

25th of January 2025

THE TRACE DENSITY BETWEEN DENSITY MATRICES A NIFTY TOOL IN NEW-PHYSICS SEARCHES



SUMMARY

[arXiv]

- density matrix = all physical information
- sensitive to new physics
- trace distance most sensitive tool

(credits to Joscha)



SUMMARY

[arXiv]

- density matrix = all physical information
- sensitive to new physics
- trace distance most sensitive tool
- but first: quantum mechanics 101

WHAT PARTICLE	PHYSICISTS DO	ACCORDING TO
$i\hbar\frac{\partial}{\partial t}\left \Psi\right\rangle=\hat{H}\left \Psi\right\rangle$	$i\hbar\frac{\partial}{\partial t}\left \Psi\right\rangle=\hat{H}\left \Psi\right\rangle$	$i\hbar\frac{\partial}{\partial t}\left \Psi\right\rangle=\hat{H}\left \Psi\right\rangle$
MY MOM	MY GRANDMA	MY FRIENDS
$i\hbar\frac{\partial}{\partial t}\left \Psi\right\rangle=\hat{H}\left \Psi\right\rangle$	$i\hbar\frac{\partial}{\partial t}\left \Psi\right\rangle=\hat{H}\left \Psi\right\rangle$	
SOCIETY	CERN DIRECTORATE	REALITY

HOW TO DO QUANTUM MECHANICS

(1) Observable \hat{O} (e.g. spin) (2) Describe system

(3) recipe expectation value

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"basic" approach

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(2) wave function $|\Psi\rangle = \sum_{i} c_{i} |\psi_{i}\rangle$ (3) $\langle \hat{O} \rangle = \langle \Psi | \hat{O} | \Psi \rangle = c_i^* O_{ij} c_i$

"advanced" approach

(2) density
$$\rho = \sum_{ij} \rho_{ij} |\psi_i\rangle\!\langle\psi_j|$$

(3) $\langle\hat{O}\rangle = \operatorname{Tr}(\rho\hat{O}) = \rho_{ij}O_{ji}$

$$\begin{aligned} |\Psi\rangle &\equiv \begin{bmatrix} c_0 & c_1 & \dots \end{bmatrix}^T \\ \langle\Psi| &\equiv \begin{bmatrix} c_0^* & c_1^* & \dots \end{bmatrix}^T & \hat{O} &\equiv \begin{bmatrix} O_{00} & O_{01} & \dots \\ O_{10} & O_{11} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} & \rho &\equiv \begin{bmatrix} \rho_{00} & \rho_{01} & \dots \\ \rho_{10} & \rho_{11} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \end{aligned}$$

(1) Observable \hat{O} (e.g. spin) (2) Describe system

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(2) wave function
$$\ket{\Psi} = \sum_i \textit{c}_i \ket{\psi_i}$$

(3)
$$\langle \hat{O} \rangle = \langle \Psi | \hat{O} | \Psi \rangle = c_j^* O_{ji} c_i = c_i c_j^* O_{ji}$$

"advanced" approach

(2) density
$$\rho = \sum_{ij} \rho_{ij} |\psi_i\rangle\!\langle\psi_j|$$

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$$\langle \hat{O} \rangle = \operatorname{Tr}(\rho \hat{O}) = \rho_{ij} O_{ji}$$

 $|\Psi
angle \Leftrightarrow
ho = |\Psi
angle \!\!\langle \Psi | \Leftrightarrow
ho_{ij} = c_i c_i^st$

HOW TO DO QUANTUM MECHANICS

(2)

(1) Observable \hat{O} (e.g. spin)

"basic" approach

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$$|\Psi\rangle = \sum_{i} c_{i} |\psi_{i}\rangle$$

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 $|\Psi
angle \Leftrightarrow
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angle\!\langle \Psi| \Leftrightarrow
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Why bother with the density?



