Quantum computing for high-energy physics simulations

Mathieu PELLEN

University of Freiburg

Based on **[Agliardi, Grossi, MP, Prati; 2201.01547]** and **[Chawdhry, MP; 2303.04818]**

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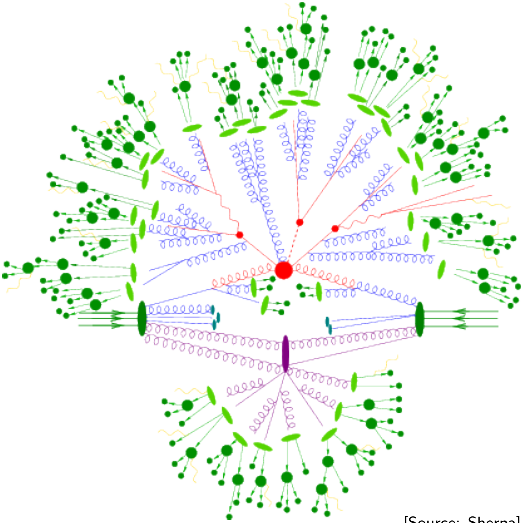
Quantum-computing applications in high-energy physics



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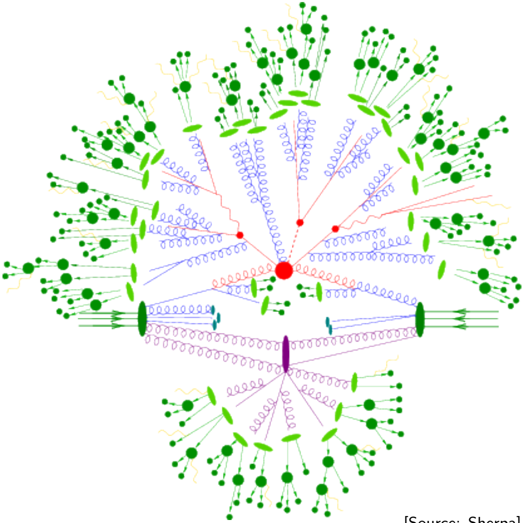

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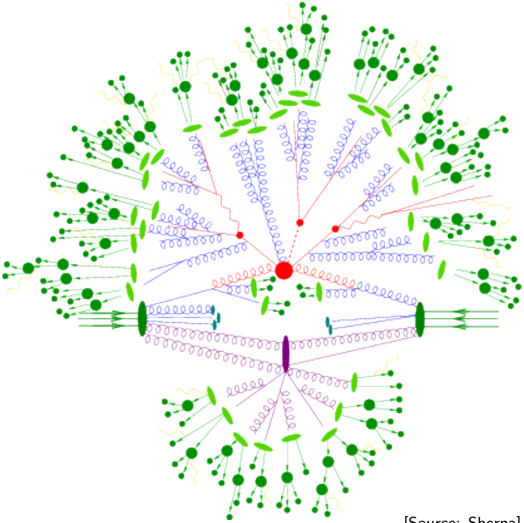

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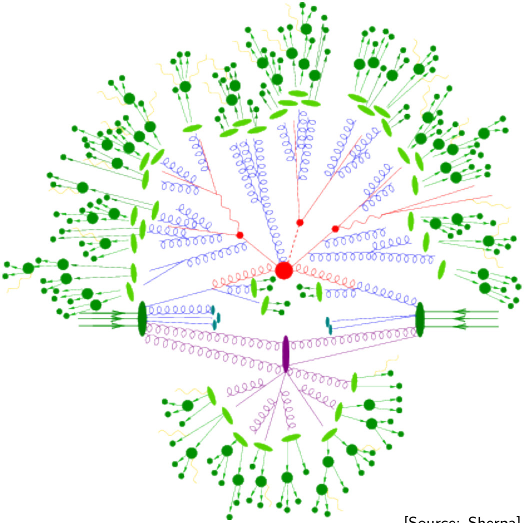
Quantum-computing applications in high-energy physics

→ Quantum applications still in their infancy!

- Is it possible?
- Is there a (theoretical) quantum advantage?
- Is it more resource efficient than CPU/GPU?

→ Look at the example of quantum simulation/integration in high-energy physics!



