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Probing topology, geometry, and localization through fluctuation-dissipation theorem in ultracold atomic gases and beyond

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Outline

1. What are topology and geometry of band structures?
2. How can we measure it?
   I. Quantum geometric tensor and topology
   II. Localization, many-body quantum metric, and fluctuation-dissipation theorem

Bloch's theorem and physics on a band

A particle (e.g. electrons) in a periodic potential

$$\hat{H} = \frac{p^2}{2m} + V(\mathbf{r}) \qquad V(\mathbf{r} + \mathbf{a}_i) = V(\mathbf{r})$$

Eigenstates are labeled by band index n and crystal momentum **k**

$$\hat{H}\psi_{n,\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\psi_{n,\mathbf{k}}(\mathbf{r})$$

Here $\psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}) \qquad u_{n,\mathbf{k}}(\mathbf{r} + \mathbf{a}_i) = u_{n,\mathbf{k}}(\mathbf{r})$

$E_n(\mathbf{k})$: Energy band structure $\quad u_{n,\mathbf{k}}(\mathbf{r}) = \langle \mathbf{r} | u_{n,\mathbf{k}} \rangle$: Bloch state

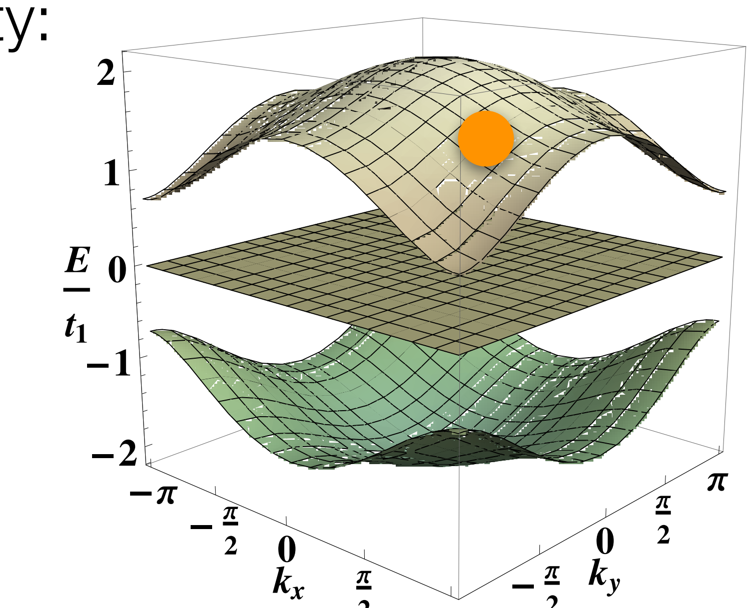
A wavepacket constructed on a band has a group velocity:

$$\dot{\mathbf{r}} = \frac{\partial E_n(\mathbf{k})}{\hbar \partial \mathbf{k}}$$

In the presence of external fields:

$$\hbar\dot{\mathbf{k}} = -e\mathbf{E}(\mathbf{r}) - e\dot{\mathbf{r}} \times \mathbf{B}$$

— semiclassical equations of motion —



[Ashcroft & Mermin (1976), page 218]

Geometric structure of bands

Geometric structure of band characterizes how much the Bloch state $|u_{n,\mathbf{k}}\rangle$ changes within the Brillouin zone

Physically meaningful quantity should be invariant under the **gauge transformation:**

$$|u_{n,\mathbf{k}}\rangle \longrightarrow e^{i\theta(\mathbf{k})}|u_{n,\mathbf{k}}\rangle$$

$\partial_{k_\mu}|u_{n,\mathbf{k}}\rangle$ is not gauge invariant, so it is not a good quantity to characterize the change of the Bloch state

Instead, we need to consider the **covariant derivative**:

$$D_{k_\mu}|u_{n,\mathbf{k}}\rangle \equiv (\partial_{k_\mu} + i\mathcal{A}^n_\mu(\mathbf{k}))|u_{n,\mathbf{k}}\rangle$$

$$\mathcal{A}^n_\mu(\mathbf{k}) \equiv i\langle u_{n,\mathbf{k}}|\partial_{k_\mu}|u_{n,\mathbf{k}}\rangle$$: Berry connection

Then, $D_{k_\mu}|u_{n,\mathbf{k}}\rangle \to e^{i\theta(\mathbf{k})}D_{k_\mu}|u_{n,\mathbf{k}}\rangle$

Its inner product is gauge invariant, and thus physically meaningful

$$\chi^n_{\mu\nu}(\mathbf{k}) \equiv \left(D_{k_\mu}\langle u_{n,\mathbf{k}}|\right)\left(D_{k_\nu}|u_{n,\mathbf{k}}\rangle\right)$$ Quantum geometric tensor

Quantum geometric tensor & Topology

Quantum geometric tensor:

$$\chi^n_{\mu\nu}(\mathbf{k}) \equiv \left\langle \frac{\partial u_{n,\mathbf{k}}}{\partial k_\mu} \middle| \frac{\partial u_{n,\mathbf{k}}}{\partial k_\nu} \right\rangle - \left\langle \frac{\partial u_{n,\mathbf{k}}}{\partial k_\mu} \middle| u_{n,\mathbf{k}} \right\rangle \left\langle u_{n,\mathbf{k}} \middle| \frac{\partial u_{n,\mathbf{k}}}{\partial k_\nu} \right\rangle$$
$$= \sum_{n' \neq n} \left\langle \frac{\partial u_{n,\mathbf{k}}}{\partial k_\mu} \middle| u_{n',\mathbf{k}} \right\rangle \left\langle u_{n',\mathbf{k}} \middle| \frac{\partial u_{n,\mathbf{k}}}{\partial k_\nu} \right\rangle$$
$$\equiv g^n_{\mu\nu}(\mathbf{k}) - i\Omega^n_{\mu\nu}(\mathbf{k})/2$$

