Quantum Geometry of Mixed States and Exact Sum Rules

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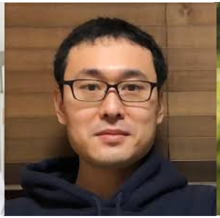

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Based on work: Density Matrix Geometry and Sum Rules (arXiv 2507.14028)
Gangue Ji, D. Palomino, N. Goldman, T. Ozawa, P. Riseborough, Jie Wang*, Bruno Mera*

Outline

Geometry in quantum physics (review)

	Geometry of wavefunction		Geometry of density matrix
Definition	Quantum metric	$\longrightarrow$	Quantum Fisher information
	Berry curvature	$\longrightarrow$	Uhlmann curvature
Application	Quantization of σ_H, localization length Stability of fractional Chern insulator		Quantum metrology Entanglement witness ......

This work

- Fully interacting
- General formalism
- Series of sum rules and outcomes

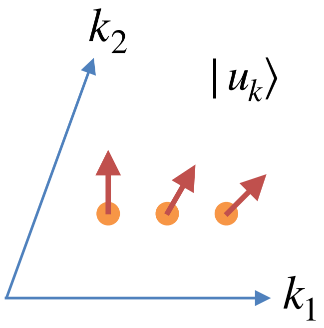
Problem setting
(standard many-body perturbation, requires thermal equilibrium)

$$H(\phi) = H_0 + \sum_a \mathcal{O}^a \phi_a + O(\phi^2)$$

Main result
(generating function of sum rules)

$$\underbrace{-\frac{1}{2\hbar}\mathcal{S}^{ij}(\omega)}_{\text{Geometry of thermal density matrix}} = \frac{\tanh^2\left(\frac{\hbar\beta\omega}{2}\right)}{1 - e^{-\hbar\beta\omega}} \underbrace{\frac{\chi^{jk}_{\mathcal{O};D}(\omega)}{(\hbar\omega)^2}}_{\text{Dissipation}}$$

Geometry of pure state (single-particle)

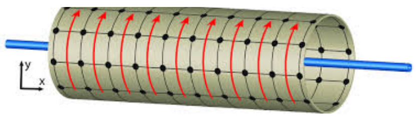


Characterizes how periodic Bloch state $|u_{\mathbf{k}}\rangle$ varies locally in the Brillouin zone $\{\mathbf{k}\}$.

Bloch state: $\psi_k(r+a) = e^{ika}\psi_k(r)$

Periodic part: $u_k(r) \equiv e^{-ikr}\psi_k(r)$

Gauge redundancy: $u_k(r) \to e^{i\theta_k}u_k(r)$



$$\mathbf{k} = \alpha + \sum_{j=1}^{d} m_j \frac{\mathbf{b}_j}{N_j}$$

α = twisted boundary condition flux
= origin of momentum grid

<u>Geometry of (single-particle) wavefunction</u>

$$|A|e^{i\alpha} = |u_{k_1}\rangle\langle u_{k_1}|\ldots|u_{k_N}\rangle\langle u_{k_N}|u_{k_1}\rangle\langle u_{k_1}|$$

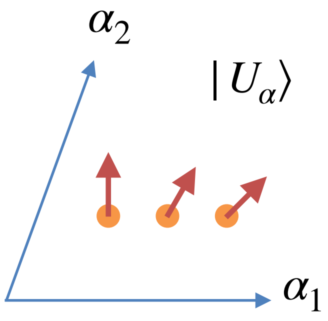
Berry curvature
(gauge invariant phase)

$$\Omega(k) = \Im\left[\langle\partial_{k_x}u_k|\partial_{k_y}u_k\rangle\right]$$

Quantum metric
(gauge invariant distance)

$$|\langle u_k|u_{k+\delta k}\rangle|^2 = 1 - g^{ab}(k)dk_a dk_b + \ldots$$

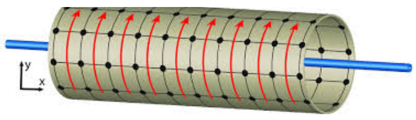
Geometry of pure state (many-particle)



How many-body state $|U_\alpha\rangle$ varies locally in the twisted boundary condition pace $\{\alpha\}$.

