

Density Matrix Geometry and Response Functions

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Guan and Bradlyn, Phys. Rev. Research 8, 013291 (2026)
Bradlyn, arXiv:2608.06326 (2026)

Background: Quantum Geometric Tensor

- Given $|\psi_0(\lambda)\rangle$ parametrized by $\lambda = (\lambda_1, \dots, \lambda_\mu, \dots, \lambda_n)$, the quantum geometric tensor (QGT) $Q_{\mu\nu}$ is defined as

$$Q_{\mu\nu}(\lambda) = \langle \partial_{\lambda_\mu} \psi_0(\lambda) | (1 - |\psi_0(\lambda)\rangle\langle\psi_0(\lambda)|) | \partial_{\lambda_\nu} \psi_0(\lambda) \rangle$$

gauge-invariant
and Hermitian

A black arrow points from the definition of $Q_{\mu\nu}$ to the equation $Q_{\mu\nu} = G_{\mu\nu} - \frac{i}{2} F_{\mu\nu}$. A blue arrow points from $G_{\mu\nu}$ to its description below. A red arrow points from $F_{\mu\nu}$ to its description below.

$$\longrightarrow Q_{\mu\nu} = G_{\mu\nu} - \frac{i}{2} F_{\mu\nu}$$

Real and symmetric
Fubini-Study (FS) metric $G_{\mu\nu}$

Imaginary and anti-symmetric
Berry curvature $F_{\mu\nu}$

Background: Berry Curvature $F_{\mu\nu}$

$$F_{\mu\nu} = 2\text{Im}\langle\partial_{\lambda_\nu}\psi_0(\boldsymbol{\lambda})|\partial_{\lambda_\mu}\psi_0(\boldsymbol{\lambda})\rangle$$

- **Noninteracting** limit: $\lambda_\mu =$ crystal momentum k_μ , $|\psi_0\rangle = |u_n(\mathbf{k})\rangle$



- **Interacting** systems: $\lambda_\mu =$ twist angle ϕ_μ , $|\psi_0\rangle = |GS(\boldsymbol{\phi})\rangle$



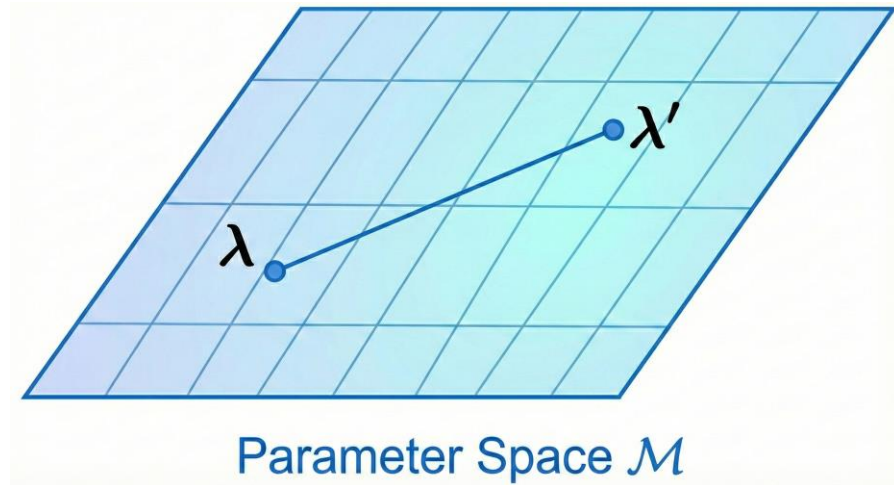
- For a non-degenerate gapped ground state of $U(1)$ -symmetric Hamiltonian with finite-range interactions, quantum Hall σ_H is

$$\sigma_H = \frac{e^2}{\hbar} 2\text{Im} \left\langle \partial_{\phi_\nu} GS \middle| \partial_{\phi_\mu} GS \right\rangle \Rightarrow \frac{e^2}{h} \sum_{n \in \text{occ}} \frac{1}{2\pi} \int_{BZ} dk_\nu dk_\mu 2\text{Im} \langle \partial_{k_\nu} u_n | \partial_{k_\mu} u_n \rangle$$

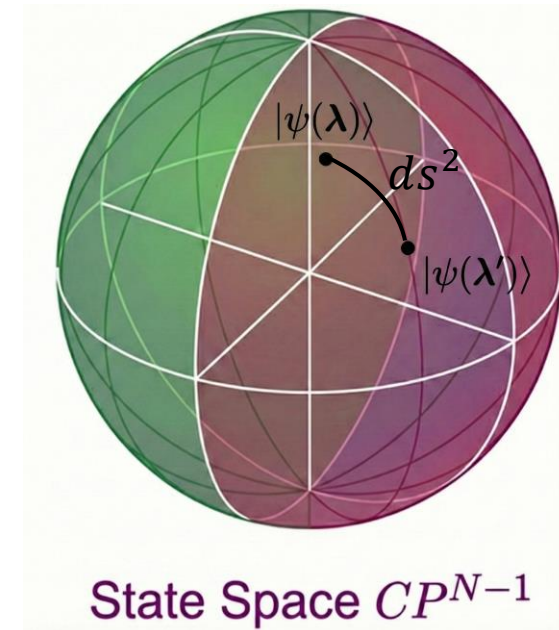
Background: Fubini-Study Metric $G_{\mu\nu}$

$$G_{\mu\nu} = \frac{1}{2} \text{Tr} \left[\partial_{\lambda_\mu} P(\lambda) \partial_{\lambda_\nu} P(\lambda) \right] \quad P(\lambda) = |\psi_0\rangle\langle\psi_0|$$

- Quantum distance between $|\psi_0(\lambda)\rangle$ and $|\psi_0(\lambda + d\lambda)\rangle$
 $ds^2 = G_{\mu\nu}(\lambda) d\lambda^\mu d\lambda^\nu$