$g^n_{\mu\nu}(\mathbf{k})$: quantum metric tensor, Fubini-Study metric

$\Omega^n_{\mu\nu}(\mathbf{k}) = \left(\nabla_\mathbf{k} \times \mathcal{A}^n(\mathbf{k})\right)_{\mu\nu}$: Berry curvature

In 2D,

$$\chi^n(\mathbf{k}) = \begin{pmatrix} g^n_{xx}(\mathbf{k}) & g^n_{xy}(\mathbf{k}) - i\Omega^n_{xy}(\mathbf{k})/2 \\ g^n_{xy}(\mathbf{k}) + i\Omega^n_{xy}(\mathbf{k})/2 & g^n_{yy}(\mathbf{k}) \end{pmatrix}$$

Semiclassical equation of motion, geometry, & topology

Taking the geometry into account, the correct semiclassical equations of motion is:

$$\dot{\mathbf{r}} = \frac{\partial E_n(\mathbf{k})}{\hbar \partial \mathbf{k}} - \underline{\dot{\mathbf{k}} \times \mathbf{\Omega}^n(\mathbf{k})}$$

$$\hbar \dot{\mathbf{k}} = -e\mathbf{E} - \underline{e\dot{\mathbf{r}} \times \mathbf{B}}$$

Looks like a Lorentz force

(ordinary) Lorentz force

where $\mathbf{\Omega}^n \equiv (\Omega^n_{yz}, \Omega^n_{zx}, \Omega^n_{xy})$

Geometric property is locally defined in each point in k-space

Topology is a **global** property of k-space

Topological invariant is an **integer** which characterizes the entire system

$$\mathcal{C}^n = \frac{1}{2\pi} \int dk_x dk_y \, \Omega^n_{xy}(\mathbf{k})$$

Chern number (topological)

Berry curvature (geometrical)

Bulk-edge correspondence:

Number of edge states within a gap = Sum of Chern number of bands under the gap

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Measuring geometry of bands through spectroscopy

We propose to measure the geometry through **excitation rate upon periodic modulation**

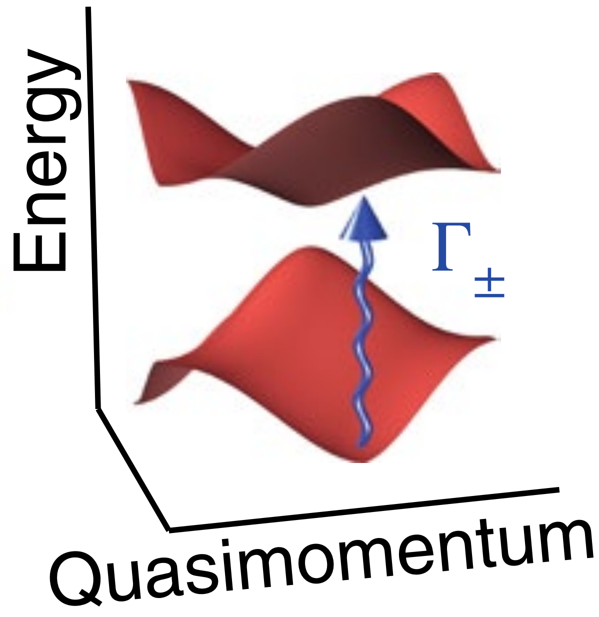
$$\hat{H}(t) = \underline{\hat{H}_{\text{lattice}}} + \underline{2E\cos(\omega t)\hat{x}}$$

We are interested in the geometry of this Hamiltonian

To probe the geometry, we add this perturbation

Steps:

1. Prepare the system in a Bloch state (or a superposition of Bloch states)
2. Add the perturbation
3. Measure the excitation rate
4. Integrate over the perturbation frequency ω
5. Then we get the quantum metric $g^{n}_{\mu\nu}$!!



Ozawa & Goldman, PRB **97**, 201117(R) (2018)

Fermi's golden rule

1. Prepare the system in a Bloch state (or a superposition of Bloch states)

   At t = 0, we start from a state $e^{i\mathbf{k}\cdot\mathbf{r}}|u_{n,\mathbf{k}}\rangle$

2. Add a perturbation

   $2E\cos(\omega t)\hat{x} = E\hat{x}e^{i\omega t} + \text{H.c.}$

3. Measure the excitation rate

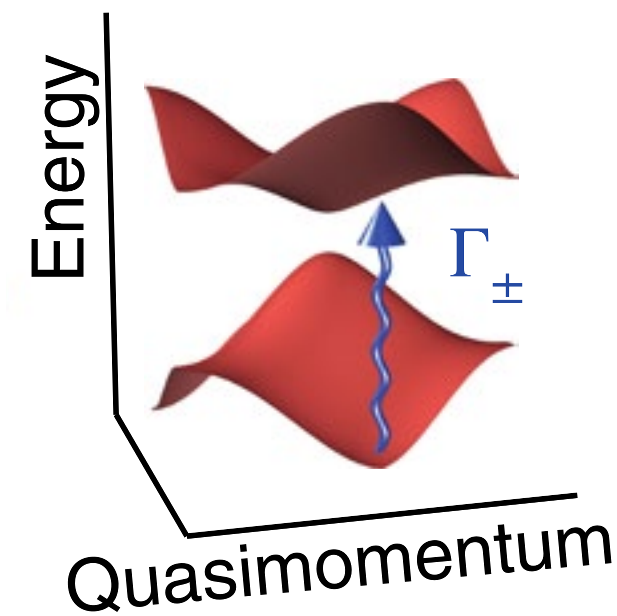
   Probability of finding the system in a state different from the original state is (Fermi's golden rule):