"Bloch state": $\Psi_\alpha(r_1, \ldots r_n + L, \ldots, r_N) = e^{i\alpha \cdot \mathbf{L}}\, \Psi_\alpha(r_1, \ldots r_n, \ldots, r_N)$

"Periodic part": $U_\alpha(r_1, \ldots, r_N) = e^{-i\alpha \cdot \sum_i \mathbf{r}_i}\, \Psi_\alpha(r_1, \ldots, r_N)$



$$\mathbf{k} = \alpha + \sum_{j=1}^{d} m_j \frac{\mathbf{b}_j}{N_j}$$

α = twisted boundary condition flux
= origin of momentum grid

Many-body Berry curvature

$$\Omega(\alpha) = \Im\left[\langle \partial_{\alpha_x} U_\alpha | \partial_{\alpha_y} U_\alpha \rangle\right]$$

Many-body quantum metric (*1st meaning*)

$$|\langle U_\alpha | U_{\alpha+\delta\alpha} \rangle|^2 = 1 - G^{ab}(\alpha) d\alpha_a d\alpha_b + \ldots$$

Comment 1 (any size): $\Omega(\alpha) = \sum_{\mathbf{k}} \Omega(\mathbf{k})$

Comment 2 (thermodynamic limit): $\Omega(\alpha) = \frac{V}{2\pi} C$

Application of quantum geometry to fractional Chern insulators

- Quantum geometric bound: $\mathrm{Tr}G(\alpha) \geq 2\sqrt{\det G(\alpha)} \geq |\Omega(\alpha)|$

R. Roy; PRB 14

- <u>Q: What happens when bound saturates $\mathrm{Tr}G(\alpha) = \Omega(\alpha)$?</u>

A: It is **Kahler condition**, the Bloch wavefunction is provable to be exactly "lowest Landau level type" (ideal band)

JW, Zhao Liu, et. al; PRL (21, 22)
Bruno Mera, Tomoki Ozawa; PRB (21,22)
Ledwith, Vishwanath, et. al; (PRR 20, 23)

$$\psi_{\mathbf{k}}(\mathbf{r}) = \mathcal{N}_{\mathbf{k}}\ \mathscr{B}(\mathbf{r})\ \Phi_{\mathbf{k}}(\mathbf{r})$$

$\Phi_{\mathbf{k}}(\mathbf{r})$ standard LLL wavefunction

$\mathscr{B}(\mathbf{r})$ determines Berry curvature distribution in Brillouin zone

Implication: FCI as Exact ground state in short-ranged interacting ideal flat band.

- See recent work for quantum geometry based classification of Bloch states and geometric conditions preferring non-Abelian states.

Theory of Generalized Landau Levels and its Implications to non-Abelian States

Z. Liu#, Bruno Mera#, M. Fujimoto, T. Ozawa, JW (PRX, 25)*

Zero temperature optical conductivity sum rule

Geometrical sum rule for optical conductivity

$$\int_0^\infty d\omega \frac{\sigma_D^{ab}(\omega, T=0)}{\omega} = \frac{\pi}{2}\frac{e^2}{V\hbar}\mathcal{Q}^{ab}(\alpha)$$

Response ⟷ Geometry

Dissipation ⟷ Fluctuation

Imaginary part: Qian Niu, D. Thouless, Yongshi Wu; PRB (85)
Real part: Souza, Wilkens, Martin; PRB (00)

Our work: finite-temperature generalization and beyond.

- *Optical absorption (hermitian)*

$$\sigma_D^{ab}(\omega) = \frac{\sigma^{ab}(\omega) + \sigma^{ba}(-\omega)}{2} = \underbrace{\begin{pmatrix} \Re\sigma_D^{xx} & \\ & \Re\sigma_D^{yy} \end{pmatrix}}_{\text{Absorption of linear light}} + i \underbrace{\begin{pmatrix} & \Im\sigma_D^{xy} \\ -\Im\sigma_D^{xy} & \end{pmatrix}}_{\text{Absorption difference of circular light}}$$