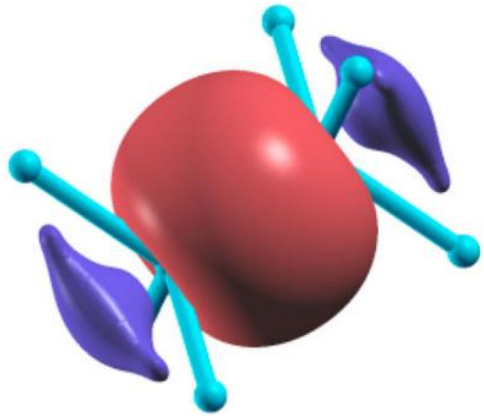


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Background: Fubini-Study Metric $G_{\mu\nu}$

- Noninteracting: measure **localizability** of Wannier function $|w_R\rangle$



$$\langle w_R | (\hat{x} - R)^2 | w_R \rangle = \frac{V_{cell}}{(2\pi)^d} \sum_{\mu=1}^d \int d^d k [G_{\mu\mu}(\mathbf{k}) + (A^\mu(k))^2]$$

Marzari & Vanderbilt (1997)

- Interacting systems: **polarization fluctuation**

$$G_{\mu\nu}(\boldsymbol{\phi}) = \frac{1}{V} \left[\langle X_\mu X_\nu \rangle_0 - \langle X_\mu \rangle \langle X_\nu \rangle_0 \right]$$

Souza et al. (2000)

Background: Several Applications

- QGT $Q_{\mu\nu}(\phi)$ probed by absorptive conductivity via SWM sum rule

$$Q_{\mu\nu} = \frac{1}{\pi} \int_0^\infty d\omega \frac{\sigma_{abs}^{\mu\nu}(\omega)}{\omega} \quad \sigma_{abs}^{\mu\nu}(\omega) = \frac{1}{2} [\sigma^{\mu\nu}(\omega) + \sigma^{\nu\mu}(\omega)^*]$$

- Topological bound via positivity of $Q_{\mu\nu}$

$$E_g \leq \frac{2\pi\hbar^2 n}{|C|m} \text{ (Chern bound)}$$

- Criteria for ideal Chern bands from GMP algebra analogy
- Superfluid weight in flat-band superconductors
- ...

Motivation

- Limitations

- (1) linear order

- (2) zero temperature

- (3) noninteracting fermions + crystal momentum

- (4) Interacting fermions + twist angle parameterization

Motivation: Current frameworks beyond noninteracting QGT

	Finite Temperature	Interaction /Disorder	Generic Parameter	Higher-Order
SWM sum rule [Souza et al. 2000]	✗	✓	✗	✗
Quantum Fisher Info [Hauke et al. 2016]	✓	✓	✓	✗
Nonlinear (Optical) Response [Ahn et al. 2021]	✗	✗	✗	✓
Time-dependent QGT [Verma et al. 2024, Ji et al. 2025, etc]	✓	✓	✗ → ✓	✗

Motivation

- Limitations

- (1) linear order

- (2) zero temperature

- (3) noninteracting fermions + crystal momentum

- (4) Interacting fermions + twist angle parameterization

- Question

Can we develop a unified geometric framework beyond all four limits?

Bures Distance

- At finite T, pure state $\rightarrow$ density matrix
- $\forall$ purification $\{(|\psi_1\rangle, |\psi_2\rangle)\}$ of (ρ_1, ρ_2) ,

$$\text{Fidelity } F(\rho_1, \rho_2) = \left(\text{Tr} \sqrt{\sqrt{\rho_2} \rho_1 \sqrt{\rho_2}} \right)^2 \geq |\langle \psi_1 | \psi_2 \rangle|^2$$

- Bures distance d_B : minimized quantum distance

$$d_B(\rho_1, \rho_2) = \sqrt{2 - 2\sqrt{F(\rho_1, \rho_2)}} \leq \sqrt{2 - 2|\langle \psi_1 | \psi_2 \rangle|}$$

Specially, if (1) $\rho_1 = \rho_2$, $d_B = 0$; (2) $\rho_1 \perp \rho_2$, $F(\rho_1, \rho_2) = 0$, $d_B = \sqrt{2}$.

Methods: Bures Distance Expansion

- In the condensed matter scenario, we start from

$$\rho(t \rightarrow -\infty) = \rho_0 = e^{-\beta H_0} / Z_0$$

- Then apply (weak) perturbation δH

$$H = H_0 + \delta H = H_0 + \lambda f^\mu(t) B_\mu \eta(t) \quad \mu = 1, \dots, N$$

- Time-evolved $\rho(t)$ can be expanded as

$$\rho(t) = \rho_0 + \lambda \rho_1(t) + \lambda^2 \rho_2(t) + \dots$$
$$\rho_n(t) = (-i)^n \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{n-1}} dt_n \prod_{i=1}^n f^{\mu_i}(t_i) \eta(t_i) \times \underbrace{[B_{\mu_1}(t_1 - t), [B_{\mu_2}(t_2 - t), [\dots [B_{\mu_n}(t_n - t), \rho_0]]]]}_{n \text{ times}}.$$

➡ Functionals of $\{\lambda f^\mu(\tau)\}_{\tau \in (-\infty, t]}$

Methods: Bures Distance Expansion

$$d_B(\rho_0, \rho(t))^2 = 2 - 2\text{Tr} \sqrt{\sqrt{\rho_0} \rho(t) \sqrt{\rho_0}}$$

measures how distinct $\rho(t)$ is from its equilibrium ρ_0

- From RHS: expand d_B^2 via perturbation

Quantum Fisher
Information $F_Q[\rho_1]$

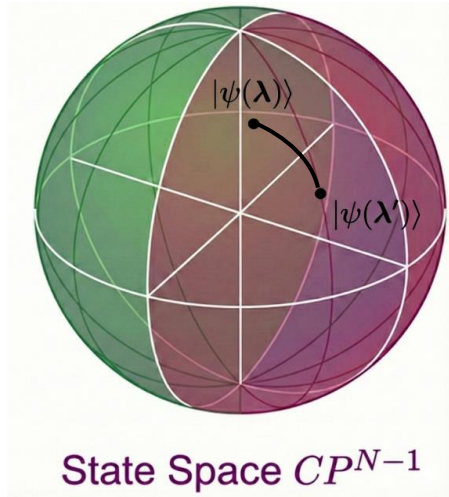
$$d_B(\rho_0, \rho(t))^2 = \frac{\lambda^2}{2} \sum_{nm} \frac{|\langle n | \rho_1 | m \rangle|^2}{p_n + p_m} + \mathcal{O}(\lambda^4)$$