$$n_{\text{ex}}(\omega, t) = \frac{2\pi t}{\hbar}E^2 \sum_{|u_{n',\mathbf{k}'}\rangle \neq |u_{n,\mathbf{k}}\rangle} |\langle u_{n',\mathbf{k}'}|e^{-i\mathbf{k}'\cdot\mathbf{r}}\hat{x}e^{i\mathbf{k}\cdot\mathbf{r}}|u_{n,\mathbf{k}}\rangle|^2 \delta^{(t)}(E_{n'}(\mathbf{k}') - E_n(\mathbf{k}) - \hbar\omega)$$

where $\delta^{(t)}(\epsilon) \equiv (2\hbar/\pi t)\sin^2(\epsilon t/2\hbar)/\epsilon^2 \longrightarrow \delta(\epsilon)$ at large t

The matrix element is (Karplus & Luttinger, 1954):

$$\langle u_{n',\mathbf{k}'}|e^{-i\mathbf{k}'\cdot\mathbf{r}}\hat{x}e^{i\mathbf{k}\cdot\mathbf{r}}|u_{n,\mathbf{k}}\rangle = i\delta_{\mathbf{k}',\mathbf{k}}\langle u_{n',\mathbf{k}}|\partial_{k_x}u_{n,\mathbf{k}}\rangle$$



Excitation rate

4. Integrate over the perturbation frequency ω

   Excitation rate is

$$\Gamma(\omega) \equiv \frac{n_{\mathrm{ex}}(\omega, t)}{t} = \frac{2\pi E^2}{\hbar} \sum_{n' \neq n} |\langle u_{n',\mathbf{k}} | \partial_{k_x} u_{n,\mathbf{k}} \rangle|^2 \delta^{(t)}(E_{n'}(\mathbf{k}) - E_n(\mathbf{k}) - \hbar\omega)$$

Integrating over the frequency, we obtain the quantum metric!!

$$\Gamma^{\mathrm{int}} \equiv \int_0^\infty \Gamma(\omega) d\omega = \frac{2\pi E^2}{\hbar^2} \sum_{n' \neq n} |\langle u_{n',\mathbf{k}} | \partial_{k_x} u_{n,\mathbf{k}} \rangle|^2 = \frac{2\pi E^2}{\hbar^2} g^n_{xx}(\mathbf{k})$$

If the initial state is fermions (partially) filling the band with density $\rho(\mathbf{k})$

$$\Gamma^{\mathrm{int}} = \frac{2\pi E^2}{\hbar^2} \sum_{\mathbf{k}} \rho(\mathbf{k}) g^n_{xx}(\mathbf{k})$$

Ozawa & Goldman, PRB **97**, 201117(R) (2018)

How to measure the Berry curvature

In fact, the proposal to measure the Berry curvature existed earlier:

Tran, Dauphin, Grushin, Zoller, & Goldman, Science Advances **3**, e1701207 (2017)

Here, one adds **circular shakings** and take a difference

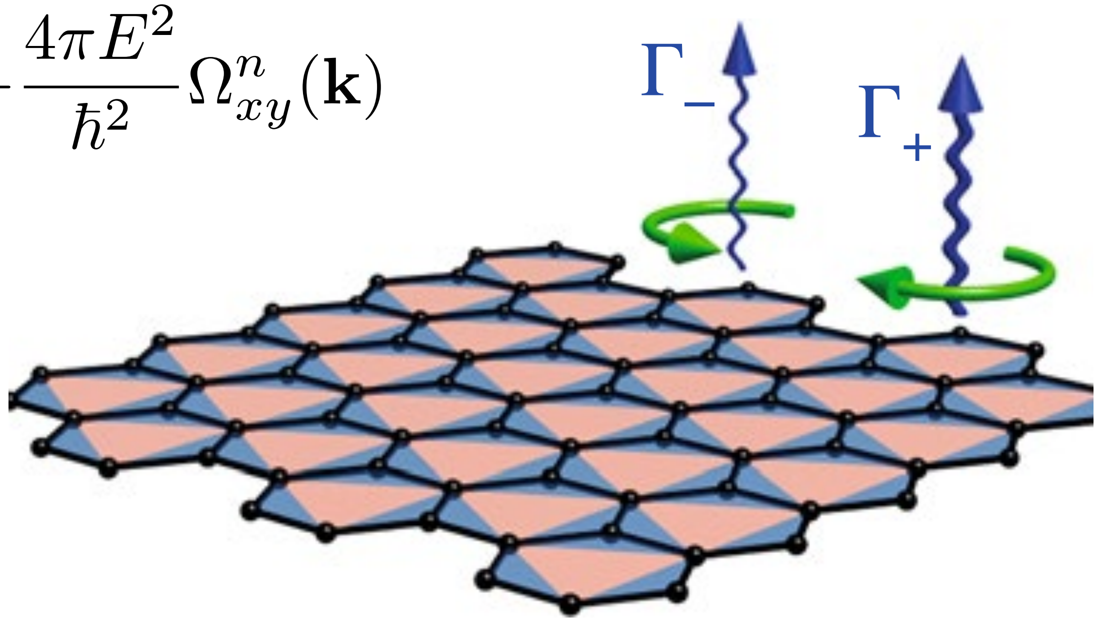
$$\hat{H}(t) = \hat{H}_{\mathrm{lattice}} + 2E\left(\hat{x}\cos(\omega t) \pm \hat{y}\sin(\omega t)\right)$$