- *Quantum geometric tensor of ground state (hermitian)*

$$\mathcal{Q}^{ab}(\alpha) = G^{ab}(\alpha) + \frac{i}{2}\epsilon^{ab}\Omega(\alpha)$$

Geometry of pure state: many-body Berry curvature

Kramers-Kronig relation

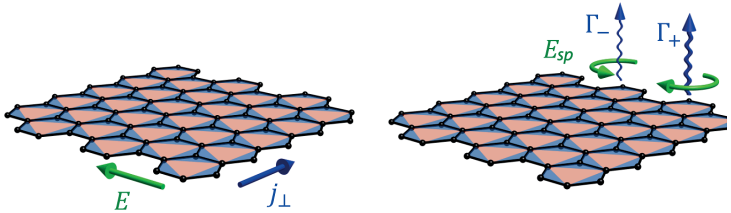
$$\sigma^{xy}(\omega=0) = -\frac{1}{\pi}\mathscr{P}\int_{-\infty}^{\infty} d\omega \frac{\Im\sigma_D^{xy}(\omega)}{\omega}$$

Quantization of 2D Hall conductivity [Niu, Wu, Thouless 85]

- Valid in the presence of interaction, disorder
- Quantization requires a gap

$$\frac{e^2}{h}C = \frac{e^2}{V\hbar}\Omega(\alpha) = \sigma^{xy}(\omega=0,\ T=0) = \frac{2}{\pi}\int_0^{\infty} d\omega \frac{\Im\sigma_D^{xy}(\omega, T=0)}{\omega}$$

Thermodynamic limit



Implication

Dynamically probe Chern number
(especially useful for neutral systems ——— cold atom)

Tran, Dauphin, Grushin, Zoller, N. Goldman (17)

Geometry of pure state: many-body quantum metric

Localization length of electronic states [Resta, Sorella 99]

$$z_N = \langle \Psi | e^{i\frac{2\pi}{L}\hat{X}} | \Psi \rangle \qquad \hat{X} = \sum_i \hat{x}_i$$

- Phase of z_N encodes *electric polarization*
- Amplitude $|z_N|$ discriminates *metal and insulator*

$$\lim_{N\to\infty} |z_N| = \begin{cases} \text{finite, insulator} \\ \infty\text{, metal} \end{cases}$$

- For insulators, $|z_N|$ is the many-body quantum metric (*2nd meaning*)

$$|z_N| = \langle \Psi | \hat{X}^2 \Psi \rangle - \langle \Psi | \hat{X} | \Psi \rangle^2 \sim \mathrm{Tr} G(\alpha)$$

Souza, Wilkens, Martin (00)

$$\int_0^\infty d\omega \frac{\Re\sigma_D^{ab}(\omega, T=0)}{\omega} = \frac{\pi}{2}\frac{e^2}{V\hbar} G^{ab}(\alpha)$$

Probed by flux insertion

↓

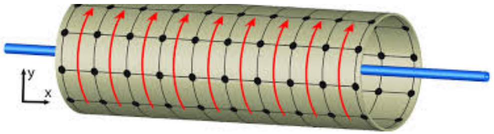
Dissipation of COM coordinates

Change of wavefunction under flux insertion

↓

Fluctuation of COM coordinates

Flux insertion, current operator, COM coordinate



The sum rule is understood as the fluctuation-dissipation relation.

Optical conductivity sum rule at zero temperature

Putting imaginary & real parts together

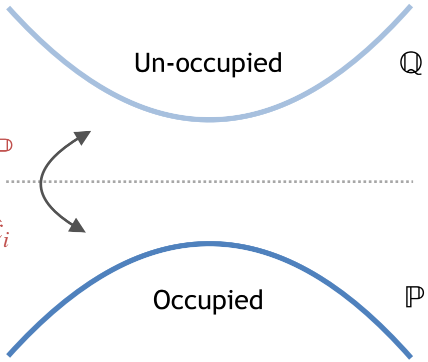
Geometrical sum rule for optical conductivity

$$\int_0^\infty d\omega \frac{\sigma_D^{ab}(\omega, T=0)}{\omega} = \frac{\pi}{2}\frac{e^2}{V\hbar}\mathcal{Q}^{ab}(\alpha)$$