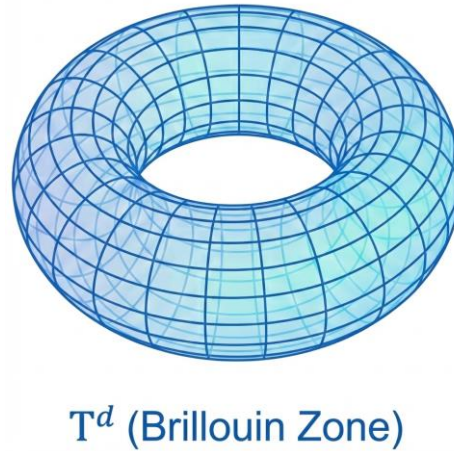
$$- \frac{\lambda^3}{2} \left(\sum_{n\ell\ell'} \frac{\langle n | \rho_1 | \ell' \rangle \langle \ell' | \rho_1 | \ell \rangle \langle \ell | \rho_1 | n \rangle}{(p_\ell + p_n)(p_n + p_{\ell'})} - \sum_{n\ell} \frac{\langle n | \rho_2 | \ell \rangle \langle \ell | \rho_1 | n \rangle + \langle n | \rho_1 | \ell \rangle \langle \ell | \rho_2 | n \rangle}{p_n + p_\ell} \right)$$

Interpretation of Geometry

Band Theory



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→



Manifold	T^d
Coordinates	$(k^1, \dots, k^d)$
Tangent vector	$\{\Delta k^\mu\}$
Distance	$ds^2 = g_{\mu\nu}(\mathbf{k}) \Delta k^\mu \Delta k^\nu$

Our framework

Space of Density Matrices D

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↓

Function Space F

Manifold	function space F (infinite-dimensional)
Coordinates	$\{f^\mu(\tau)\}_{\tau \in (-\infty, t]}$
Tangent vector	$\{\delta f^\mu(\tau)\}_{\tau \in (-\infty, t]}$
Distance	$ds^2 = \int dt_1 dt_2 \, \underline{g_{(\mu, t_1)(\nu, t_2)}[\mathbf{f}(\tau)]} \delta f^\mu(t_1) \delta f^\nu(t_2)$ $\nearrow g_{\mu\nu}(\mathbf{f}, t, t_1, t_2)$

Methods: Bures Distance Expansion

$$d_B(\rho_0, \rho(t))^2 = 2 - 2\text{Tr} \sqrt{\sqrt{\rho_0} \rho(t) \sqrt{\rho_0}}$$

- From LHS: treat $\{\lambda f^\mu(t)\}$ as coordinates on a manifold

$$d_B(\rho_0, \rho(t)) = \int_0^\lambda d\lambda' \sqrt{\int dt_1 dt_2 g_{\mu\nu}(\lambda \mathbf{f}, t, t_1, t_2) f^\mu(t_1) f^\nu(t_2)}$$

infinitesimal line element

Methods: Bures Distance Expansion

$$d_B(\rho_0, \rho(t))^2 = 2 - 2\text{Tr}\sqrt{\sqrt{\rho_0}\rho(t)\sqrt{\rho_0}}$$

- From LHS: expanding $g_{\mu\nu}(\lambda\mathbf{f}, t, t_1, t_2)$ near $\lambda\mathbf{f} = 0$ yields

$$\begin{aligned} d_B(\rho_0, \rho(t))^2 = & \lambda^2 \int dt_1 dt_2 g_{\mu\nu}(t, t_1, t_2) f^\mu(t_1) f^\nu(t_2) \\ & + \lambda^3 \int dt_1 dt_2 dt_3 \Gamma_{\mu\lambda\nu}(0, t, t_1, t_3, t_2) f^\mu(t_1) f^\nu(t_2) f^\lambda(t_3) + \mathcal{O}(\lambda^4) \end{aligned}$$

Methods: Bures Distance Expansion

Matching LHS and RHS of d_B^2 order-by-order gives

(1) Bures Metric at $\mathcal{O}(\lambda^2)$

$$\int dt_1 dt_2 g_{\mu\nu}(t, t_1, t_2) f^\mu(t_1) f^\nu(t_2) = \frac{1}{2} \sum_{nm} \frac{|\langle n | \rho_1 | m \rangle|^2}{p_n + p_m}$$

$$g_{\mu\nu}(t, t_1, t_2) = -\frac{1}{2\pi} \underbrace{\prod_{i=1}^2 e^{\epsilon(t_i - t)} \Theta(t - t_i)}_{\text{Causality}} \operatorname{Re} \left[\int d\omega e^{i\omega(t_1 - t_2)} \underbrace{\tanh \frac{\beta\omega}{2}}_{\text{Thermal Weight}} \underbrace{\chi''_{\nu\mu}(\omega)}_{\text{Spectral density}} \right]$$

$$\text{spectral density } \chi''_{\nu\mu}(\omega) = -\frac{1}{2} \int dt e^{i\omega t} \langle [B_\nu(t), B_\mu(0)] \rangle_0$$

Methods: Bures Distance Expansion

(2) **Bures Connection** at $\mathcal{O}(\lambda^3)$

$$\int dt_1 dt_2 dt_3 \Gamma_{\lambda\mu\nu}(t, t_1, t_2, t_3) f^\mu(t_1) f^\nu(t_2) f^\lambda(t_3) \equiv \Gamma^f(t) + \Gamma^{\text{in}}(t)$$

Methods: Bures Distance Expansion

(2) Bures Connection at $\mathcal{O}(\lambda^3)$

- Fisher term

$$\Gamma^f(t) = \frac{1}{2} \sum_{n\ell} \frac{\langle n | \rho_2 | \ell \rangle \langle \ell | \rho_1 | n \rangle + \langle n | \rho_1 | \ell \rangle \langle \ell | \rho_2 | n \rangle}{p_n + p_\ell}$$

accessible from expanding **Quantum Fisher Information**

$$\frac{1}{4} F_Q[\delta\rho] = \frac{1}{2} \sum_{n\ell} \frac{|\langle n | \delta\rho | \ell \rangle|^2}{p_n + p_\ell} \quad \delta\rho = \lambda\rho_1 + \lambda^2\rho_2 + \dots$$