When the initial state is a Bloch state $e^{i\mathbf{k}\cdot\mathbf{r}}|u_{n,\mathbf{k}}\rangle$, the integrated excitation rate is

$$\Gamma_{\pm}^{\mathrm{int}} = \frac{2\pi E^2}{\hbar^2}\left(g_{xx}^n(\mathbf{k}) + g_{yy}^n(\mathbf{k}) \mp \Omega_{xy}^n(\mathbf{k})\right)$$

So, the difference between the clockwise and anticlockwise shaking is

$$\Delta\Gamma^{\mathrm{int}} \equiv \Gamma_{+}^{\mathrm{int}} - \Gamma_{-}^{\mathrm{int}} = -\frac{4\pi E^2}{\hbar^2}\Omega_{xy}^n(\mathbf{k})$$

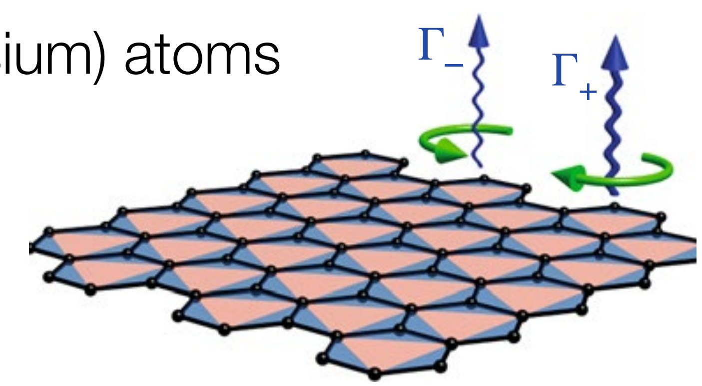


If the initial state covers a whole band, the difference of the integrated excitation rate gives the topological Chern number

Experiment (ultracold atoms @ Hamburg)

Asteria, Tran, TO, et al., Nature Physics **15**, 449–454 (2019)