Dissipation　　　　　Fluctuation

$\hat{D} \equiv \mathbb{Q}\hat{X}\mathbb{P}$

$\hat{X} \equiv \sum_i \hat{x}_i$



$\mathbb{Q} = 1 - \mathbb{P}$

$\mathbb{P} = \sum_{\mathbf{k}} |u_{\mathbf{k}}\rangle\langle u_{\mathbf{k}}|$

Important point (second meaning of geometry):

Geometry = two-point correlation function

$$\mathcal{Q}^{ab}(\alpha) = \langle \hat{D}^{a\dagger}\hat{D}^b \rangle$$

$$\hat{D}^a = \mathbb{Q}\ \hat{X}^a\ \mathbb{P}$$

dipole transition operator

COM coordinate connecting ground state and its excitations

Time dependent geometry at zero temperature

Static wavefunction's geometric tensor $\mathcal{Q}^{ab} \equiv \langle \hat{D}^{\dagger a} \hat{D}^{b} \rangle$

Time dependent geometric tensor

$$\mathcal{Q}^{ab}(t-t') \equiv \langle \hat{D}^{\dagger a}(t) \hat{D}^{b}(t') \rangle$$

$$\hat{D}^{a}(t) = e^{iHt/\hbar} \hat{D}^{a} e^{-iHt/\hbar}$$

Generating function for $T = 0$ sum rules
(formally from F-D theorem)

$$\frac{1}{2V} \frac{e^2}{\hbar} \mathcal{Q}^{ab}(\omega) = \frac{\sigma_D^{ab}(\omega)}{\omega}$$

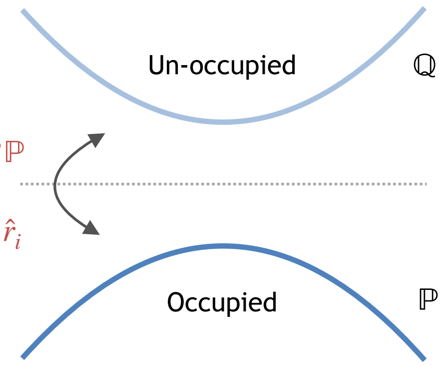
Various sum rules

$$\frac{1}{2V} \frac{e^2}{\hbar} \mathcal{Q}^{ab}_{(n)} = \int_{-\infty}^{\infty} d\omega \, \sigma_D^{ab}(\omega) \omega^{n-1}$$

$$\mathcal{Q}^{ab}_{(n)} = (i\partial_t)^n \mathcal{Q}^{ab}(t)|_{t=0}$$

$\hat{D} \equiv \mathbb{Q} \hat{R} \mathbb{P}$

$\hat{R} \equiv \sum_i \hat{r}_i$



$\mathbb{Q} = 1 - \mathbb{P}$

$\mathbb{P} = \sum_{\mathbf{k}} |u_{\mathbf{k}}\rangle\langle u_{\mathbf{k}}|$

What about finite temperature, and what is new?

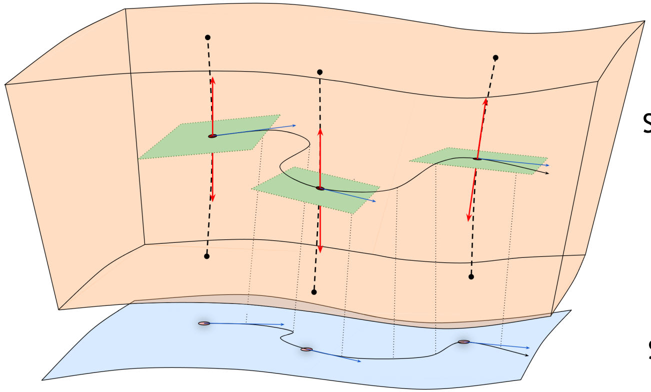
Wavefunction $\Rightarrow$ **density matrix.**

Nishchhal Verma, Raquel Queiroz (23).