Methods: Bures Distance Expansion

(2) Bures Connection at $\mathcal{O}(\lambda^3)$

- Fisher term

$$\Gamma_{\mu_1\mu_2\mu_3}^f(t, t_1, t_2, t_3) = \frac{\Theta(t_1 - t_2)}{6\pi^2} \prod_i \Theta(t - t_i) e^{\epsilon t_i} \operatorname{Im} \left[\int d\omega_1 d\omega_2 \tanh \frac{\beta(\omega_1 - \omega_2)}{2} \right. \\ \left. \times e^{i[(\omega_1 - \omega_2)t_3 + \omega_2 t_2 - \omega_1 t_1]} \chi''_{\mu_1\mu_3\mu_2}(\omega_1, \omega_2) \right] + \{(\mu_i, t_i) \leftrightarrow (\mu_j, t_j)\}$$

second-order spectral density

$$\chi''_{\mu_1\mu_3\mu_2}(\omega_1, \omega_2) = \frac{1}{4} \int dt_1 dt_2 e^{i\omega_1 t_1} e^{i\omega_2 t_2} \times \langle [[B_{\mu_1}(0), B_{\mu_3}(-t_1)], B_{\mu_2}(-t_1 - t_2)] \rangle_0$$

Bradlyn & Abbamonte, Phys. Rev. B 110, 245132 (2024).

Methods: Bures Distance Expansion

(2) **Bures Connection** at $\mathcal{O}(\lambda^3)$

- Intrinsic term

$$\Gamma^{\text{in}}(t) = -\frac{1}{2} \sum_{n\ell\ell'} \frac{\langle n | \rho_1 | \ell' \rangle \langle \ell' | \rho_1 | \ell \rangle \langle \ell | \rho_1 | n \rangle}{(p_\ell + p_n)(p_n + p_{\ell'})}$$

appears at each order of the Bures distance expansion.

Methods: Bures Distance Expansion

(2) Bures Connection at $\mathcal{O}(\lambda^3)$

- Intrinsic term

$$\Gamma_{\mu_1\mu_2\mu_3}^{\text{in}}(t, t_1, t_2, t_3) = -\frac{1}{12} \prod_i \Theta(t - t_i) e^{\epsilon t_i} \text{Im} \left[\int d\omega_1 d\omega_2 \tanh \frac{\beta\omega_1}{2} \tanh \frac{\beta(\omega_1 - \omega_2)}{2} \right. \\ \left. \times e^{i[(\omega_1 - \omega_2)t_3 + \omega_2 t_2 - \omega_1 t_1]} S_{\mu_1\mu_3\mu_2}(\omega_1, \omega_2) \right] + \{(\mu_i, t_i) \leftrightarrow (\mu_j, t_j)\}.$$

$$\chi''_{\mu_1\mu_3\mu_2}(\omega_1, \omega_2) = -\pi^2 \left[S_{\mu_1\mu_3\mu_2}(\omega_1, \omega_2) - S_{\mu_3\mu_1\mu_2}(\omega_2 - \omega_1, \omega_2) \right]$$

$$S_{\mu_1\mu_3\mu_2}(\omega_1, \omega_2) = \frac{1}{4\pi^2} \int dt_1 dt_2 e^{i\omega_1 t_1} e^{i\omega_2 t_2} \langle [B_{\mu_3}(-t_1) B_{\mu_1}(0), B_{\mu_2}(-t_1 - t_2)] \rangle_0$$

independent of second-order response

Advantages of Our Framework

	Finite Temperature	Interaction /Disorder	Generic Parameter	Higher-Order
SWM Sum Rule	✗	✓	✗	✗
Quantum Fisher Info	✓	✓	✓	✗
Nonlinear (Optical/Hall) Response	✗	✗	✗	✓
Time-dependent QGT	✓	✓	✗ → ✓	✗
Our Framework	✓	✓	✓	✓

Advantages of Our Framework

	Finite Temperature	Interaction /Disorder	Generic Parameter	Higher-Order
SWM Sum Rule	×	✓	×	×
Quantum Fisher Info	✓	✓	✓	×
Nonlinear (Optical/Hall) Response	×	×	×	✓
Time-dependent QGT	✓	✓	× → ✓	×
Our Framework	✓	✓	✓	✓

Bures Metric
$$g_{\mu\nu}(t - t_1, t - t_2) = -\frac{1}{2\pi} \prod_{i=1}^2 e^{\epsilon(t_i - t)} \Theta(t - t_i) \text{Re} \left[\int d\omega e^{i\omega(t_1 - t_2)} \tanh \frac{\beta\omega}{2} \chi''_{\nu\mu}(\omega) \right]$$

Advantages of Our Framework

	Finite Temperature	Interaction /Disorder	Generic Parameter	Higher-Order
SWM Sum Rule	×	✓	×	×
Quantum Fisher Info	✓	✓	✓	×
Nonlinear (Optical/Hall) Response	×	×	×	✓
Time-dependent QGT	✓	✓	× → ✓	×
Our Framework	✓	✓	✓	✓

Bures connection $\Gamma_{\mu\nu\lambda} \leftrightarrow S_{\mu\nu\lambda}(\omega_1, \omega_2)$

Advantages of Our Framework

	Finite Temperature	Interaction /Disorder	Generic Parameter	Higher-Order
SWM Sum Rule	×	✓	×	×

Apply it to three **experimentally relevant limits**

independent QGT	✓	✓	∧ → ✓	×
Our Framework	✓	✓	✓	✓

Applications of the Bures Metric

- Quasistatic limit: $f^\mu(t) = f^\mu$

$$g_{\mu\nu}^{\text{q.s.}} = -\frac{1}{2\pi} \int d\omega \frac{1}{\omega^2} \tanh \frac{\beta\omega}{2} \text{Re} \chi''_{\nu\mu}(\omega)$$

Ji et al. (2025)

- Instantaneous limit: $f^\mu(t) = f^\mu \delta(t)$

$$g_{\mu\nu}^{\text{inst}}(t) = -\frac{1}{2\pi} \Theta(t) \int d\omega \tanh \frac{\beta\omega}{2} \text{Re} \chi''_{\nu\mu}(\omega)$$

Hauke et al. (2016)

Results in different limits are unified in our framework.