We experimentally implemented the protocol using ultracold K (potassium) atoms

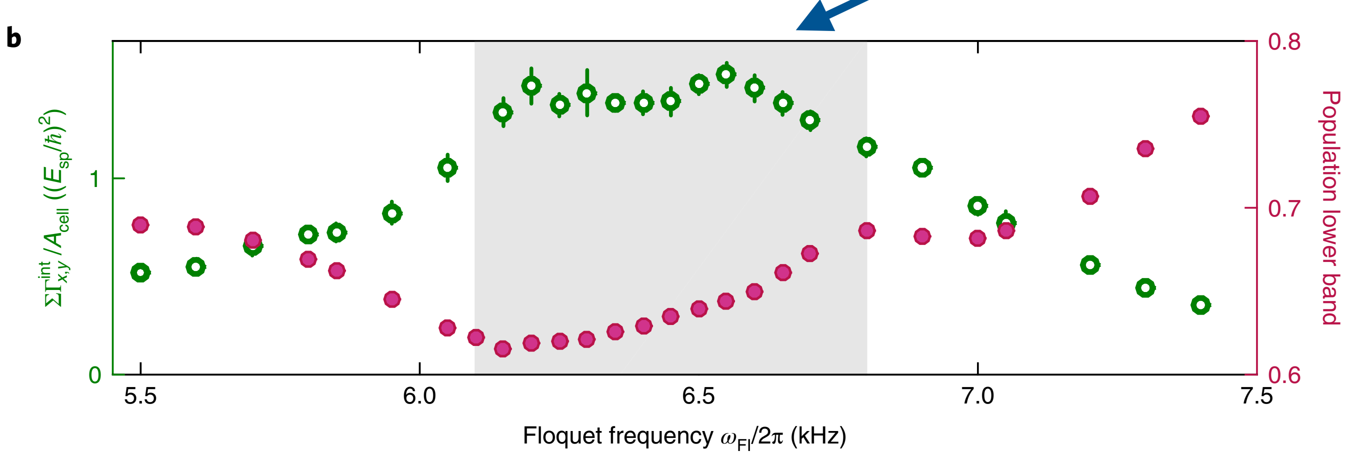


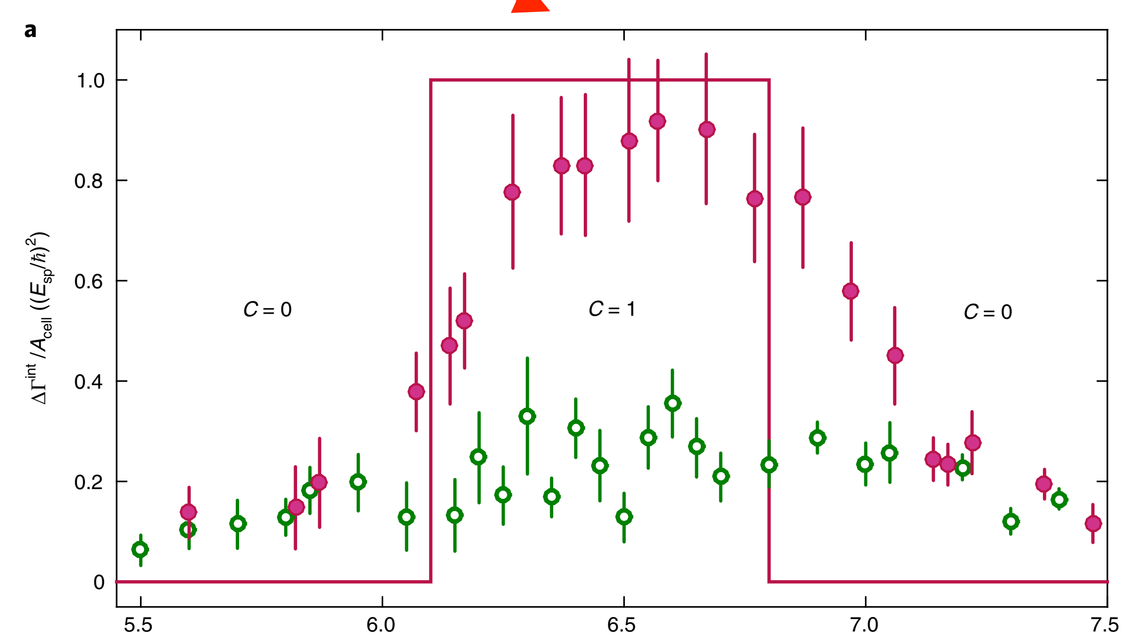
We prepare the Haldane model

And then shake linearly / circularly and detect excitation

We change the system parameter and observed **topological phase transitions**

and also the first ever estimate of **quantum metric**





More quantitative measurement in progress in collaboration with Y. Takahashi group in Kyoto

Experiment (diamond NV Center @ Wuhan)

Suppose Hamiltonian $\hat{H}(\boldsymbol{\lambda})$ and its eigenstates $\psi(\boldsymbol{\lambda})$ depends on parameters: $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \cdots)$

Quantum geometric tensor can also be defined in this **general parameters space**:

$$\chi_{\mu\nu}(\boldsymbol{\lambda}) \equiv \langle \partial_{\lambda_\mu} \psi(\boldsymbol{\lambda}) | \partial_{\lambda_\nu} \psi(\boldsymbol{\lambda}) \rangle - \langle \partial_{\lambda_\mu} \psi(\boldsymbol{\lambda}) | \psi(\boldsymbol{\lambda}) \rangle \langle \psi(\boldsymbol{\lambda}) | \partial_{\lambda_\nu} \psi(\boldsymbol{\lambda}) \rangle$$

To measure it, we now modulate **parameters** in time $\lambda_1(t) = \lambda_1^0 + 2(E/\hbar\omega)\cos(\omega t)$

Starting from an eigenstate $|\psi_{\mathrm{ini}}\rangle$ of the Hamiltonian $\hat{H}(\boldsymbol{\lambda}^0)$, the integrated excitation rate is then

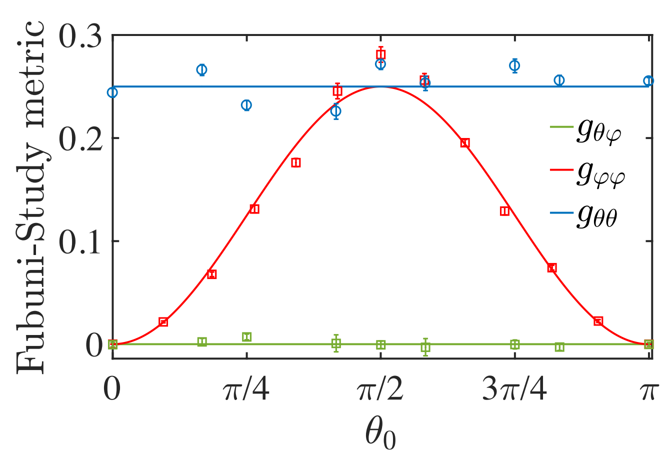
$$\Gamma^{\mathrm{int}} = \frac{2\pi E^2}{\hbar^2} g_{\lambda_1\lambda_1}(\boldsymbol{\lambda}^0)$$

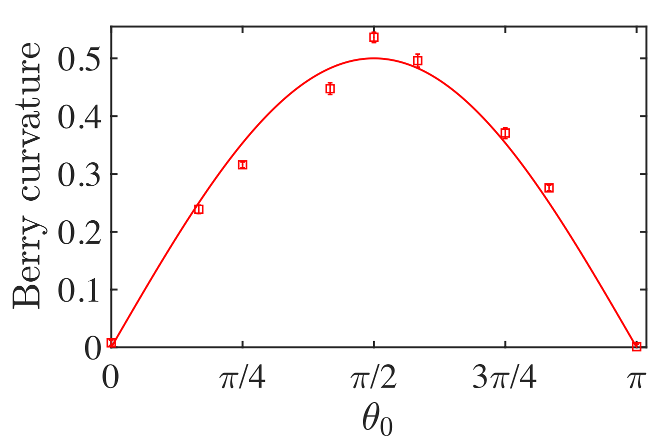
With qubits in diamond NV centers, the Hamiltonian $\hat{H}(\theta, \phi) = H_0 \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}$

Is realized and the **quantum geometric tensor** is **quantitatively measured for the first time**

Ozawa & Goldman, PRB **97**, 201117(R) (2018)

Yu, *et al*., arXiv:1811.12840





cf. superconducting qubit: Tan, *et al*. (Nanjing), Phys. Rev. Lett. **122**, 210401 (2019)

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Reconsider the argument

What we had was a time periodic modulation of the following form:

$$\hat{H}(t) = \hat{H}_0 + 2E\cos(\omega t)\hat{x}$$

We started from a Bloch state and looked at the excitation rate.