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Computing problem in high-energy physics

→ Event generation:
$\sim$ 15% of $\sim$ 3 billion cpuh.y^{-1} for ATLAS
→ More in: [Buckley; 1908.00167], [Valassi et al.; 2004.13687]

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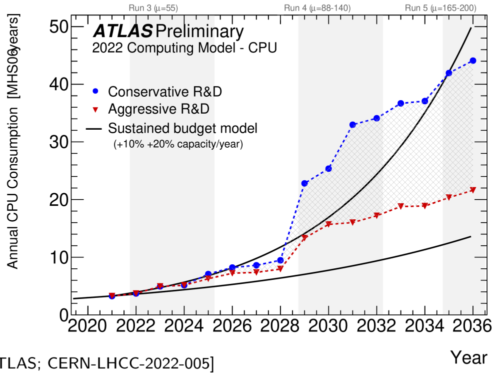

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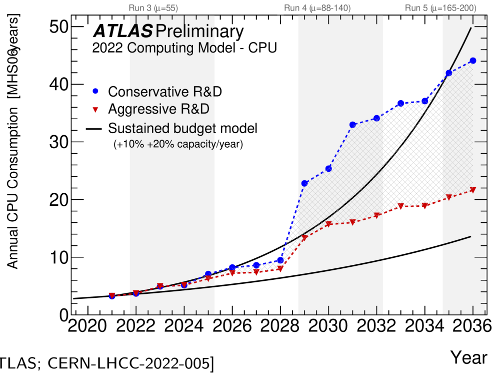

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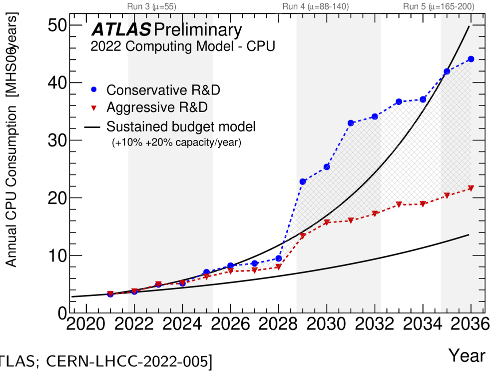

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- Can quantum computing be of any use in HEP?
  → to compute things faster/more efficiently?
  → to compute new things?

Cross section

- → Probability to measure scattering process
- → Predictable theoretically and measurable experimentally!
- → Monte Carlo techniques with error scaling as $1/\sqrt{N}$

$$\sigma \propto \int \mathrm{d}\Phi |\mathcal{M}|^2$$

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→ In general:

$$\sigma \propto \int_0^1 \mathrm{d}x_1 \cdots \int_0^1 \mathrm{d}x_n \, f(x_1, \cdots, x_n) \, \Theta(g(x_1, \cdots, x_n))$$

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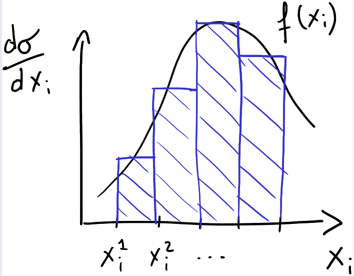
- For a given observable $\mathcal{O} = \mathcal{O}(x_1, \cdots, x_n)$:

$$\sigma = \sum_i \frac{\mathrm{d}\sigma}{\mathrm{d}\mathcal{O}^i} = \sum_{i,l} c_{il} \frac{\mathrm{d}\sigma}{\mathrm{d}x_l^i}$$

- **Integrating = guessing the values of a function at specific points (Riemann sum)**



State

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle = \begin{pmatrix}\alpha \\ \beta\end{pmatrix},$$

with $\alpha^2 + \beta^2 = 1$

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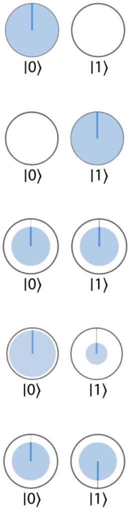
→ Representation

Possible values of a qubit	Graphical representation
$\|0\rangle$	
$\|1\rangle$	
$0.707\|0\rangle + 0.707\|1\rangle$	
$0.95\|0\rangle + 0.35\|1\rangle$	
$0.707\|0\rangle - 0.707\|1\rangle$	