- Infinite-time limit: $f^\mu(|t| \rightarrow \infty) \rightarrow 0$

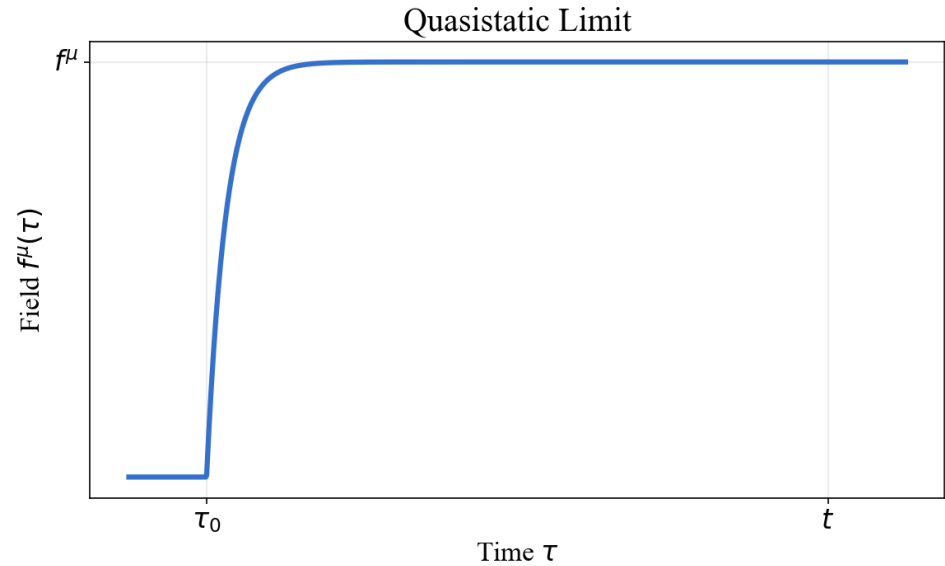
$$d_B^2(\rho_0, \rho(t \rightarrow \infty)) = -\frac{\kappa^2}{2\pi} \int d\omega \tanh \frac{\beta\omega}{2} \boxed{\bar{f}^\nu(-\omega) \chi''_{\nu\mu}(\omega) \bar{f}^\mu(\omega)} + \mathcal{O}(\kappa^3)$$

A new geometric interpretation of Fermi's golden rule

Applications of the Bures Metric

- Quasistatic Limit $f^\mu(t) \rightarrow f^\mu$
- Current perturbation

$$H_A = H_0 - \sum_{n=1}^{\infty} \frac{1}{n!} j^{\mu_1 \dots \mu_n} A_{\mu_1} \dots A_{\mu_n}$$



- **Finite-temperature** twist-angle metric and SWM sum rule

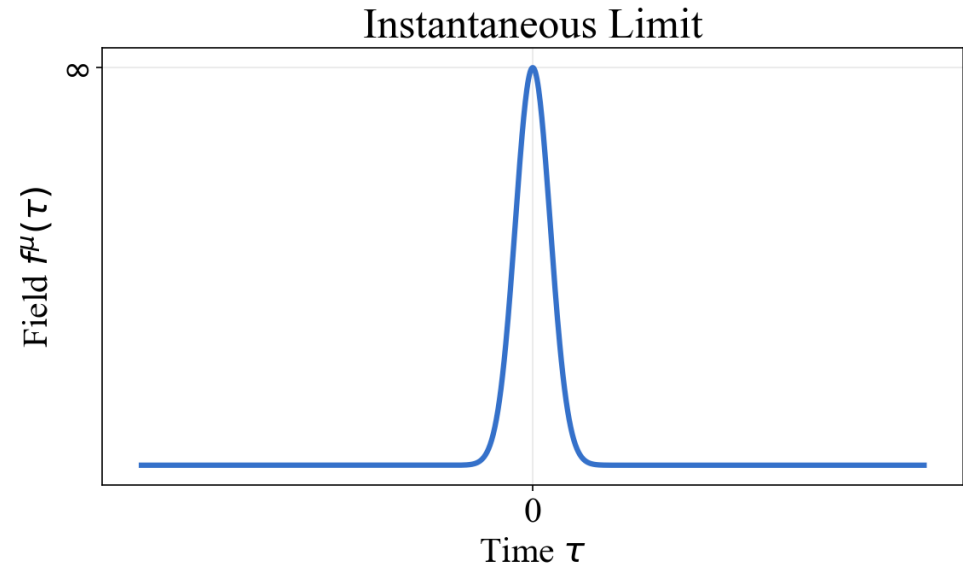
$$g_{\mu\nu}^{\text{q.s.}} = \frac{V}{\pi} \int_{0+}^{\infty} d\omega \frac{1}{\omega} \tanh \frac{\beta\omega}{2} \text{Re} \sigma_{\text{abs}}^{\mu\nu}(\omega)$$

Dissipative conductivity $\sigma_{\text{abs}}^{\mu\nu}(\omega) = \pi \delta(\omega) D^{\mu\nu} - \text{P} \frac{1}{V\omega} [\chi'']^{\mu\nu}(\omega)$

Applications of the Bures Metric

- Instantaneous Limit $f^\mu(t) = f^\mu \delta(t)$
- Density perturbation

$$\delta H = \frac{1}{V} \sum_{\mathbf{q}} \phi_{\mathbf{q}} \delta(t) \rho_{-\mathbf{q}}$$



- Instantaneous metric

$$g_{\mathbf{q}}(t) = \frac{\Theta(t)}{4\pi} \int_0^\infty d\omega \tanh \frac{\beta\omega}{2} (1 - e^{-\beta\omega}) [S(\mathbf{q}, \omega) + S(-\mathbf{q}, \omega)]$$

Dynamic structure factor $S(\mathbf{q}, \omega) = \frac{1}{V} \int dt e^{i\omega t} \langle \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) \rangle_c$