Now, assume that the Hamiltonian is the many-body Hamiltonian, and we start from an arbitrary eigenstate $|\alpha\rangle$

The probability of the system being excited is:

$$n_{\mathrm{ex}}(\omega, t) = \frac{2\pi E^2 t}{\hbar} \sum_{\beta\neq\alpha} |\langle\beta|\hat{x}|\alpha\rangle|^2 \delta^{(t)}(\epsilon_\beta - \epsilon_\alpha - \hbar\omega)$$

And thus the integrated excitation rate is:

$$\Gamma^{\mathrm{int}} \equiv \int_0^\infty \frac{n_{\mathrm{ex}}(\omega, t)}{t} d\omega = \frac{2\pi E^2}{\hbar^2} \boxed{\sum_{\beta\neq\alpha} |\langle\beta|\hat{x}|\alpha\rangle|^2}$$

$$\sum_{\beta\neq\alpha} |\langle\beta|\hat{x}|\alpha\rangle|^2 = \sum_{\beta\neq\alpha} \langle\alpha|\hat{x}|\beta\rangle\langle\beta|\hat{x}|\alpha\rangle = \langle\alpha|\hat{x}^2|\alpha\rangle - \langle\alpha|\hat{x}|\alpha\rangle^2 \equiv \mathrm{Var}(\hat{x})$$

Variance of position!

Ozawa & Goldman, arXiv:1904.11764

Fluctuation-dissipation theorem

We can derive the same formula from the fluctuation-dissipation theorem

Upon adding a modulation $2E\cos(\omega t)\hat{x}$, the **fluctuation-dissipation theorem** tells that

$$\langle \hat{x}^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty \underline{\alpha''(\omega)} \coth \frac{\hbar\omega}{2T} d\omega$$

Landau-Lifshitz “Statistical Physics” eq. (124.10)

Imaginary part of the generalized susceptibility

On the other hand, the rate of energy absorption by the system is $P(\omega) = 2\omega E^2 \alpha''(\omega)$

Landau-Lifshitz “Statistical Physics” eq. (123.11)

The rate of exciting the system is then $\Gamma(\omega) = P(\omega)/\hbar\omega$ and thus

$$\langle \hat{x}^2 \rangle = \frac{\hbar^2}{2\pi E^2} \int_0^\infty \Gamma(\omega) \coth \frac{\hbar\omega}{2T} d\omega$$

In the limit of T = 0, we re-obtain

$$\Gamma^{\mathrm{int}} = \int_0^\infty \Gamma(\omega) d\omega = \frac{2\pi E^2}{\hbar^2} \langle \hat{x}^2 \rangle = \frac{2\pi E^2}{\hbar^2} \mathrm{Var}(\hat{x})$$

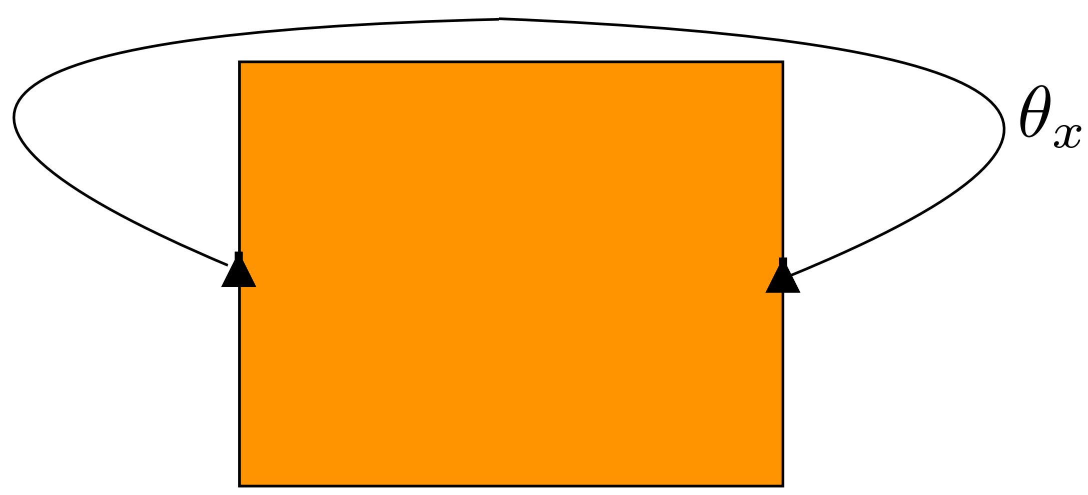
Many-body quantum geometric tensor

We can connect the variance of the position and geometry by introducing the concept of **many-body quantum geometric tensor**

Historically, Berry curvature was extended to many-body cases by Niu-Thouless-Wu (1985) by defining the Berry curvature in the parameter space of **twisted boundary condition**

Here, we consider a many-body wave function $\Psi(\{\mathbf{r}_a\})$ with

$$\Psi(\{x_a + L_x, y_a, \cdots\}) = e^{i\theta_x}\Psi(\{x_a, y_a, \cdots\})$$



Many-body quantum geometric tensor is defined in this twist space as

$$\chi_{\mu\nu}(\boldsymbol{\theta}) \equiv \left\langle \frac{\partial \Psi(\boldsymbol{\theta})}{\partial \theta_\mu} \middle| \frac{\partial \Psi(\boldsymbol{\theta})}{\partial \theta_\nu} \right\rangle - \left\langle \frac{\partial \Psi(\boldsymbol{\theta})}{\partial \theta_\mu} \middle| \Psi(\boldsymbol{\theta}) \right\rangle \left\langle \Psi(\boldsymbol{\theta}) \middle| \frac{\partial \Psi(\boldsymbol{\theta})}{\partial \theta_\nu} \right\rangle$$
$$\equiv g_{\mu\nu}(\boldsymbol{\theta}) - i\Omega_{\mu\nu}(\boldsymbol{\theta})/2$$