→ Basic of quantum mechanics

State

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle = \begin{pmatrix}\alpha \\ \beta\end{pmatrix},$$

with $\alpha^2 + \beta^2 = 1$

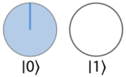
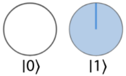
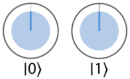
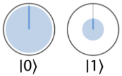
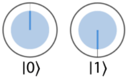
Operation

$$\psi \xrightarrow{A} \psi'$$

$A\,|\psi\rangle = |\psi'\rangle$ with A unitary

$$|\psi\rangle \; — \boxed{A} — \; |\psi'\rangle$$

→ Representation

Possible values of a qubit	Graphical representation
$\lvert 0\rangle$	
$\lvert 1\rangle$	
$0.707\lvert 0\rangle + 0.707\lvert 1\rangle$	
$0.95\lvert 0\rangle + 0.35\lvert 1\rangle$	
$0.707\lvert 0\rangle - 0.707\lvert 1\rangle$	

Example of gates

Pauli-X (X)

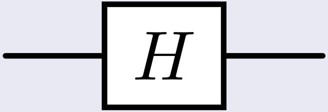
$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\alpha |0\rangle + \beta |1\rangle \to \alpha |1\rangle + \beta |0\rangle$$

Hadamard (H)

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$\alpha |0\rangle + \beta |1\rangle \to \alpha \frac{|0\rangle + |1\rangle}{\sqrt{2}} + \beta \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

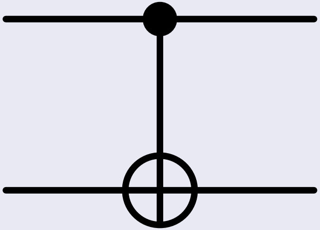


Example of gates

Controlled not (CNOT, CX)

$$CX = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$|00\rangle \rightarrow |00\rangle$; $|01\rangle \rightarrow |01\rangle$;
$|10\rangle \rightarrow |11\rangle$; $|11\rangle \rightarrow |10\rangle$.



- If 0 nothing happens, if 1 CX!
- *Control* qubit (top) and *target* qubit (bottom)

Grover algorithm/iteration

- Very general quantum algorithm
- Quadratic speed up $\rightarrow \mathcal{O}(\sqrt{N})$ operations instead of $\mathcal{O}(N)$
- Most famous example: unstructured database search

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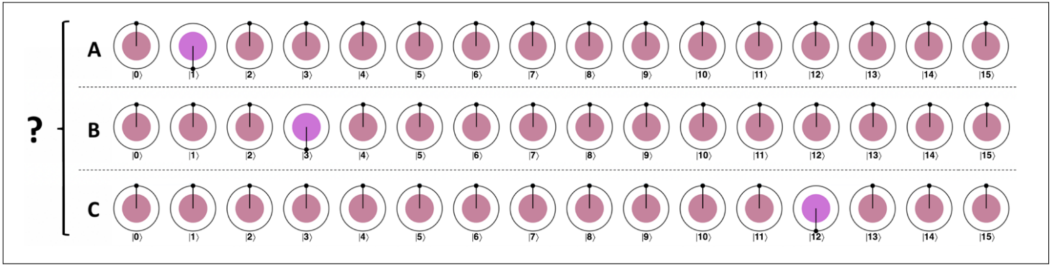
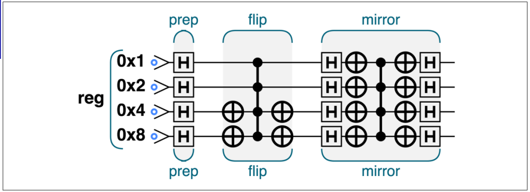
- Example (from [Johnston, Harrigan, Gimeno-Segovia; Programming Quantum Computers])

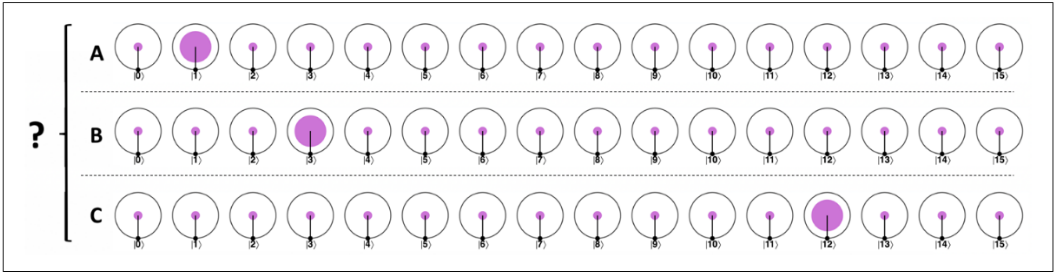


→ What solution is contained in our quantum register?