wave function describes closed system



wave function describes closed system

ightarrow system with states $|\psi_i
angle$



wave function describes closed system

- ightarrow system with states $|\psi_i
 angle$
- ightarrow rest universe with states $|\mathcal{U}_i
 angle$



wave function describes closed system

- ightarrow system with states $|\psi_i
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- $\rightarrow \,$ state of each independent



total universe

 $\ket{\Phi} = \ket{\textit{U}} \ket{\Psi}$

wave function describes closed system

- ightarrow system with states $|\psi_i
 angle$
- ightarrow rest universe with states $|\mathcal{U}_i
 angle$
- ightarrow state of each independent observable \hat{O} on system:

$$\left<\hat{O}\right> = \left<\Phi\right|\hat{O}\left|\Phi\right> = \left<\Psi\right|\hat{O}\left|\Psi\right>\underbrace{\left}_{=1}$$



total universe

 $\ket{\Phi} = \ket{\textit{U}} \ket{\Psi}$

what if **open**?

- ightarrow system with states $|\psi_i
 angle$
- ightarrow rest universe with states $|\mathcal{U}_i
 angle$



$$\ket{\Phi} = \sum_{ij} f_{ij} \ket{\psi_i} \ket{\mathcal{U}_j}$$

what if open?

- ightarrow system with states $|\psi_i
 angle$
- ightarrow rest universe with states $|\mathcal{U}_i
 angle$
- $\rightarrow\,$ no well defined independent states: mixed! observable \hat{O} on system:

$$egin{aligned} &\langle \hat{O}
angle = \langle \Phi | \ \hat{O} \, | \Phi
angle = \sum_{ijk\ell} f_{k\ell}^* f_{ij} ig \langle \psi_k | \ \hat{O} \, | \psi_i
angle \underbrace{\langle \mathcal{U}_\ell | \mathcal{U}_j
angle}_{= \delta_{\ell j}} \ \end{array} \ = \sum_{ijk} f_{kj}^* f_{ij} ig \langle \psi_k | \ \hat{O} \, | \psi_i
angle \end{aligned}$$



$$\ket{\Phi} = \sum_{ij} f_{ij} \ket{\psi_i} \ket{\mathcal{U}_j}$$

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angle &= \langle \Phi | \ \hat{m{O}} \, | \Phi
angle &= \sum_{ijk} f_{kj}^* f_{ij} \left\langle \psi_k | \ \hat{m{O}} \, | \psi_i
ight
angle \ &= \mathsf{Tr} \left(\sum_{ijk} f_{kj}^* f_{ij} \left| \psi_i
ight
angle \! \langle \psi_k | \ \hat{m{O}}
ight) \end{aligned}$$



$$\left|\Phi\right\rangle = \sum_{ij} f_{ij} \left|\psi_{i}\right\rangle \left|\mathcal{U}_{j}\right\rangle$$

what if open?

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angle \ &= \mathsf{Tr} \left(\sum_{ijk} f_{kj}^* f_{ij} \, | \psi_i
angle \! \langle \psi_k | \ \hat{\mathcal{O}}
ight) \end{aligned}$$



$$ho_{\Phi} = \sum_{ijk\ell} f_{ij} f_{k\ell}^* \ket{\psi_i} \ket{\mathcal{U}_j} ig \langle \psi_k | ig \langle \mathcal{U}_\ell |$$

MIXED SYSTEM: QUANTUM EFFECTS

Pure state: only two types

- \blacksquare classical product state $\left|\psi\right\rangle \left|\phi\right\rangle$
- entangled states: $\sum_{i} |\psi_i\rangle |\phi_i\rangle$

Mixed state: rich categorization / observables

 \rightarrow concurrence, discord, magic...



