Thermodynamic Geometry Emerges From Thermal pure quantum state

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Thermal Pure Quantum States

SS and A. Shimizu, PRL 108, 240401 (2012)
SS and A. Shimizu, PRL 111, 010401 (2013)

The canonical thermal pure quantum (TPQ) state at temperature $1/\beta$ is defined by

$$|\beta\rangle \equiv \frac{1}{\sqrt{Z}} \sum_i z_i \exp\left[-\frac{1}{2}\beta \hat{H}\right] |i\rangle$$

Random number — High energy cut-off — Arbitrary basis

$Z \equiv \sum_i |z_i|^2 e^{-\beta \hat{H}}$, $\{|i\rangle\}_i$: arbitrary orthonormal basis

$\{z_i\}_i$: random complex numbers s.t. $z_i \equiv \frac{x_i + i y_i}{\sqrt{2}}$

(x_i and y_i obey normal distribution with mean = 0 and variance = 1)

No resevoir. Not the "purification" of Gibbs state $e^{-\beta \hat{H}}/Z$.

✔ Equilibrium value

For $^\forall \epsilon > 0$,

$$\mathrm{P}\left(\left|\langle\beta|\hat{A}|\beta\rangle - \langle\hat{A}\rangle_\beta^{\mathrm{ens}}\right| \geq \epsilon\right) \leq \frac{1}{\epsilon^2} \frac{\langle(\Delta\hat{A})^2\rangle_{2\beta}^{\mathrm{ens}} + (\langle A\rangle_{2\beta}^{\mathrm{ens}} - \langle A\rangle_\beta^{\mathrm{ens}})^2}{\exp[2V\beta\{f(2\beta) - f(\beta)\}]}$$

$$\leq \frac{1}{\epsilon^2} \frac{V^{3m}}{\exp[O(V)]}$$

"Typicality"

$f(\beta;V) \equiv \frac{F(\beta,V)}{V}$: Free energy density

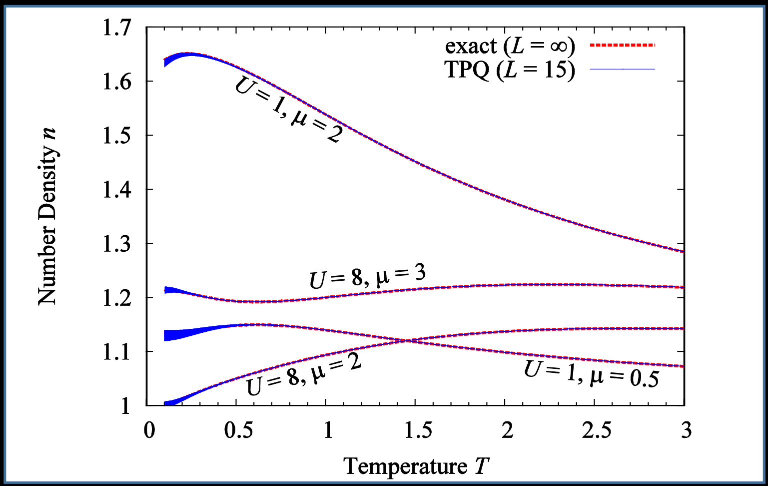
$\langle\hat{A}\rangle_\beta^{\mathrm{ens}}$: Ensemble average, $\langle(\Delta\hat{A})^2\rangle_\beta^{\mathrm{ens}}$:Variance of $\hat{A}$