Applications of the Bures Metric

- In the zero temperature and **long-wavelength** limit,

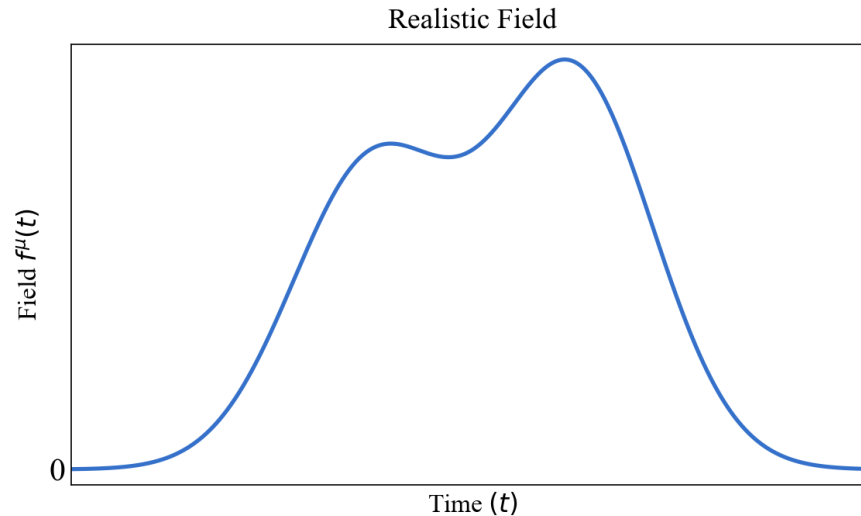
$$g_{\mathbf{q}}(t) = \Theta(t) q_{\mu} q_{\nu} \frac{1}{V} g_{\text{q.s.}}^{\mu\nu}.$$

- For any pair of operators B_{μ} and C_{μ} satisfying $C_{\mu} = \partial_t B_{\mu} = i [H_0, B_{\mu}]$

$$g_{B_{\mu} B_{\nu}}^{\text{inst}}(t) = \Theta(t) g_{C_{\mu} C_{\nu}}^{\text{q.s.}}$$

Applications of the Bures Metric

- Infinite-time limit $f^\mu(|t| \rightarrow \infty) \rightarrow 0$ and $t \rightarrow +\infty$



$$\lim_{t \rightarrow \infty} \int dt_1 dt_2 g_{\mu\nu}(t - t_1, t - t_2) f^\mu(t_1) f^\nu(t_2) = -\frac{1}{2\pi} \int d\omega \tanh \frac{\beta\omega}{2} \bar{f}^\nu(-\omega) \chi''_{\nu\mu}(\omega) \bar{f}^\mu(\omega)$$

- Taking derivative w.r.t. $\bar{f}^\mu(\omega)$ yields

$$\bar{g}_{\mu\nu}(\omega_1, \omega_2) = -\frac{1}{2\pi} \delta(\omega_1 + \omega_2) \tanh \frac{\beta\omega_1}{2} \chi''_{\mu\nu}(\omega_1)$$

Applications of the Bures Metric

Limits	Perturbations	Bures metric
Quasistatic	$-j^\mu A_\mu + \mathcal{O}(A^2)$	$\frac{V}{\pi} \int_0^\infty d\omega \frac{1}{\omega} \tanh \frac{\beta\omega}{2} \text{Re}\sigma_{\text{abs}}^{\mu\nu}(\omega)$
Instantaneous	$\frac{1}{V} \sum_{\mathbf{q}} \phi_{\mathbf{q}} \delta(t) \rho_{-\mathbf{q}}$	$\frac{\Theta(t)}{4\pi} \int_0^\infty d\omega \tanh \frac{\beta\omega}{2} (1 - e^{-\beta\omega}) [S(\mathbf{q}, \omega) + S(-\mathbf{q}, \omega)]$
Infinite Time	any	$-\frac{1}{2\pi} \delta(\omega_1 + \omega_2) \tanh \frac{\beta\omega_1}{2} \chi''_{\mu\nu}(\omega_1)$

Application: Bures Connection

- Quasistatic limit + current perturbation $H_A = H_0 - \sum_{n=1}^{\infty} \frac{1}{n!} j^{\mu_1 \dots \mu_n} A_{\mu_1} \dots A_{\mu_n}$

Must consider **diamagnetic contributions** beyond $\lambda f^\mu(t) B_\mu \eta(t)$!

$$\rho_1(t) = i \int_{-\infty}^t dt_1 A_\mu(t_1) [j^\mu(t_1 - t), \rho_0]$$

$$\rho_2(t) = - \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \left(A_\mu(t_1) A_\nu(t_2) [j^\mu(t_1 - t), [j^\nu(t_2 - t), \rho_0]] \right)$$

$$+ \left[\frac{i}{2} \int_{-\infty}^t dt_1 A_\mu(t_1) A_\nu(t_1) [j^{\mu\nu}(t_1 - t), \rho_0] \right],$$

Bures Connection: free fermions at $T = 0$

- Band-theoretic Christoffel symbol

Definitions:

$$r_{\alpha\beta\mathbf{k}}^{\mu} = \langle u_{\alpha\mathbf{k}} | i\partial_{k_{\mu}} | u_{\beta\mathbf{k}} \rangle$$

$$\Gamma^{\mu\nu\lambda}(\mathbf{k}) = \frac{1}{2} (\partial^{\nu} g^{\mu\lambda}(\mathbf{k}) + \partial^{\lambda} g^{\mu\nu}(\mathbf{k}) - \partial^{\mu} g^{\nu\lambda}(\mathbf{k}))$$

$$g^{\mu\nu}(\mathbf{k}) = \sum_{\substack{\alpha \in \text{unocc} \\ \beta \in \text{occ}}} \text{Re}(r_{\alpha\beta\mathbf{k}}^{\mu} r_{\beta\alpha\mathbf{k}}^{\nu})$$

- Under quasistatic current perturbation:

$$\Gamma_{\text{q.s.}} = -V A_{\mu} A_{\nu} A_{\lambda} \int \frac{d^d \mathbf{k}}{(2\pi)^d} \Gamma^{\mu\nu\lambda}(\mathbf{k})$$

BZ average of the totally symmetric Christoffel symbol

- **Quasistatic Bures connection** is a many-body generalization of the Christoffel symbol, valid for **interacting systems at finite T** .

