}{\partial x_\alpha}\right\rangle - \left\langle \frac{\partial u}{\partial x_\alpha}\middle|\frac{\partial u}{\partial t}\right\rangle\right]$$

Adiabatic Pumping and Polarization

Adiabatic pumping: $\beta(\boldsymbol{x}, t) = \beta(t)$

Equation of motion: $\dot{k} = 0\,, \qquad \dot{x} = \frac{\partial \varepsilon}{\partial k} + \Omega_{tk}$

Current: $j = -e \int_0^{2\pi/a} \frac{dk}{2\pi} \Omega_{tk}$

Charge pumping
(A complete cycle in T)

$$Q = -e \int_0^T dt \int_0^{2\pi/a} \frac{dk}{2\pi} i \Big[\Big\langle \frac{\partial u}{\partial t} \Big| \frac{\partial u}{\partial k} \Big\rangle - \Big\langle \frac{\partial u}{\partial k} \Big| \frac{\partial u}{\partial t} \Big\rangle \Big]$$

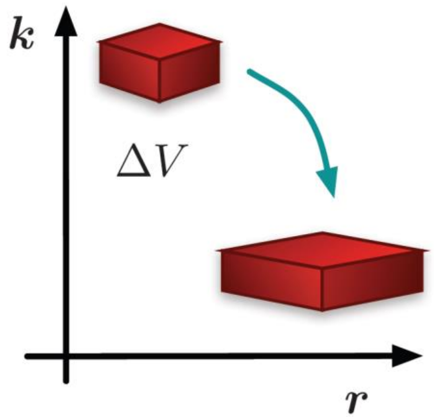
Thouless, PRB (1983)

Polarization
$\lambda = \lambda(t)$

$$\Delta P = -e \int_0^1 d\lambda \int_0^{2\pi/a} \frac{dk}{2\pi} i \Big[\Big\langle \frac{\partial u}{\partial \lambda} \Big| \frac{\partial u}{\partial k} \Big\rangle - \Big\langle \frac{\partial u}{\partial k} \Big| \frac{\partial u}{\partial \lambda} \Big\rangle \Big]$$

King-Smith & Vanderbilt, PRB (1983)

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 the Berry curvature field $\frac{1}{\Delta V}\frac{d\Delta V}{dt} \neq 0$

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

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

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

Berry-Phase Modified Density of States

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

Special cases

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

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

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)

Adiabatic current with inhomogeneity

Adiabatic current for a filled band of electrons

$$\boldsymbol{j} = -e \int_{\mathrm{BZ}} d\boldsymbol{k} D(\boldsymbol{k}, \boldsymbol{r}) \dot{\boldsymbol{r}},$$

DOS:

$$D(\boldsymbol{k}, \boldsymbol{r}) = (1 + \Omega^{kr}_{\alpha\alpha})/(2\pi)^d$$

$$\dot{r}_\alpha = \nabla^k_\alpha \varepsilon - \Omega^{kr}_{\alpha\beta} \dot{r}_\beta - \Omega^{kk}_{\alpha\beta} \dot{k}_\beta - \dot{\lambda} \Omega^{k\lambda}_\alpha,$$

$$\dot{k}_\alpha = -\nabla^r_\alpha \varepsilon + \Omega^{rr}_{\alpha\beta} \dot{r}_\beta + \Omega^{rk}_{\alpha\beta} \dot{k}_\beta + \dot{\lambda} \Omega^{r\lambda}_\alpha,$$

To first order in the gradient:

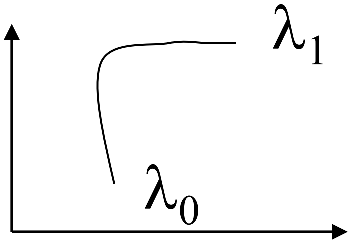
$$j^{(2)}_\alpha = e\dot{\lambda} \int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} (\Omega^{kk}_{\alpha\beta} \Omega^{r\lambda}_\beta + \Omega^{kr}_{\beta\beta} \Omega^{k\lambda}_\alpha - \Omega^{kr}_{\alpha\beta} \Omega^{k\lambda}_\beta)$$

Xiao, Shi, Clougherty & Q.N., PRL (2009)

Polarization to first order in gradients

- Integrate the adiabatic current over time

$$P_{\alpha}^{(1)} = e \int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \int_0^1 d\lambda \left(\Omega_{\beta\beta}^{kr} \Omega_{\alpha}^{k\lambda} - \Omega_{\alpha\beta}^{kr} \Omega_{\beta}^{k\lambda} + \Omega_{\alpha\beta}^{kk} \Omega_{\beta}^{r\lambda} \right)$$



- Two-point formula:

$$P_{\alpha}^{(1)} = e \int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \left(\mathcal{A}_{\alpha}^{k} \nabla_{\beta}^{r} \mathcal{A}_{\beta}^{k} + \mathcal{A}_{\beta}^{k} \nabla_{\alpha}^{k} \mathcal{A}_{\beta}^{r} + \mathcal{A}_{\beta}^{r} \nabla_{\beta}^{k} \qquad \right) \Big|_0^1$$

Chern-Simons field in $(k_{\alpha},k_{\beta},r_{\beta})$ space

Electric Polarization by B field

- Treat vector potential in Hamiltonian as an inhomogeneity.
- Spatial derivative becomes k derivative

$$\boldsymbol{k} \to \boldsymbol{k} + e\boldsymbol{a} \qquad \partial_x \to \partial_x a_i \partial_{k_i}$$

$$\langle P_x^{(\mathrm{in})} \rangle = \frac{Be^2}{\hbar} \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\, \epsilon_{ijk}\, \mathrm{Tr}[\mathcal{A}_i \partial_j \mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i \mathcal{A}_j \mathcal{A}_k] \quad (6)$$