Numerical Applications of TPQ state

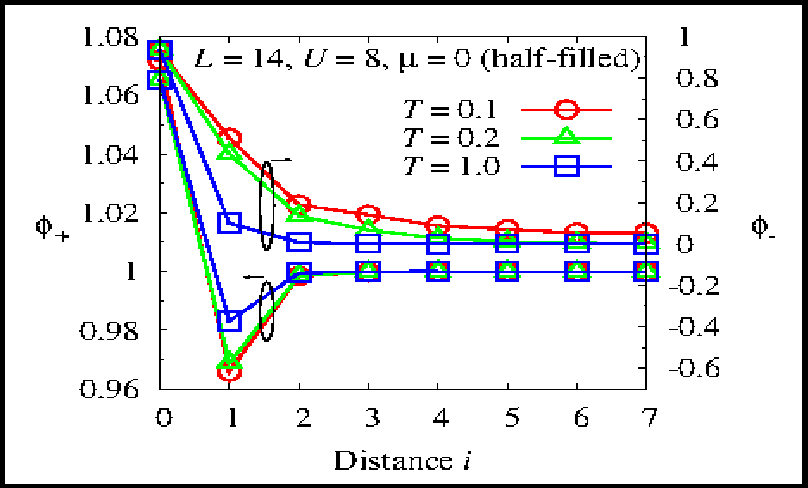
SS and A.Shimizu, arXiv:1312.5145

M. Hyuga, SS, K. Sakai, A.Shimizu ,PRB 90, 121110(R) (2014)

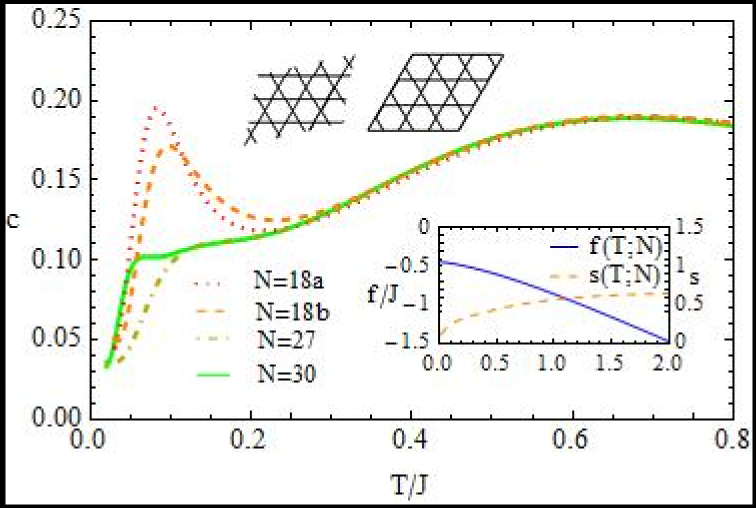
Number Density



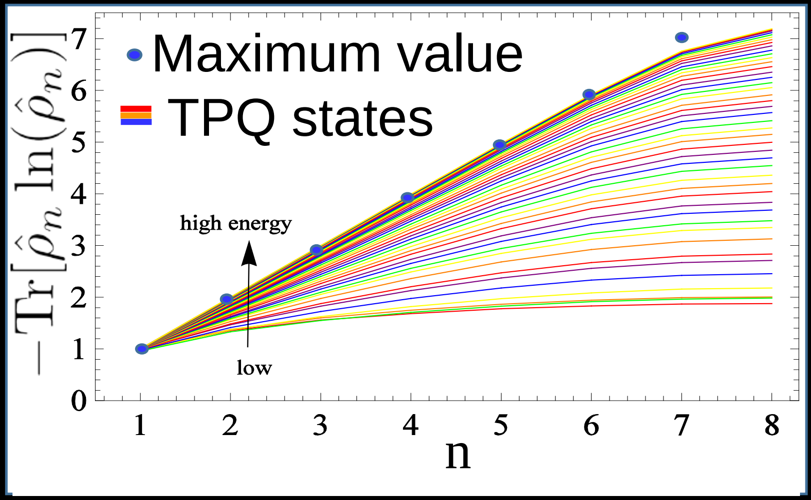
Correlation Function



Specific Heat



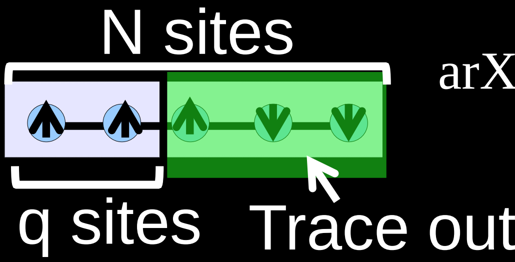
von Neumann Entropy

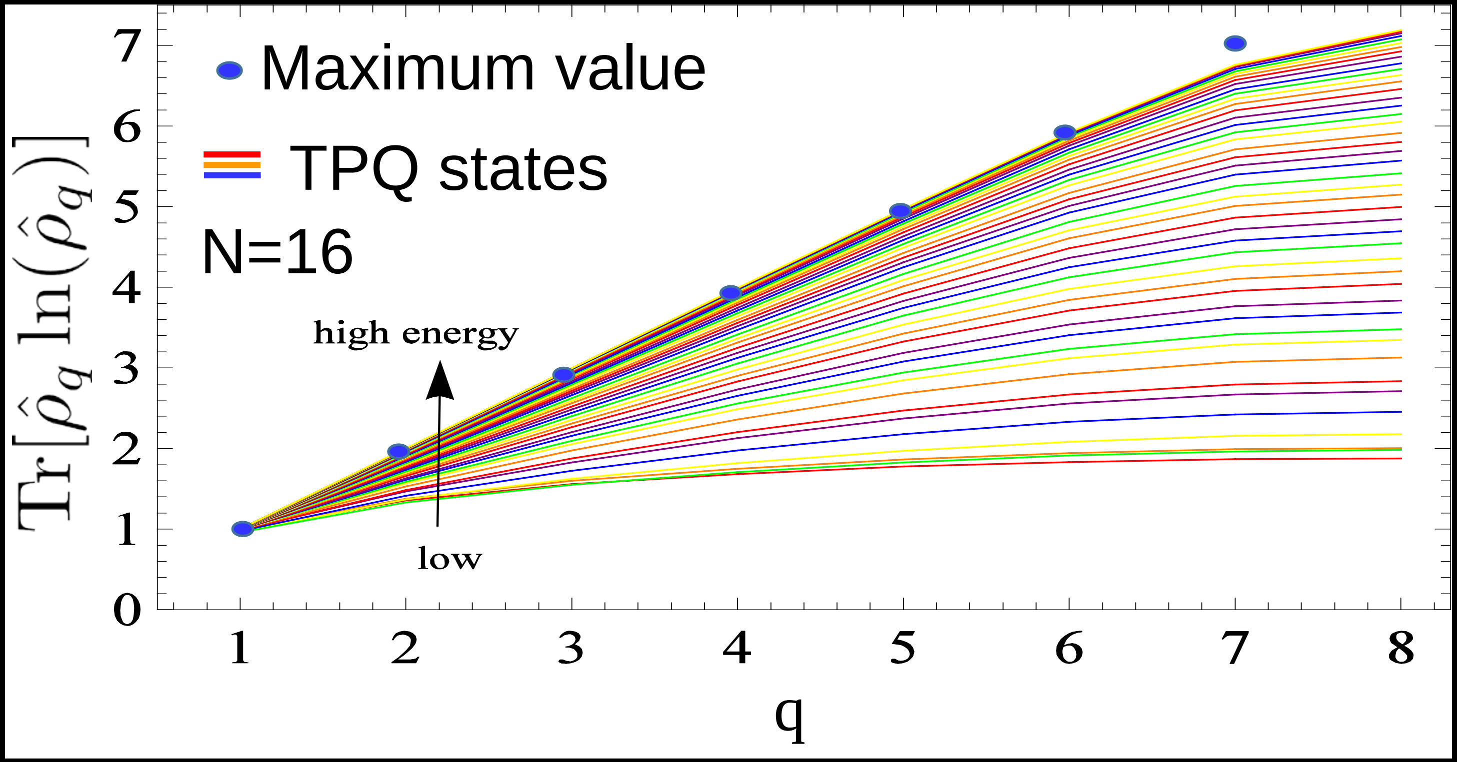


A single realization of the TPQ state gives equilibrium values of all macrocscopic quantities.

von Neumann's Entropy

arXiv:1312.5145





TPQ states are almost maximally entangled

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Fubini-Study metric

Quantum distance

$$\mathrm{d}s^2 = 1 - |\langle \psi(\gamma + \mathrm{d}\gamma) - \psi(\gamma) \rangle|^2 = \sum_{\mu\nu} g_{\mu\nu} \mathrm{d}\gamma_\mu \mathrm{d}\gamma_\nu$$

Metric tensor

For mathematical simplicity, I employ Fubini-Study metric.

Def) Fubini-Study metric

$$\chi_{\mu\nu} \equiv \left\langle \frac{\partial}{\partial \gamma_\mu}\psi \middle| \frac{\partial}{\partial \gamma_\nu}\psi \right\rangle - \underbrace{\left\langle \frac{\partial}{\partial \gamma_\mu}\psi \middle| \psi \right\rangle \left\langle \psi \middle| \frac{\partial}{\partial \gamma_\nu}\psi \right\rangle}$$

↘ Removes Berry connection to keep it gauge invariant

[$|\psi(\gamma)\rangle$: pure quantum state with set of parameters γ]