Geometry of density matrices

Pure state geometry	*mixed state geometry*
Band projector $\mathbb{P}_\alpha \equiv \lvert U_\alpha \rangle \langle U_\alpha \rvert$	Density matrix $\rho_\alpha = \exp(-\beta H_\alpha)$
Wavefunction $\lvert U_\alpha \rangle$	Purification ("wavefunction of DM") $\rho_\alpha = W_\alpha W_\alpha^\dagger$
Gauge transformation $\lvert U_\alpha \rangle \to e^{i\theta_\alpha} \lvert U_\alpha \rangle$	Gauge transformation $W_\alpha \to W_\alpha V_\alpha, \quad V_\alpha V_\alpha^\dagger = 1$

"Purification" restores the "wavefunction" (gauge structure) of mixed state.



Practical ways of deriving DM's geometry:

- Symmetric log derivative operator $\partial \rho(\alpha)/\partial \alpha = \{\rho, L\}$
- $\mathcal{S}^{ab} \equiv \mathrm{Tr}\left[\rho L^a L^b\right] = \mathcal{F}^{ab} + i\mathcal{U}^{ab}$

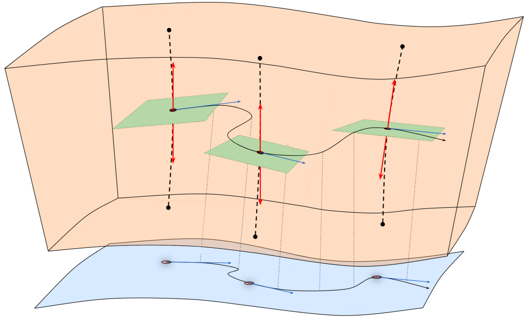
Uhlmann's parallel transport condition

$$W^\dagger \frac{\partial}{\partial t} W - \frac{\partial}{\partial t} W^\dagger W = 0$$

Armin Uhlmann (91): A Gauge Field Governing Parallel Transport Along Mixed States.

Geometry of density matrices

Purification $\rho_\alpha = W_\alpha W_\alpha^\dagger$



Practical ways of deriving DM's geometry:

- Symmetric log derivative operator

$$\frac{\partial \rho}{\partial \alpha_a} = \{\rho, L^a\}$$

- $\mathcal{S}^{ab} \equiv \mathrm{Tr}\left[\rho L^a L^b\right] = \underbrace{\mathcal{F}^{ab}}_{\text{Fisher info}} + i\underbrace{\mathcal{U}^{ab}}_{\text{Uhlmann curvature}}$

Fisher information as the distance measure of density matrices

Fidelity of DMs: $f(\rho, \rho') = \mathrm{Tr}\sqrt{\sqrt{\rho}\rho'\sqrt{\rho}}$ Wf's overlap: $|\langle u | u' \rangle|^2$

Bures distance: $D_B^2(\rho, \rho') = 1 - f(\rho, \rho')$ Wf's distance: $D^2 = 1 - |\langle u | u' \rangle|^2$

Fisher info: $D_B^2\left[\rho(\alpha), \rho(\alpha + \delta\alpha)\right] = \mathcal{F}^{ab}(\alpha) d\alpha_a d\alpha_b$ Wf's metric: $D^2 = g^{ab}(k) dk_a dk_b$

Fisher information and quantum metrology: Cramér-Rao bound

Set the lower bound of the parameter estimation: $|\Delta\alpha|^2 \geq 1/\left[N\,\mathrm{Tr}\mathcal{F}(\alpha)\right]$.

Entanglement witness and observable

Tell if a system is N-particle entangled.

Theory: Hauke, Heyl, Tagliacozzo and Zoller, Nat-Phy (16); Qimiao Si group (25);

Experiment: Jianming Cai group; Matteo Mitrano group, ……

Phase transition in the absence of order parameter (B. Mera et al PRL 17)

Geometrical sum rules for all temperature

Setting: Hamiltonian parameterized by ϕ at inverse temperature β: $H(\phi) = H_0 + \sum_a \mathcal{O}^a \phi_a + O(\phi^2)$

On the geometry side:

$\partial\rho/\partial\phi_a = \{\rho, L^a\}$

$L^a(t) = e^{iHt/\hbar} L^a e^{-iHt/\hbar}$

$\mathcal{S}_L^{ab}(t-t') \equiv \langle L^a(t) L^b(t') \rangle$

On the response side:

$\chi_{\mathcal{O}}^{ab}(t-t') = -i\Theta(t-t')\langle [\mathcal{O}^a(t), \mathcal{O}^b(t')] \rangle$

$\chi_{\mathcal{O};D}^{ab}(\omega) = [\chi^{ab}(\omega) - \chi^{ba}(-\omega)]/2i$

$\mathcal{S}_{\mathcal{O}}^{ab}(t-t') \equiv \langle \mathcal{O}^a(t) \mathcal{O}^b(t') \rangle$

Applying fluctuation-dissipation theorem

$$\chi_{\mathcal{O};D}^{ab}(\omega) = -\frac{1}{2}\left(1 - e^{-\beta\omega}\right) \mathcal{S}_{\mathcal{O}}^{ab}(\omega)$$

And relation of two-point functions

$$\mathcal{S}_{\mathcal{O}}^{ab}(\omega) = \omega^2 \coth^2\left(\frac{\beta\omega}{2}\right) \mathcal{S}_L^{ab}(\omega)$$

Generating function for sum rules

$$-\frac{1}{2\hbar} S^{ab}(\omega) = \frac{\tanh^2(\beta\omega/2)}{1 - e^{-\beta\omega}} \frac{\chi_D^{ab}(\omega)}{\omega^2}$$

New results for orbital magnetization sum rules

0_{th} **moment** $\int_{-\infty}^{\infty} d\omega$

Hauke, Heyl, Tahliacozzo, Zoller 16

$$\frac{\pi}{2V}\frac{e^2}{\hbar}F^{ab} = \int_0^\infty d\omega\ \tanh\left(\frac{\hbar\beta\omega}{2}\right)\frac{\Re\sigma_D^{ab}(\omega)}{\omega}$$

Zero T limit

$$\frac{\pi}{2V}\frac{e^2}{\hbar}\mathcal{Q}^{ab} = \int_0^\infty d\omega \frac{\sigma_D^{ab}(\omega, T=0)}{\omega}$$

Leonforte, Valenti, Spagnolo, Carollo 19

$$\frac{\pi}{2V}\frac{e^2}{\hbar}U^{ab} = \int_0^\infty d\omega\ \tanh^2\left(\frac{\hbar\beta\omega}{2}\right)\frac{\Im\sigma_D^{ab}(\omega)}{\omega}$$

$$\frac{\tanh^2\left(\frac{\beta\omega}{2}\right)}{1-e^{-\beta\omega}}\frac{\sigma_D^{ab}(\omega)}{\omega} = \frac{1}{2}S^{ab}(\omega)$$

Dissipation Geometry

$$-\frac{\pi e}{\hbar}\mathcal{M}(T=0) = \frac{\pi}{2V}\frac{e^2}{\hbar}\epsilon_{ab}\mathcal{U}_{(1)}^{ab}(T=0)$$

Resta (20) $= \epsilon_{ab}\int_0^\infty d\omega\ \Im[\sigma_D^{ab}(\omega)]$

[Orbital magnetization sum rule (new)]()

Zero T limit

1_{st} **moment** $\int_{-\infty}^{\infty} d\omega \times \omega$

$$-\frac{\pi e}{\hbar}\mathcal{M} = \epsilon_{ab}\int_0^\infty d\omega\ \coth\left(\frac{\beta\omega}{2}\right)\Im[\sigma_D^{ab}(\omega)]$$

$$\frac{\pi}{2V}\frac{e^2}{\hbar}\mathcal{U}_{(1)}^{ab} = \int_0^\infty d\omega\ \tanh\left(\frac{\hbar\beta\omega}{2}\right)\Im[\sigma_D^{ab}(\omega)]$$

Reduces to T=0 OM sum rule Resta (20)

Positivity of geometry and constrains

Time-dependent geometry is a “non-negative function”

$$\mathcal{S}^{ab}(t-t') \equiv \langle \mathcal{O}^a(t)\mathcal{O}^b(t')\rangle$$

For any $X_a(t)$, there is $\int dt \int dt' X_a^\dagger(t)\mathcal{S}^{ab}(t-t')X_b(t') \geq 0$