Meaning of the many-body quantum geometry

Niu-Thouless-Wu (1985): Many-body Berry curvature is related to the many-body Chern number

$$\mathcal{C}_{\mathrm{MB}} = \frac{1}{2\pi}\int d\theta_x d\theta_y \Omega_{xy}(\theta_x, \theta_y)$$

This integer enters the Hall conductance

If there is a degeneracy of states, it can signal fractional quantum Hall effect

Souza-Wilkens-Martin (2000): Many-body quantum metric is related to the localization

Matrix element of the (properly defined) position operator satisfies $\langle\alpha|\hat{x}|\beta\rangle = -iL_x\langle\partial_{\theta_x}\alpha|\beta\rangle$

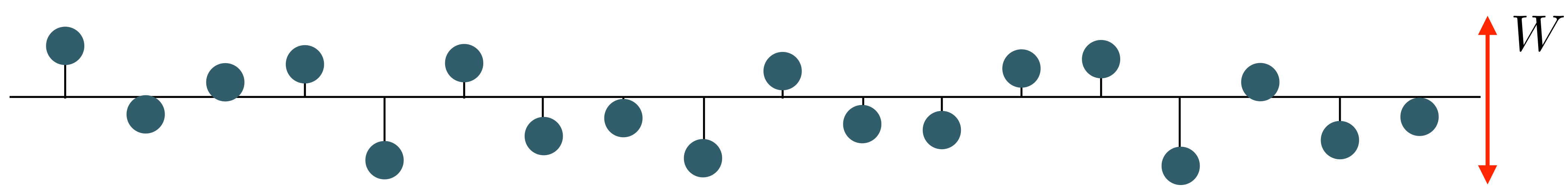
$$\begin{aligned} g_{xx} &= \langle\partial_{\theta_x}\alpha|\partial_{\theta_x}\alpha\rangle - \langle\partial_{\theta_x}\alpha|\alpha\rangle\langle\alpha|\partial_{\theta_x}\alpha\rangle \\ &= \sum_{\beta\neq\alpha}\langle\partial_{\theta_x}\alpha|\beta\rangle\langle\beta|\partial_{\theta_x}\alpha\rangle = \sum_{\beta\neq\alpha}\langle\alpha|\hat{x}|\beta\rangle\langle\beta|\hat{x}|\alpha\rangle/L_x^2 \\ &= \left(\langle\alpha|\hat{x}^2|\alpha\rangle - \langle\alpha|\hat{x}|\alpha\rangle^2\right)/L_x^2 = \mathrm{Var}(\hat{x})/L_x^2 \end{aligned}$$

And thus

$$\Gamma^{\mathrm{int}} = \frac{2\pi E^2}{\hbar^2}\mathrm{Var}(\hat{x}) = \frac{2\pi E^2}{\hbar^2}L_x^2 g_{xx}$$

Example I: Anderson model

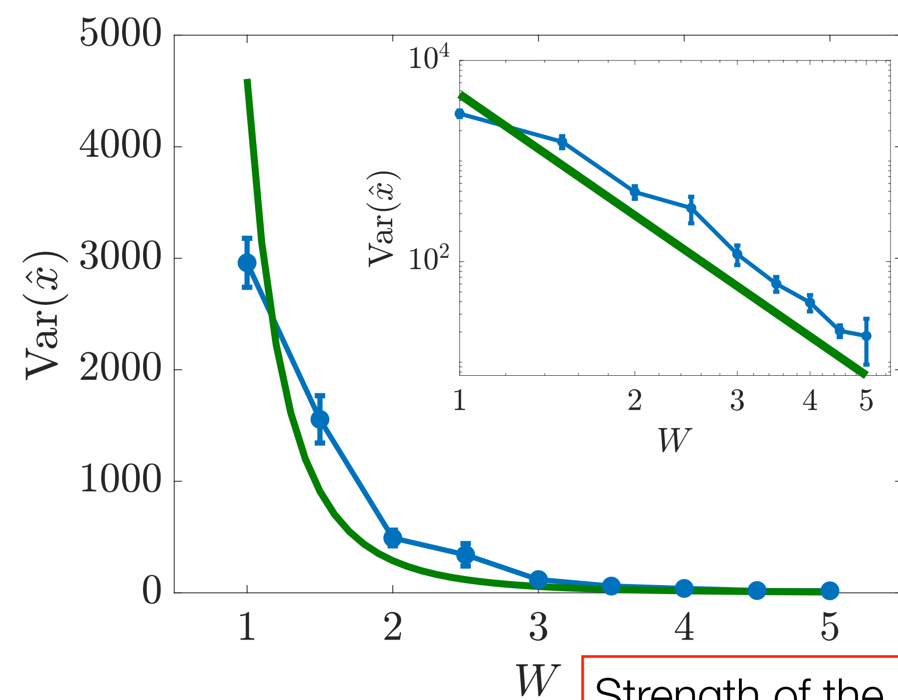
We theoretically apply our method to the one-dimensional Anderson model



One dimensional lattice with **uniform hopping** and **random onsite energy**

Eigenstates are localized (Anderson localization)