Multi-State Geometry of Density Matrices and Rectification Sum Rules

Barry Bradlyn, arXiv:2608.06326 (2026)

- The same formalism can be extended to the other quantities in quantum information geometry.
- In QIG, the mixture/exponential connection is not compatible with the metric.

Amari & Nagaoka, Methods of Information Geometry (2000)

- This **non-metricity term** is exactly the **multi-state geometric contribution** in the sum rule for the **shift current** conductivity.

Nonlinear Optical Response

- A weak electric field induces a second-order current density

$$j_{(2)}^{\mu}(\omega) = \int d\omega_1 d\omega_2 \delta(\omega - \omega_1 - \omega_2) \sigma^{\mu;\nu\lambda}(\omega_1, \omega_2) E_{\nu}(\omega_1) E_{\lambda}(\omega_2)$$

$$E_{\nu}(t) = \int d\omega E_{\nu}(\omega) e^{-i\omega t}$$

Monochromatic input at $\pm\omega$	Output frequency	Current response
$\omega_1 = \omega_2 = \pm\omega$	$\pm 2\omega$	Second harmonic
$\omega_1 = -\omega_2$	0	Rectification

Rectification: Drude, Injection, and Shift

Selected Contribution	Physical picture
Nonlinear Drude	Low-frequency acceleration of mobile carriers
Injection current	Current grows during illumination until relaxation
Shift current	Polarization changes during an optical transition

And additional frequency-dependent terms

Next step: a sum rule for the shift current contribution

Motivation: A Nonlinear SWM Sum Rule

Linear SWM sum rule at T=0

$$G_{\mu\nu}(\phi) = \frac{1}{\pi} \int_0^\infty d\omega \frac{\text{Re}\sigma_{abs}^{\mu\nu}(\omega)}{\omega} = \frac{1}{V} \left[\langle X_\mu X_\nu \rangle_0 - \langle X_\mu \rangle \langle X_\nu \rangle_0 \right]$$

Nonlinear shift current sum rule

Band theory limit: the integrated shift response contains skewness of X_μ and a multi-state geometric contribution.

**What is this multi-state contribution
when interactions and disorder are present?**

Shift Response Beyond Band Theory

Consider a large but finite system with open boundaries

$$H_0|a\rangle = E_a|a\rangle, \quad p_a = e^{-\beta E_a}/Z, \quad X_{ac}^\mu = \langle a|X^\mu|c\rangle$$

X is the total position operator, V is the volume, and $\beta = 1/T$.

$$H'(t) = E_\nu(t)X^\nu, \quad J^\mu = i[H_0, X^\mu]$$

$$\sigma_{\text{shift}}^{\mu;\nu\lambda}(\omega) = \frac{2\pi}{V} \sum_{E_a > E_c} (p_a - p_c)(X_{cc}^\mu - X_{aa}^\mu)X_{ac}^\nu X_{ca}^\lambda \delta(\omega - E_a + E_c)$$

$$\langle J^\mu \rangle_{\text{DC}}/V = \int_0^\infty d\omega \sigma_{\text{shift}}^{\mu;\nu\lambda}(\omega) E_\nu(\omega) E_\lambda^*(\omega)$$

The Many-Body Rectification Sum Rule

Let $|0\rangle$ denote the ground state. Define its position fluctuation and skewness

$$\delta X^\mu = X^\mu - \langle X^\mu \rangle_0, \quad c_{\lambda\mu\nu}^{(3)} = \langle \delta X^\lambda \delta X^\mu \delta X^\nu \rangle_0$$

The zero-temperature complex distortion contains virtual excited states

$$S_{\lambda\mu\nu} \equiv \lim_{T \rightarrow 0} S_{\lambda\mu\nu}(T) = \sum'_{a,b>0} X_{0a}^\lambda X_{ab}^\mu X_{b0}^\nu$$

The prime excludes $E_\alpha = E_\beta$ terms.

$$\lim_{T \rightarrow 0} \frac{1}{\pi} \int_0^\infty d\omega \, \sigma_{\text{shift}}^{\mu;\nu\lambda}(\omega) = \frac{2}{V} (c_{\lambda\mu\nu}^{(3)} - S_{\lambda\mu\nu})$$

No assumption of clean bands or noninteracting electrons

Why Multi-State?

The correction contains matrix elements between two excited states

$$S_{\lambda\mu\nu} = \sum'_{a,b>0} X_{0a}^{\lambda} X_{ab}^{\mu} X_{b0}^{\nu}$$



The product follows the closed virtual path $0 \rightarrow b \rightarrow a \rightarrow 0$.

$S_{\lambda\mu\nu}$ cannot be written as a ground state quantity.

What the Optical Sum Rule Measures

Commuting position operators make the skewness real and symmetric

$$\frac{1}{\pi} \int_0^\infty d\omega \operatorname{Re} \sigma_{\text{shift}}^{\mu;\nu\lambda}(\omega) = \frac{2}{V} (c_{\lambda\mu\nu}^{(3)} - \operatorname{Re} S_{\lambda\mu\nu})$$

$$\frac{1}{\pi} \int_0^\infty d\omega \operatorname{Im} \sigma_{\text{shift}}^{\mu;\nu\lambda}(\omega) = -\frac{2}{V} \operatorname{Im} S_{\lambda\mu\nu}$$

Linear polarization probes the symmetric combination.

Circular polarization isolates the antisymmetric part of S.

Density Matrix Geometry: Notation

Use external fields $\lambda(t)$ as coordinates and $\partial_\mu = \delta/\delta\lambda^\mu(t)$

$$\rho(\lambda) = U(\lambda)\rho_0U^\dagger(\lambda), \quad \rho_\mu \equiv \partial_\mu\rho = \{G_\mu, \rho\}$$

G_μ is half the symmetric logarithmic derivative (SLD) at $T > 0$.