This means its “Hankel matrix” and its “principle minors” are non-negative

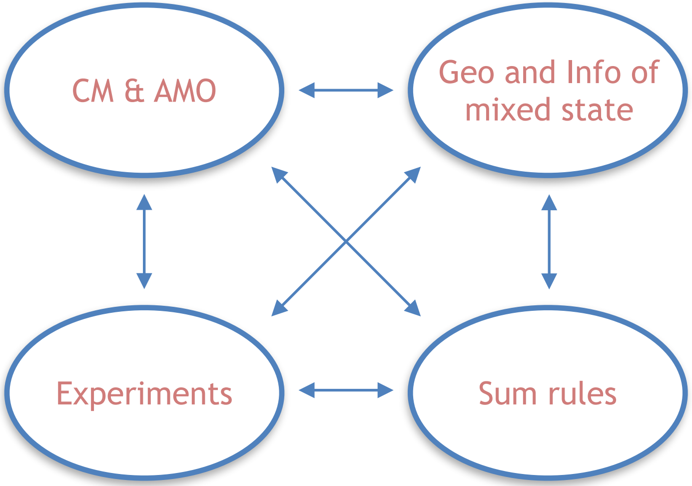
$$\mathcal{S}^{ab}_{(n)} = \partial_t^n \mathcal{S}^{ab}(t)|_{t=0}$$

$$\begin{bmatrix} \begin{bmatrix} \mathcal{S}^{11}_{(0)} & \mathcal{S}^{11}_{(1)} & \mathcal{S}^{11}_{(2)} & \cdots \\ \mathcal{S}^{11}_{(1)} & \mathcal{S}^{11}_{(2)} & \mathcal{S}^{11}_{(3)} & \cdots \\ \mathcal{S}^{11}_{(2)} & \mathcal{S}^{11}_{(3)} & \mathcal{S}^{11}_{(4)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} & \begin{bmatrix} \mathcal{S}^{12}_{(0)} & \mathcal{S}^{12}_{(1)} & \mathcal{S}^{12}_{(2)} & \cdots \\ \mathcal{S}^{12}_{(1)} & \mathcal{S}^{12}_{(2)} & \mathcal{S}^{12}_{(3)} & \cdots \\ \mathcal{S}^{12}_{(2)} & \mathcal{S}^{12}_{(3)} & \mathcal{S}^{12}_{(4)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} & \cdots \\ \begin{bmatrix} \mathcal{S}^{21}_{(0)} & \mathcal{S}^{21}_{(1)} & \mathcal{S}^{21}_{(2)} & \cdots \\ \mathcal{S}^{21}_{(1)} & \mathcal{S}^{21}_{(2)} & \mathcal{S}^{21}_{(3)} & \cdots \\ \mathcal{S}^{21}_{(2)} & \mathcal{S}^{21}_{(3)} & \mathcal{S}^{21}_{(4)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} & \begin{bmatrix} \mathcal{S}^{22}_{(0)} & \mathcal{S}^{22}_{(1)} & \mathcal{S}^{22}_{(2)} & \cdots \\ \mathcal{S}^{22}_{(1)} & \mathcal{S}^{22}_{(2)} & \mathcal{S}^{22}_{(3)} & \cdots \\ \mathcal{S}^{22}_{(2)} & \mathcal{S}^{22}_{(3)} & \mathcal{S}^{22}_{(4)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

Consequences (infinity number of bounds):

- $\mathcal{S}^{ii}_{(n)} \geq 0$
- $\det \mathcal{S}_{(2n)} \geq 0$
- **Cauchy-Schawtz** $\mathcal{S}^{jj}_{(2m)}\mathcal{S}^{kk}_{(2n)} - |\mathcal{S}^{jk}_{(m+n)}|^2 \geq 0$
- ……

Conclusion and acknowledgements



Density matrix geometry and sum rules

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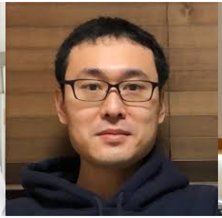
Tomoki Ozawa


Bruno Mera

Thank you for your attention!