• wave function $\Psi \rightarrow$ density matrix ho

 \blacksquare wave function $\Psi \rightarrow$ density matrix ρ

 \blacksquare braket \rightarrow trace

$$\begin{array}{l} \bullet \quad \langle \Psi | \Psi \rangle = \mathsf{1} \to \mathsf{Tr} \, \rho = \mathsf{1} \\ \bullet \quad \langle \hat{O} \rangle = \langle \Psi | \, \hat{O} \, | \Psi \rangle \to \langle \hat{O} \rangle = \mathsf{Tr} \big(\rho \hat{O} \big) \end{array}$$

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$$\begin{array}{l} \bullet \quad |\Psi\rangle = \sum_{i} c_{i} |\psi_{i}\rangle \text{ with } c_{i} = \langle \psi_{i} |\Psi\rangle, \\ \langle \psi_{i} |\psi_{j}\rangle = \delta_{ij} \end{array}$$

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- $|\Psi\rangle = \sum_{i} c_{i} |\psi_{i}\rangle$ with $c_{i} = \langle \psi_{i} |\Psi\rangle$, $\langle \psi_{i} |\psi_{j}\rangle = \delta_{ij}$ • $\rho = \sum_{i} r_{i} |\rho_{i}\rangle$ with $r_{i} = \operatorname{Tr}(\rho_{i}\rho)$, $\operatorname{Tr}(\rho_{i}\rho_{j}) = \delta_{ij}$
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- ightarrow basis elements \equiv observables
- \blacksquare product states: $\left|\phi\right\rangle \left|\psi\right\rangle
 ightarrow
 ho_{\phi}\otimes
 ho_{\psi}$

$$\rightarrow (A \otimes B)_{ijkl} = A_{ij}B_{kl}$$
$$Tr(A \otimes B) = Tr A Tr B$$









Correlation $\propto \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$ so $C_{ij} \equiv$ correlation only if unpolarized ($B^{0,1} = 0$)

$$\rho = \frac{1}{4} \left(\mathbb{1} \otimes \mathbb{1} + \sum_{i} B_{i}^{0} \sigma_{i} \otimes \mathbb{1} + \sum_{i} B_{i}^{1} \mathbb{1} \otimes \sigma_{i} + \sum_{ij} C_{ij} \sigma_{i} \otimes \sigma_{j} \right)$$

$$\sum_{ijk\ell} r_{ij} |s_{i}s_{j}\rangle\langle s_{k}s_{\ell}| = \begin{pmatrix} s_{00} \otimes s_$$

1

individua

$$1 \equiv \text{no mea}$$

$$p = \frac{1}{4} \left(1 \otimes 1 + \sum_{i} B_{i}^{0} \sigma_{i} \otimes 1 + \sum_{i} B_{i}$$
normalization

$$Tr(1_{2} \otimes 1_{2}) = Tr 1_{4} = 4$$
alternatively, $\hat{\Sigma}_{z}$ eige

$$\rho = \sum_{ijk\ell} r_{ij} |s_{i}s_{j}\rangle\langle s_{k}s_{\ell}| = \begin{pmatrix} s_{00} \\ s_{01} \\ s_{10} \\ s_{1100} \\ s_{1101} \\ s_{1101} \\ s_{1110} \\ s_{1110} \\ s_{1111} \end{pmatrix}$$

density



initial state, e.g. e^+e^-



density



- initial state, e.g. e^+e^-
- transition matrix $|e^+e^angle o \hat{\mathcal{T}}\,|e^+e^angle$



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- matrix element: $\mathcal{M} \propto \langle \mu^+ \mu^- | \, \hat{\mathcal{T}} \, | {\it e}^+ {\it e}^-
 angle$



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• xsec:
$$\frac{d\sigma}{d\Omega} \propto \left| \langle \mu^+ \mu^- | \hat{\mathcal{T}} | e^+ e^- \rangle \right|^2$$



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density approach



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density approach

• initial density $ho_{ee} = |e^+e^-\rangle\!\langle e^+e^-|$



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density approach

 \blacksquare initial density $ho_{ee} = |e^+e^angle \langle e^+e^-|$

• transition:
$$\rho_{ee}^{\rm in} \rightarrow \rho_{ee}^{\rm out} = \hat{\mathcal{T}} \rho_{ee} \hat{\mathcal{T}}$$