Object	Construction	Meaning
$Q_{\mu\nu}$	$G_\mu\rho G_\nu$	QGT operator
$g_{\mu\nu}$	$\text{Tr}(\rho\{G_\mu, G_\nu\})/2$	Bures metric
$\mathcal{F}_{\mu\nu}$	$-i\text{Tr}(\rho[G_\mu, G_\nu])/2$	Uhlmann curvature

$$\text{Tr } Q_{\mu\nu} = g_{\mu\nu} - i\mathcal{F}_{\mu\nu}$$

Mixture and Exponential Connections

A connection specifies how to compare tangent vectors at nearby states.

$$\rho_\nu = \partial_\nu \rho = \{G_\nu, \rho\}, \quad \Gamma_{\mu\nu\sigma} \equiv g(\nabla_{\partial_\mu} \partial_\nu, \partial_\sigma)$$

Mixture (m): differentiate the density matrix tangent vector ρ_ν

$$\Gamma_{\mu\nu\sigma}^{(m)} = \frac{1}{2} \text{Tr}(G_\sigma \rho_{\mu\nu}), \quad \rho_{\mu\nu} \equiv \partial_\mu \partial_\nu \rho$$

Exponential (e): differentiate the tangent vector G_ν

$$\Gamma_{\mu\nu\sigma}^{(e)} = \frac{1}{2} \text{Tr}(\rho_\sigma \partial_\mu G_\nu)$$

They form a dual pair with respect to the Bures metric:

$$\partial_\mu g_{\nu\sigma} = \Gamma_{\mu\nu\sigma}^{(m)} + \Gamma_{\mu\sigma\nu}^{(e)}$$

Non-Metricity of the Connection

Metric compatibility means $\nabla g = 0$ for the Bures metric

$$(\nabla_\sigma g)_{\mu\nu} = \partial_\sigma g_{\mu\nu} - \Gamma_{\sigma\mu\nu} - \Gamma_{\sigma\nu\mu}$$

Define the quantum Amari–Chentsov (QAC) tensor:

$$T_{\sigma\mu\nu} \equiv \Gamma_{\sigma\mu\nu}^{(m)} - \Gamma_{\sigma\mu\nu}^{(e)} = \frac{1}{2} \text{Tr}(\rho\{G_\sigma, \{G_\mu, G_\nu\}\})$$

$$(\nabla_\sigma^{(m)} g)_{\mu\nu} = -T_{\sigma\mu\nu}, \quad (\nabla_\sigma^{(e)} g)_{\mu\nu} = +T_{\sigma\mu\nu}$$

$$\nabla^{(0)} \equiv \frac{1}{2} (\nabla^{(m)} + \nabla^{(e)}), \quad \nabla^{(0)} g = \nabla^{\text{LC}} g = 0$$

Both preserve the metric. $\nabla^{(0)}$ generally has torsion, whereas Levi-Civita is torsion-free.

Connection to the Bures Expansion

The Levi-Civita connection follows from the Fisher connection and QAC

$$\Gamma_{\mu\nu\sigma}^{\text{LC}} = \underbrace{\Gamma_{\mu\nu\sigma}^{(m)}}_{\text{Fisher term}} - \underbrace{\frac{1}{2}(T_{\mu\nu\sigma} + T_{\nu\sigma\mu} - T_{\sigma\mu\nu})}_{\text{Intrinsic term (distortion)}}$$

$$\Gamma_{\mu\nu\sigma}^{(m)} = \frac{1}{2} \text{Tr}(G_{\sigma} \rho_{\mu\nu}), \quad \rho_{\mu\nu} \equiv \partial_{\mu} \partial_{\nu} \rho$$

$\Gamma_{\mu\nu\sigma}^{\text{LC}}$ and $\Gamma_{\mu\nu\sigma}^{(m)}$ are both torsion-free

non-metricity = distortion

The cQAC Tensor

The derivative of the QGT contains a density matrix variation

$$\partial_\sigma Q_{\mu\nu} = (\partial_\sigma G_\mu) \rho G_\nu + G_\mu \rho_\sigma G_\nu + G_\mu \rho (\partial_\sigma G_\nu)$$

The trace of the middle term defines the complex QAC (cQAC) tensor.

Object	Definition	Meaning
$T_{\sigma\mu\nu}$	$\frac{1}{2} \text{Tr}(\rho \{G_\sigma, \{G_\mu, G_\nu\}\})$	QAC tensor
$\Phi_{\sigma\mu\nu}$	$-\frac{i}{2} \text{Tr}(\rho \{G_\sigma, [G_\mu, G_\nu]\})$	Uhlmann curvature dipole
$Z_{\sigma\mu\nu}$	$\text{Tr}(G_\mu \rho_\sigma G_\nu) = T_{\sigma\mu\nu} - i\Phi_{\sigma\mu\nu}$	Complex QAC tensor

$$Z_{\sigma\mu\nu} = [\nabla_\sigma^{(e)} (g - i\mathcal{F})]_{\mu\nu}$$

The Complex Distortion Tensor

In the eigenbasis of ρ , let p_m denote its eigenvalues.

J rotates off-diagonal tangent directions and satisfies $J^2 = -1$.

$$(G_{J\partial_\mu})_{mn} = -i \operatorname{sgn}(p_m - p_n) (G_\mu)_{mn} \quad (p_m \neq p_n)$$

For tangent vectors u, v, w :

$$Z(u, v, w) \equiv \operatorname{Tr}[G_v u(\rho) G_w]$$

Object	Construction	Meaning
$\tilde{S}_{\sigma\mu\nu}$	$Z(J\partial_\sigma, J\partial_\mu, J\partial_\nu)$	J-rotated cQAC
$S_{\mu\sigma\nu}$	$\frac{1}{2} (\tilde{S}_{\mu\nu\sigma} + \tilde{S}_{\nu\sigma\mu} - \tilde{S}_{\sigma\mu\nu})$	Complex distortion

Complex distortion tensor enters the sum rule at $T \rightarrow 0$ limit.

Summary

$$\lim_{T \rightarrow 0} \frac{1}{\pi} \int_0^\infty d\omega \, \sigma_{\text{shift}}^{\mu;\nu\lambda}(\omega) = \frac{2}{V} (c_{\lambda\mu\nu}^{(3)} - S_{\lambda\mu\nu})$$

$$S_{\lambda\mu\nu} = \sum'_{a,b>0} X_{0a}^\lambda X_{ab}^\mu X_{b0}^\nu = \text{Complex Distortion}$$

- The multi-state term depends on virtual excited-state transitions
 - Its band limit separates into particle and hole contributions
 - The complex distortion has an origin of non-metricity
- * At nonzero temperature, in general, the exact split into distortion and skewness fails.