Polarziation induced by a magnetic field
PRL (2009): Essin, Moore, Vanderbilt

Phonon induced electronic current

Chiral Phonon: circular motion of $(u_x(t), u_y(t))$

Substitute λ → $(u_x(t), u_y(t))$

$$j_\alpha^{(2)} = e\dot{u}_x \int \frac{d\boldsymbol{k}}{(2\pi)^2} \Omega_{k_\alpha k_\beta r_\beta u_x} + e\dot{u}_y \int \frac{d\boldsymbol{k}}{(2\pi)^2} \Omega_{k_\alpha k_\beta r_\beta u_y}$$

with $\Omega_{\alpha\beta\gamma\delta} = \Omega_{\alpha\beta}\Omega_{\gamma\delta} + \Omega_{\beta\gamma}\Omega_{\alpha\delta} - \Omega_{\alpha\gamma}\Omega_{\beta\delta}$

Taylor expansion near $\boldsymbol{u} = 0$

$$j_\alpha^{(2)} = \sum_\delta e\dot{u}_\delta \int \frac{d\boldsymbol{k}}{(2\pi)^2} \Omega_{k_\alpha k_\beta r_\beta u_\delta}|_{\boldsymbol{u}=0}$$

→ Polarization current
Vanishes after time average

$$+ \sum_{\delta\gamma} e\dot{u}_\delta u_\gamma \int \frac{d\boldsymbol{k}}{(2\pi)^2} \partial_{u_\gamma} \Omega_{k_\alpha k_\beta r_\beta u_\delta}|_{\boldsymbol{u}=0}$$

summation of δ, γ runs over u_x, u_y

Phonon Induced Electronic Orbital Magnetization

$$\sum_{\delta\gamma} e\dot{u}_\delta u_\gamma \int \frac{d\boldsymbol{k}}{(2\pi)^2} \partial_{u_\gamma} \Omega_{k_\alpha k_\beta r_\beta u_\delta} |_{\boldsymbol{u}=0}$$

Only antisymmetric part can survive after time average

$$\frac{e}{2}(\boldsymbol{u} \times \dot{\boldsymbol{u}})_z \int \frac{d\boldsymbol{k}}{(2\pi)^2} (\partial_{u_x} \Omega_{k_\alpha k_\beta r_\beta u_y} - \partial_{u_y} \Omega_{k_\alpha k_\beta r_\beta u_x})$$

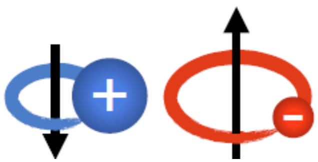
$$\boxed{\partial_{k_\alpha} \Omega_{u_x k_\beta r_\beta u_y} + \partial_{k_\beta} \Omega_{k_\alpha u_x r_\beta u_y}} + \partial_{r_\beta} \Omega_{k_\alpha k_\beta u_x u_y} \xrightarrow{j_\alpha = \partial_\beta M_{\alpha\beta}} M_{xy} = \frac{e}{2m_{\mathrm{I}}} L_{\mathrm{I}} \int \frac{d\boldsymbol{k}}{(2\pi)^2} \Omega_{k_\alpha k_\beta u_x u_y}$$

Total derivative, vanishes after integrating over $k_{x,y}$

$$L_{\mathrm{I}} = \frac{m_{\mathrm{I}}}{T} \int_0^T (\boldsymbol{u} \times \dot{\boldsymbol{u}})_z dt$$

Phonon magnetic moment

- Old theory



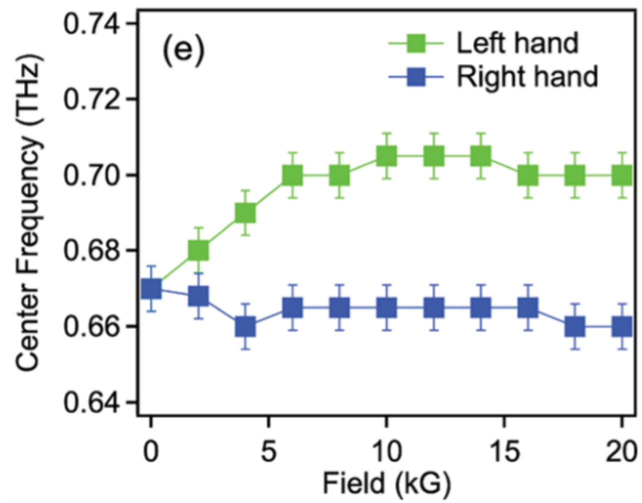
$$\boldsymbol{L} = m_{\mathrm{I}} \boldsymbol{u} \times \dot{\boldsymbol{u}}$$

Contribution to magnetic moment

$$\boldsymbol{M} = \gamma \boldsymbol{L}$$

$$\gamma = eZ_{\mathrm{I}}^{*}/2m_{\mathrm{I}}$$

Cd_3As_2



Cheng … Armitage, Nano Lett. **20**, 5991 (2020)

Born effective charge tensor :

$P_i = eZ_{ij}^{*} u_j$

$Z_{ij}^{*} = \int \frac{d\boldsymbol{k}}{(2\pi)^d} \Omega_{k_i u_j}$

Gonze & Lee, PRB **55**, 10355 (1997)

- Our theory

$$M_z = (\boldsymbol{u} \times \dot{\boldsymbol{u}})_z \frac{1}{2} e \int \frac{d\boldsymbol{k}}{(2\pi)^2} [\Omega_{k_x u_y} \Omega_{k_y u_x} - \Omega_{k_x u_x} \Omega_{k_y u_y} + \Omega_{k_x k_y} \Omega_{u_x u_y}]$$

Ren, Xiao, Saparov & Q.N., PRL (2021)