$\Re\{\chi_{\mu\nu}\} = g_{\mu\nu}$: Metric tensor

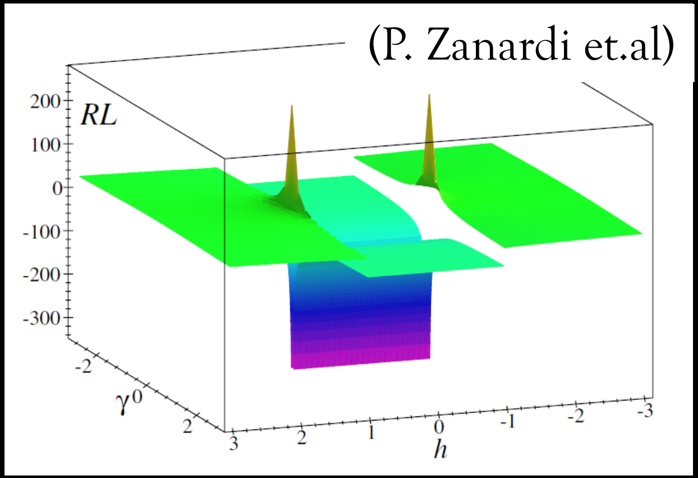
$\Im\{\chi_{\mu\nu}\} = A_{\mu\nu}$: Berry curvature

Fubini-Study metric for Ground State

P Zanardi, P. Giorda, M. Cozzini, PRL 99, 100603 (2007)

M Kolodrubetz, V. Gritsev, A. Polkovnikov, PRB 88, 064304 (2013)

Fubini-Study metric: $\chi_{\mu\nu} \equiv \left\langle \frac{\partial}{\partial\gamma_\mu}\psi \middle| \frac{\partial}{\partial\gamma_\nu}\psi \right\rangle - \left\langle \frac{\partial}{\partial\gamma_\mu}\psi \middle| \psi \right\rangle \left\langle \psi \middle| \frac{\partial}{\partial\gamma_\nu}\psi \right\rangle$



- ✓ Singularity captures Quantum Phase Transition

- ✓ Bulk and Boundary Euler integrals:

$$\chi_{\rm bulk}(\mathcal{M}) = \frac{1}{2\pi}\int_{\mathcal{M}} K \mathrm{d}S, \quad \chi_{\rm boundary}(\mathcal{M}) = \frac{1}{2\pi}\int_{\partial\mathcal{M}} k_g \mathrm{d}l$$

They are protected against various perturbations

We will obtain FS metric at finite temperature using TPQ state

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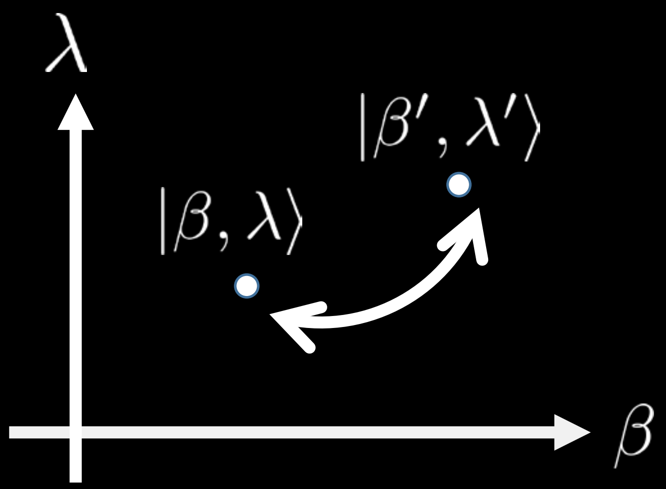
Geometry of cTPQ states



Consider special case of the cTPQ state

$$|\beta,\lambda\rangle \equiv \frac{1}{\sqrt{Z(\beta,\lambda)}} \sum_n e^{i\phi_n} e^{-\frac{1}{2}\beta\hat{H}(\lambda)} |n(\lambda)\rangle$$

Random Phase ($e^{i\phi_n}$), Fixed Amplitude ($e^{-\frac{1}{2}\beta\hat{H}(\lambda)}$), Energy Eigenstates ($|n(\lambda)\rangle$)

$$|\beta',\lambda'\rangle \equiv \frac{1}{\sqrt{Z(\beta',\lambda')}} \sum_n e^{i\theta_n} e^{-\frac{1}{2}\beta\hat{H}(\lambda')} |n(\lambda)\rangle$$

(λ : set of parameters of Hamiltonian, $\beta' \equiv \beta + \mathrm{d}\beta,\ \lambda' \equiv \lambda + \mathrm{d}\lambda,$
$\{\phi_n\},\{\theta_n\}$: set of random real numbers, $\{|n\rangle\}$: Energy eigenstates)

However, $\overline{|\langle\beta,\lambda|\beta',\lambda'\rangle|} \sim O(e^{-\frac{S}{2}}) \ll 1$