We try to detect the variance of the localized eigenstates through excitation rate simulation



Strength of the random onsite energy

The measurement of the many-body quantum metric can be used to detect the localization without directly looking at real-space wave function

Ozawa & Goldman, arXiv:1904.11764

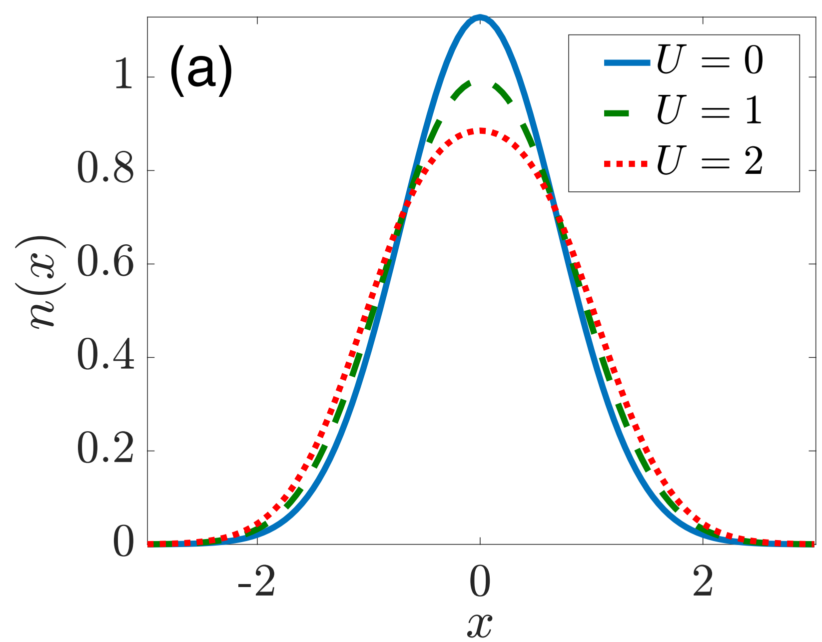
Example II: two particles in a harmonic trap

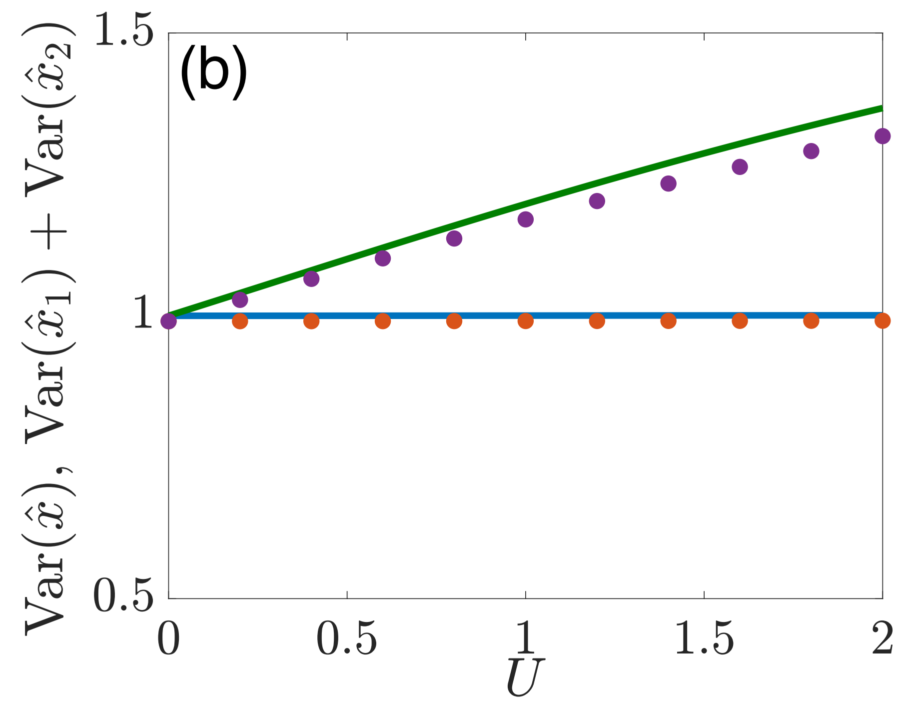
We consider two interacting particles in a harmonic trap

In the presence of repulsive interactions, the wavefunction becomes a bit spread

We try to detect this spread through simulating periodic modulation and looking at the excitation rate

As a function of the repulsive interaction U,
we can estimate the spread via excitation rate simulation





Ozawa & Goldman, arXiv:1904.11764

Summary

- **Quantum geometric tensor** characterizes the gauge invariant structure of a quantum state on a parameter space, and it is made of two parts: Quantum metric and Berry curvature
- Quantum geometric tensor can be extracted through excitation rate upon periodic modulation
- In many-body or disordered situation, **fluctuation-dissipation theorem** relates excitation rate and the fluctuation of position, which in turn is related to quantum metric in twist-boundary condition space

- Theory collaboration: Nathan Goldman (Université Libre de Bruxelles)
- Experiment collaboration (cold atom): Klaus Sengstock & Christof Weitenberg (Hamburg)
- Experiment collaboration (NV center): Jianming Cai (Huazhong University)
- Ongoing experimental collaboration (cold atom): Yoshiro Takahashi (Kyoto)

Ozawa & Goldman, PRB **97**, 201117(R) (2018)
Asteria, *et al*., Nature Physics **15**, 449–454 (2019)
Yu, *et al*., arXiv:1811.12840
Ozawa & Goldman, arXiv:1904.11764