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- lacksquare transition matrix $|e^+e^angle o \hat{\mathcal{T}}\,|e^+e^angle$
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- $\begin{array}{l} \bullet \quad \text{matrix element: } \mathcal{M} \propto \left\langle \mu^{+} \mu^{-} \right| \hat{\mathcal{T}} \left| e^{+} e^{-} \right\rangle \\ \bullet \quad \text{xsec: } \frac{d\sigma}{d\Omega} \propto \left| \left\langle \mu^{+} \mu^{-} \right| \hat{\mathcal{T}} \left| e^{+} e^{-} \right\rangle \right|^{2} \end{array}$

density approach

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- $\begin{array}{l} \bullet \quad \text{xsec:} \ \frac{d\sigma}{d\Omega} \propto \langle \mu^+ \mu^- | \ \rho_{ee}^{\text{out}} | \mu^+ \mu^- \rangle \\ = \langle \mu^+ \mu^- | \ \hat{\mathcal{T}} | e^+ e^- \rangle \ \langle e^+ e^- | \ \hat{\mathcal{T}} | \mu^+ \mu^- \rangle \end{array} \end{array}$



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density approach

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 ightarrow \rho_{ee}^{\rm out} = \hat{\mathcal{T}} \rho_{ee} \hat{\mathcal{T}}$
- \blacksquare xsec: $\frac{d\sigma}{d\Omega}\propto \left<\mu^+\mu^-\right|\rho_{ee}^{\rm out}\left|\mu^+\mu^-\right>$
- diagonal elements \equiv differential xsec
- Tr $ho_{ee}^{
 m out}\equiv rac{d\sigma}{d\Omega}(e^+e^ightarrow X)$ (unnormalized)

1 unpolarized, uncorrelated initial state: $\rho_{ee}^{in} = \frac{1}{4} \sum_{s_e^+ s_e^-} |s_e^+ s_e^- \rangle \langle s_e^+ s_e^- |$

$$\rho_{ee}^{\mathsf{in}} = \frac{1}{4} \begin{pmatrix} +\sum_{i} B_{i}^{\mathsf{in}+} \sigma_{i} \otimes \mathbb{1} \\ \mathbb{1} \otimes \mathbb{1} + \sum_{i} B_{i}^{\mathsf{in}-} \mathbb{1} \otimes \sigma_{i} \\ +\sum_{ij} C_{ij}^{\mathsf{in}} \sigma_{i} \otimes \sigma_{j} \\ = 0 \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \\ & & & 1 \end{pmatrix}$$

1 unpolarized, uncorrelated initial state: $\rho_{ee}^{in} = \frac{1}{4} \sum_{s_e^+ s_e^-} |s_e^+ s_e^- \rangle \langle s_e^+ s_e^- |$ 2 transition $\rho_{ee}^{in} \rightarrow \rho_{ee}^{out} = \hat{\mathcal{T}}^{\dagger} \rho_{ee} \hat{\mathcal{T}}$ and take final state $\mu^+ \mu^-$

$$\left\langle \mu^{+}\mu^{-} \right| \rho_{ee}^{\text{out}} \left| \mu^{+}\mu^{-} \right\rangle \propto \frac{1}{4} \frac{d\sigma}{d\Omega} \begin{pmatrix} +\sum_{i} B_{i}^{\text{out}+}\sigma_{i} \otimes \mathbb{1} \\ \mathbb{1} \otimes \mathbb{1} + \sum_{i} B_{i}^{\text{out}-} \mathbb{1} \otimes \sigma_{i} \\ +\sum_{ij} C_{ij}^{\text{out}}\sigma_{i} \otimes \sigma_{j} \end{pmatrix} = \frac{1}{4} \frac{d\sigma}{d\Omega} \begin{pmatrix} \mathcal{B}^{++} & \cdots & \cdots & \mathcal{B}^{+-} \\ \mathcal{B}^{+-} & \cdots & \mathcal{B}^{-+} \\ \cdots & \mathcal{B}^{--} \end{pmatrix}$$

1 unpolarized, uncorrelated initial state: $\rho_{ee}^{in} = \frac{1}{4} \sum_{s_e^+ s_e^-} |s_e^+ s_e^- \rangle \langle s_e^+ s_e^- |$ 2 transition $\rho_{ee}^{in} \to \rho_{ee}^{out} = \hat{\mathcal{T}}^{\dagger} \rho_{ee} \hat{\mathcal{T}}$ and take final state $\mu^+ \mu^-$