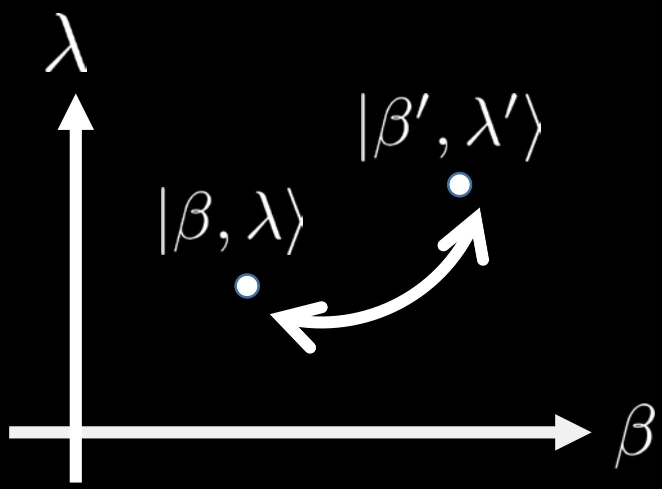
($\overline{X}$: Random Average of X
S : Entropy)

→ Geometric tensor $g_{\mu\nu}$ diverges…

$$\left(\mathrm{d}s^2 = 1 - |\langle\beta,\lambda|\beta',\lambda'\rangle|^2 = \sum_{\mu\nu} g_{\mu\nu}\mathrm{d}\gamma_\mu \mathrm{d}\gamma_\nu \right)$$

Because microstates can be completely different even when they are macroscopically same equilibrium state

Geometry of cTPQ states



Consider special case of the cTPQ state

$$|\beta,\lambda\rangle \equiv \frac{1}{\sqrt{Z(\beta,\lambda)}} \sum_n e^{i\phi_n} e^{-\frac{1}{2}\beta\hat{H}(\lambda)} |n(\lambda)\rangle$$

Random Phase ($e^{i\phi_n}$) — Fixed Amplitude ($e^{-\frac{1}{2}\beta\hat{H}(\lambda)}$) — Energy Eigenstates ($|n(\lambda)\rangle$)

$$|\beta',\lambda'\rangle \equiv \frac{1}{\sqrt{Z(\beta',\lambda')}} \sum_n e^{i\theta_n} e^{-\frac{1}{2}\beta\hat{H}(\lambda')} |n(\lambda)\rangle$$

Fix $\{\phi_n\}_n$ and minimize the quantum distance by tuning $\{\theta_n\}_n$

→ We find $\theta_n = \phi_n + \Theta_\beta \mathrm{d}\beta + \Theta_\lambda \mathrm{d}\lambda$ [$\Theta_\beta, \Theta_\lambda$: real constant independent of *n*]

→ $\partial_\nu |\beta,\lambda\rangle \equiv \frac{|\beta',\lambda'\rangle - |\beta,\lambda\rangle}{\mathrm{d}\gamma_\nu}$ [$\gamma_0 \equiv \beta, \gamma_1 \equiv \lambda$]

$$= \sum_n \frac{1}{\mathrm{d}\gamma_\nu} \left(e^{i\theta_n} \frac{e^{-\frac{1}{2}\beta\hat{H}(\lambda')}}{\sqrt{Z(\beta',\lambda')}} - e^{i\phi_n} \frac{e^{-\frac{1}{2}\beta\hat{H}(\lambda)}}{\sqrt{Z(\beta,\lambda)}} \right) |n(\lambda)\rangle$$

$$= \underbrace{\sum_n e^{i\phi_n} \left(\partial_\nu \frac{e^{-\frac{1}{2}\beta\hat{H}(\lambda)}}{\sqrt{Z(\beta,\lambda)}} \right)}_{} |n(\lambda)\rangle + \underbrace{i\Theta_\nu}_{} |\beta,\lambda\rangle$$

Geometry of cTPQ states

$$\partial_\nu|\beta,\lambda\rangle = \sum_n e^{i\phi_n} \underbrace{\left(\partial_\nu \frac{e^{-\frac{1}{2}\beta\hat{H}}}{\sqrt{Z}}\right)}|n\rangle + \underbrace{i\Theta_\nu}|\beta,\lambda\rangle$$