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(!) actual meaning of

- "average over initial states"
- "sum over final states"

- ightarrow use initial density matrix
- $ightarrow \,$ trace final density matrix

1 unpolarized, uncorrelated initial state: $\rho_{ee}^{in} = \frac{1}{4} \sum_{s_e^+ s_e^-} |s_e^+ s_e^- \rangle \langle s_e^+ s_e^- |$ 2 transition $\rho_{ee}^{in} \to \rho_{ee}^{out} = \hat{T}^{\dagger} \rho_{ee} \hat{T}$ and take final state $\mu^+ \mu^-$

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(!) actual meaning of

"average over initial states"

 \rightarrow use initial density matrix

"sum over final states"

 $ightarrow \,$ trace final density matrix

(!) normalized density: (quantum) probability density (on the diagonal)

Trace distance

$$\mathcal{D}^{\mathsf{T}}(
ho,\zeta) = rac{1}{2} \operatorname{Tr} \sqrt{(
ho-\zeta)^{\dagger}(
ho-\zeta)}$$

Fidelity

$$\mathcal{F}(
ho,\zeta) = \mathsf{Tr}\,\sqrt{\sqrt{
ho}\zeta\sqrt{
ho}}$$

Trace distance

$$\mathcal{D}^{\mathsf{T}}(\rho,\zeta) = rac{1}{2}\operatorname{Tr}\sqrt{(
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$$ightarrow \mathcal{D}^{\mathsf{T}}(
ho,\zeta) = rac{1}{2}\sum_{i} |\lambda_{i}|$$
 with λ_{i} the eigenvalues of $ho - \zeta$

 $ightarrow \mathcal{F}(
ho,\zeta) = \sum_i \sqrt{\lambda_i}$ with λ_i the eigenvalues of $ho\zeta$

Trace distance

$$\mathcal{D}^{ au}(
ho,\zeta)=rac{1}{2}\operatorname{Tr}\sqrt{(
ho-\zeta)^{\dagger}(
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$$\mathcal{F}(\rho,\zeta) = \operatorname{Tr}\sqrt{\sqrt{
ho}\zeta\sqrt{
ho}}$$

$$\rightarrow \mathcal{D}^{T}(\rho,\zeta) = \frac{1}{2} \sum_{i} |\lambda_{i}| \text{ with } \lambda_{i} \text{ the eigenvalues of } \rho - \zeta$$

 $\rightarrow \mathcal{D}^{\mathsf{T}}(\rho,\zeta) = \mathbf{0} \Leftrightarrow \lambda_i = \mathbf{0} \forall \lambda_i \Leftrightarrow \rho - \zeta = \mathbf{0} \qquad \rightarrow \mathcal{F}(\rho,\zeta) = \mathbf{1} \Leftrightarrow \rho = \zeta$

 $\begin{array}{l} \rightarrow \ \mathcal{F}(\rho,\zeta) = \sum_{i} \sqrt{\lambda_{i}} \text{ with } \lambda_{i} \text{ the eigenvalues} \\ \text{ of } \rho\zeta \\ \rightarrow \ \mathcal{F}(\rho,\zeta) = \mathbf{1} \Leftrightarrow \rho = \zeta \end{array}$

Trace distance

$$\mathcal{D}^{\mathsf{T}}(\rho,\zeta) = \frac{1}{2} \operatorname{Tr} \sqrt{(\rho-\zeta)^{\dagger}(\rho-\zeta)}$$

$$\rightarrow \mathcal{D}^{\mathcal{T}}(\rho,\zeta) = \frac{1}{2} \sum_{i} |\lambda_{i}| \text{ with } \lambda_{i} \text{ the eigenvalues of } \rho - \zeta$$

$$\rightarrow \mathcal{D}^{\mathsf{T}}(\rho,\zeta) = \mathbf{0} \Leftrightarrow \lambda_i = \mathbf{0} \forall \lambda_i \Leftrightarrow \rho - \zeta = \mathbf{0}$$

 \rightarrow classical interpretation: $\frac{1}{2}\sum_{i} |p_i - q_i|$

Fidelity

$$\mathcal{F}(
ho,\zeta) = \mathsf{Tr}\,\sqrt{\sqrt{
ho}\zeta\sqrt{
ho}}$$

 $ightarrow \mathcal{F}(
ho,\zeta) = \sum_i \sqrt{\lambda_i}$ with λ_i the eigenvalues of $ho\zeta$

$$\rightarrow \mathcal{F}(\rho,\zeta) = \mathbf{1} \Leftrightarrow \rho = \zeta$$

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Trace distance

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$$o \ \mathcal{D}^{\intercal}(
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ho - \zeta = \mathbf{0}$$

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- ightarrow pure state: $\sqrt{1 |\langle \psi | \phi \rangle|^2}$

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- ightarrow pure state: $|\langle \psi | \phi
 angle|$



new physics searches using $\mathcal{D}^{T}(
ho,
ho_{\mathrm{SM}})$ or $\mathcal{F}(
ho,
ho_{\mathrm{SM}})$

SEARCHING NEW PHYSICS

$$\chi^2(\lambda) = \left(rac{\mathcal{D}^{ au}[
ho_{
m NP}(\lambda) -
ho_{
m SM}]}{\sigma_{\mathcal{D}^{ au}}}
ight)^2 + \left(rac{\sigma_{
m NP} - \sigma_{
m SM}}{\sigma_{\sigma}}
ight)^2$$



EXAMPLE: TOP QUARK CHROMOMAGNETIC DIPOLE MOMENT



or equivalently in SMEFT (before EW symmetry breaking)

$$\mathcal{L}_{\mathsf{dip}} = rac{m{c}_{tG}}{\lambda^2}(\mathcal{O}_{tG} + \mathcal{O}_{tG}^{\dagger})$$

Benchmark limit:

inclusive xsec

LHC (7 and 8 TeV) and tevatron (1.96 TeV)

$$-0.046 \le \mu_t \le 0.040$$





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- $-0.046 \le \mu_t \le 0.040$



 $-0.025 \leq |\mu_t| \leq 0.037$

EXAMPLE: ANOMALOUS au COUPLING AT FCC-ee

$$\mathcal{L}_{ au Z}^{\mathrm{NP}} \propto \overline{ au} \begin{bmatrix} \gamma^{\mu} q^{2} / m_{ au}^{2} \left(\mathcal{C}_{1}^{V} + \gamma_{5} \mathcal{C}_{1}^{A}
ight) \\ + i \sigma^{\mu
u} q_{
u} / (2m_{ au}) \left(\mathcal{F}_{2} + \gamma_{5} \mathcal{F}_{3}
ight) \end{bmatrix} au Z_{\mu}$$

Benchmark limit:

- FCC-ee simulation at $s = m_Z^2$
- combines concurrence, incl xsec, ...
- $\begin{array}{||c||} \bullet & \left| C_1^V \right| < 0.01, \left| C_1^A \right| < 0.001 \\ |F_2| < 0.003, |F_3| < 0.001 \end{array}$



COMPARISON OF DIFFERENT METRICS





- $^{*}\mathcal{C}$ measures entanglement
- * \mathcal{M}_2 measures diffculty to classically simulate







QUANTUM PROBABILITY

positive definite matrix: $\rho \ge 0$

- $ho_{ij} = \sum_{k} c_{ik} c_{jk}^{*} = (\mathcal{CC}^{\dagger})_{ij} \rightarrow \langle \phi | \rho | \phi \rangle = \left\langle \mathcal{C}^{\dagger} \phi \middle| \mathcal{C}^{\dagger} \phi \right\rangle \geq 0$
- diagonalizable: $ho = \sum_i p_i |\phi_i \rangle \langle \phi_i |$ with $p_i \ge 0$
- **system in state** ϕ_i with probability p_i
- $ightarrow \,$ quantum probability distribution

classical merchanics: density matrix always diagonal