✓ Berry connection

$$\langle\beta,\lambda|\partial_\nu|\beta,\lambda\rangle$$

$$= \sum_{n,m} \underset{\delta_{n,m}}{\underset{\wr|}{e^{i(\phi_n-\phi_m)}}} \langle m|\frac{e^{-\frac{1}{2}\beta\hat{H}}}{\sqrt{Z}}\left(\partial_\nu \frac{e^{-\frac{1}{2}\beta\hat{H}}}{\sqrt{Z}}\right)|n\rangle + i\Theta_\nu$$

$$\simeq \underbrace{i\Theta_\nu}$$

It can have $U(1)$ phase degree of freedom

✓ Fubini-Study metric

$$\chi_{\nu\mu} = \langle\beta,\lambda|\overleftarrow{\partial_\nu}\partial_\mu|\beta,\lambda\rangle - \langle\beta,\lambda|\overleftarrow{\partial_\nu}|\beta,\lambda\rangle\langle\beta,\lambda|\partial_\mu|\beta,\lambda\rangle$$

$$\simeq \sum_n \langle n|\underbrace{\left(\partial_\nu \frac{e^{-\frac{1}{2}\beta\hat{H}}}{\sqrt{Z}}\right)\left(\partial_\nu \frac{e^{-\frac{1}{2}\beta\hat{H}}}{\sqrt{Z}}\right)}|n\rangle$$

What's the meaning of this metric?

✔ Fubini-Study metric

$$\chi_{\nu\mu} \simeq \sum_n \langle n| \left(\partial_\nu \frac{e^{-\frac{1}{2}\beta \hat{H}}}{\sqrt{Z}} \right) \left(\partial_\nu \frac{e^{-\frac{1}{2}\beta \hat{H}}}{\sqrt{Z}} \right) |n\rangle$$

$$\chi_{\beta\beta} = \frac{1}{4}\left\langle \Delta \hat{H}(\lambda)^2 \right\rangle_{\beta\lambda} = \frac{1}{4}\partial_\beta^2(\beta F(\beta,\lambda))$$

$$\chi_{\beta\lambda} = \frac{\beta}{4}\left\langle \Delta \hat{H}(\lambda)\Delta(\partial_\lambda \hat{H}(\lambda)) \right\rangle_{\beta\lambda} = \frac{\beta}{4}\ \partial_\beta\partial_\lambda(\beta F(\beta,\lambda))$$

$\langle \hat{X} \rangle_{\beta\lambda}$: canonical ensemble average at (β,λ)

$$\Delta\hat{X} \equiv \hat{X} - \langle \hat{X} \rangle_{\beta\lambda}$$

$$F(\beta,\lambda) \equiv \frac{1}{\beta}\ln Z(\beta,\lambda)$$

$$\chi_{\lambda\lambda} = \mathrm{Tr}\left[\int_{\frac{-\beta}{2}}^{\frac{\beta}{2}} \left(\frac{\beta}{2} - |\tau|\right) e^{-(\frac{\beta}{2}+\tau)\hat{H}(\lambda)}\ \Delta\left(\partial_\lambda \hat{H}(\lambda)\right) e^{-(\frac{\beta}{2}-\tau)\hat{H}(\lambda)}\ \Delta\left(\partial_\lambda \hat{H}(\lambda)\right) \mathrm{d}\tau\right]$$

"generalized correlation" (cf: Linear Response theory)

When $[\hat{H}, \partial_\lambda \hat{H}] = 0$,

$$= \frac{\beta^2}{4}\partial_\lambda^2(\beta F(\beta,\lambda))$$

This is Thermodynamic Geometry

Quantum Distance between TPQ states are determined by thermodynamics

Thermodynamic Geometry

F.Weinhold, J. Chem. Phys., 63, 2479 (1975)
G.Ruppeiner, Phys. Rev. A, 20, 1608 (1979)
G.E.Crooks, Phys. Rev. Lett, 99, 100602 (2007)

Hessian of thermodynamic function gives Riemannian metric:

$$\mathrm{d}s^2 = g_{\nu\mu}\mathrm{d}\gamma_\nu \mathrm{d}\gamma_\mu \qquad \left[\begin{array}{l} g_{\nu\mu} \equiv \partial_\nu \partial_\mu (\beta F(\beta, \lambda_1, \lambda_2, \cdots)) \\ \gamma_0 = \beta, \gamma_i = \lambda_i \end{array}\right]$$

(Many variations: Ruppeiner metric, Weinhold metric …)

- ✓ Curvature singularities signal critical behaviors
- ✓ Flat for systems with noninteracting underlying statistical mechanics such as ideal gas

Thermodynamic Length

$$L \equiv \int_0^T \sqrt{\frac{\mathrm{d}\gamma_\nu}{\mathrm{d}t} g_{\nu\mu} \frac{\mathrm{d}\gamma_\mu}{\mathrm{d}t}}$$

- ✓ Minimum distanced paths are geodesics for $g_{\nu\mu}$
- ✓ Geodesics path minimize dissipation under thermodynamic operations

What's the meaning of this metric?

✓ Fubini-Study metric

However, when $[\hat{H}, \partial_\lambda \hat{H}] \neq 0$,

$$\chi_{\lambda\lambda} = \mathrm{Tr}\left[\int_{\frac{-\beta}{2}}^{\frac{\beta}{2}} (\tfrac{\beta}{2} - |\tau|) e^{-(\frac{\beta}{2}+\tau)\hat{H}(\lambda)}\, \Delta\left(\partial_\lambda \hat{H}(\lambda)\right) e^{-(\frac{\beta}{2}-\tau)\hat{H}(\lambda)}\, \Delta\left(\partial_\lambda \hat{H}(\lambda)\right) \mathrm{d}\tau\right]$$

$$\neq \frac{\beta^2}{4}\partial_\lambda^2(\beta F(\beta,\lambda))$$

$$= \frac{\beta^2}{4}\partial_\lambda^2(\beta F(\beta,\lambda)) + C(\beta,\lambda)$$

Quantum correction term

$$\left(C(\beta,\lambda) \equiv \mathrm{Tr}[\int_{\frac{-\beta}{2}}^{\frac{\beta}{2}} (\tfrac{\beta}{4} - |\tau|)\, e^{-(\frac{\beta}{2}+\tau)\hat{H}(\lambda)}\, \Delta\left(\partial_\lambda \hat{H}(\lambda)\right) e^{-(\frac{\beta}{2}-\tau)\hat{H}(\lambda)}\, \Delta\left(\partial_\lambda \hat{H}(\lambda)\right) \mathrm{d}\tau] \right)$$

- ✓ I believe that it relates to dissipative dynamics in quantum statistical mechanics.
- ✓ Does this kind of correlation generically appear?

  ⟶ Similar metric is obtained from Gibbs state.
- ✓ Many parameters case is straightforward

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Bures metric of Gibbs states

Bures metric : Extension of FS metric to mixed quantum states (Equilavent to Quantum Fisher metric)

$$\mathrm{d}s_B^2 \equiv 1 - \mathcal{F}(\hat{\rho}, \hat{\rho} + \mathrm{d}\hat{\rho}) = \chi^B_{\nu\mu}\mathrm{d}\gamma_\nu \mathrm{d}\gamma_\mu$$

$\left(\mathcal{F}(\hat{\rho}, \hat{\sigma}) \equiv \mathrm{Tr}\left[\sqrt{\sqrt{\hat{\rho}}\hat{\sigma}\sqrt{\hat{\rho}}}\right] \right.$: Fidelity for mixed states. $\Big)$

Consider Bures metric for two Gibbs states

$$\hat{\rho} \equiv \frac{e^{-\beta \hat{H}}}{Z(\beta,\lambda)},\ \hat{\rho} + \mathrm{d}\hat{\rho} \equiv \frac{e^{-\beta + \mathrm{d}\beta \hat{H}(\lambda + \mathrm{d}\lambda)}}{Z(\beta + \mathrm{d}\beta, \lambda + \mathrm{d}\lambda)}.$$

Using the relation

$$\chi^B_{\nu\mu}\mathrm{d}\gamma_\nu \mathrm{d}\gamma_\mu = \frac{1}{2}\sum_{n,m=1}^{D} \frac{|\langle n|\mathrm{d}\hat{\rho}|m\rangle|^2}{w_n + w_m},$$

we get

$$\chi^B_{nm} = \sum_{n,m} \frac{(e^{-\frac{\beta}{2}E_n} + e^{-\frac{\beta}{2}E_m})^2}{2(e^{-\beta E_n} + e^{-\beta E_m})} \langle n| \left(\partial_n \frac{e^{-\frac{\beta}{2}\hat{H}}}{\sqrt{Z}} \right) |m\rangle\langle m| \left(\partial_m \frac{e^{-\frac{\beta}{2}\hat{H}}}{\sqrt{Z}} \right) |n\rangle.$$

Comparison of thermodynamic metrics

Fubini- Study metric of TPQ state:

$$\chi_{\nu\mu} \simeq \sum_n \langle n| \left(\partial_\nu \frac{e^{-\frac{1}{2}\beta \hat{H}}}{\sqrt{Z}} \right) \left(\partial_\nu \frac{e^{-\frac{1}{2}\beta \hat{H}}}{\sqrt{Z}} \right) |n\rangle$$

Bures metric of Gibbs state:

$$\chi^B_{nm} = \sum_{n,m} \frac{(e^{-\frac{\beta}{2}E_n} + e^{-\frac{\beta}{2}E_m})^2}{2(e^{-\beta E_n} + e^{-\beta E_m})} \langle n| \left(\partial_n \frac{e^{-\frac{\beta}{2}\hat{H}}}{\sqrt{Z}} \right) |m\rangle\langle m| \left(\partial_m \frac{e^{-\frac{\beta}{2}\hat{H}}}{Z} \right) |n\rangle .$$

→ Since $\frac{1}{2} \leq \frac{(e^{-\frac{\beta}{2}E_n} + e^{-\frac{\beta}{2}E_m})^2}{2(e^{-\beta E_n} + e^{-\beta E_m})} < 1$ holds,

$$\frac{1}{2}\chi_{\nu\mu} \leq \chi^{\mathrm{B}}_{\nu\mu} < \chi_{\nu\mu}$$

- ✓ This kind of correlation generically appear in quantum statisitical-mechanical geometry.
- ✓ Practically, metric induced from TPQ state is easier to calculate.
- ✓ This Bures metric will change its behavior between integrable model and non-integrable model.

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Example

Consider XY model with anisotropy η and magnetic field h.

$$\hat{H} = -\sum_j J\left(\frac{1+\eta}{2}\right) s_j^x s_{j+1}^{-} + J\left(\frac{1-\eta}{2}\right) s_j^y s_{j+1}^y + h s_j^z$$

Jordan-Wigner transformation

$$= -\sum_k \begin{bmatrix} A_k & B_k \\ B_k & -A_k \end{bmatrix} \qquad \left(\begin{aligned} A_k &\equiv h - \cos k \\ B_k &\equiv \eta \sin k \end{aligned} \right)$$

Diagonalization

$$= -\sum_k \begin{bmatrix} -E_k & 0 \\ 0 & E_k \end{bmatrix} \qquad \left(E_k \equiv \sqrt{A_k^2 + B_k^2} \right)$$

Metric Tensor

$$\chi_{\beta\beta} = \sum_k \frac{1}{(e^{-\beta E_k} + e^{\beta E_k})^2}$$

$$\chi_{hh} = \sum_k \frac{B_k^2}{2{E_k}^4} \frac{\left(e^{\frac{-\beta E_k}{2}} - e^{\frac{\gamma_0 E_k}{2}}\right)^2}{e^{-\beta E_k} + e^{\beta E_k}} + \frac{A_k^2}{{E_k}^2} \frac{\gamma_0^2}{(e^{-\beta E_k} + e^{\beta E_k})^2}$$

$$\chi_{\eta\eta} = \sin^2 k \sum_k \frac{A_k^2}{2{E_k}^4} \frac{\left(e^{\frac{-\beta E_k}{2}} - e^{\frac{\beta E_k}{2}}\right)^2}{e^{-\beta E_k} + e^{\beta E_k}} + \frac{B_k^2}{{E_k}^2} \frac{\beta^2}{(e^{-\beta E_k} + e^{\beta E_k})^2}$$

$$\chi_{\beta h}, \chi_{\beta\eta}, \chi_{h\eta}$$

Summary

Thermal Pure Quantum State:

$$|\beta\rangle \equiv \frac{1}{\sqrt{Z}} \sum_i z_i \ \exp\left[-\frac{1}{2}\beta\hat{H}\right] \ |i\rangle$$

Fubini-Study Metric:

$$\chi_{\mu\nu} \equiv \left\langle \frac{\partial}{\partial\gamma_\mu}\psi \middle| \frac{\partial}{\partial\gamma_\nu}\psi \right\rangle - \left\langle \frac{\partial}{\partial\gamma_\mu}\psi \middle| \psi \right\rangle \left\langle \psi \middle| \frac{\partial}{\partial\gamma_\nu}\psi \right\rangle$$

- ✓ Metric is obtained from TPQ state by minimizing quantum distance
- ✓ Minimization washes out microscopic details and Themodynamic geometry (plus, quantum correction) determine distance between TPQ states
- ✓ Similar metric for Gibbs state is obtained using Bures metric
- ✓ As an illustration , metric for XY model is derived