Grover algorithm/iteration

→ Applying a Grover iteration





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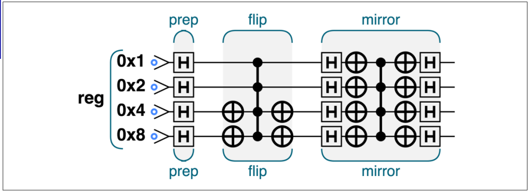

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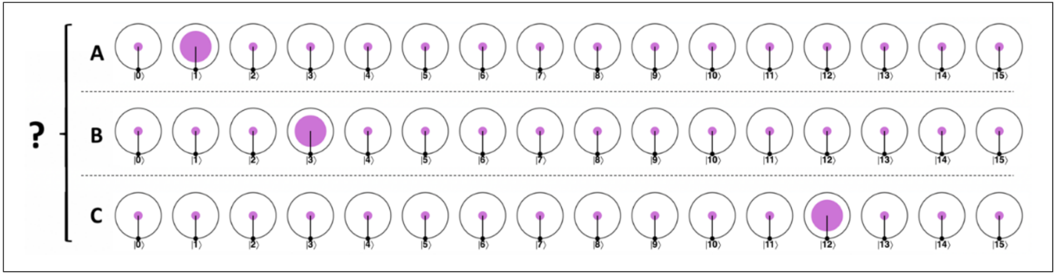
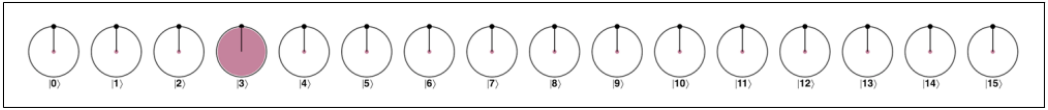


→ Applying it twice



Quantum Amplitude Estimate (QAE) [Brassard, Hoyer, Mosca, Tapp; quant-ph/0005055]

$$\mathcal{A}|0\rangle = \sqrt{1-a}|\Psi_0\rangle + \sqrt{a}|\Psi_1\rangle$$

$\rightarrow$ QAE estimates a with high probability such that the estimation error scales as $\mathcal{O}(1/M)$ [as opposed to $\mathcal{O}(1/\sqrt{M})$]

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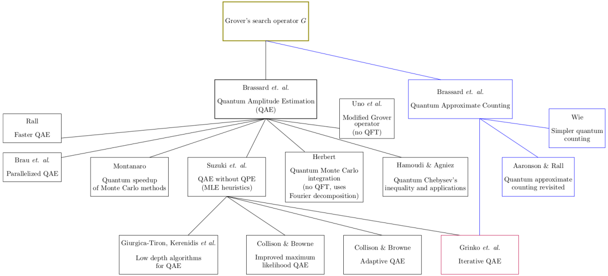

[Intallura et al.; 2303.04945]

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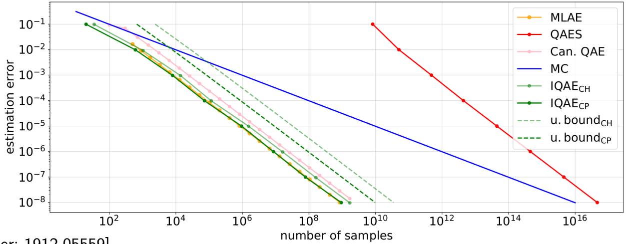
→ QAE estimates a with high probability such that the estimation error scales as $\mathcal{O}(1/M)$ [as opposed to $\mathcal{O}(1/\sqrt{M})$]
→ Various algorithms/implementations available
→ Basis of quantum Monte Carlo integration and $\mathcal{O}(1/M)$ scaling



[Grinko, Gacon, Zoufal, Woerner; 1912.05559]

Resulting estimation error for $a = 1/2$ and 95% confidence level with respect to the required total number of oracle queries.

Quantum integration

Extension to

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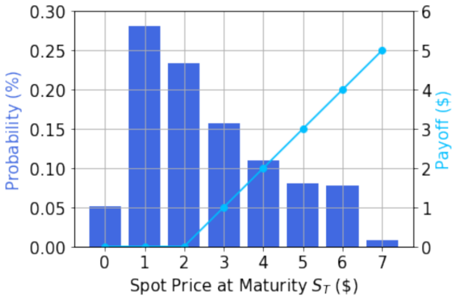
[Woerner and Egger; 1806.06893], [Stamatopoulos et al.; 1905.02666, 2111.12509], [Rebentrost, Gupt, Bromley; Phys.Rev.A 98 (2018) 022321]

→ Applicable to HEP? What are the limitations?



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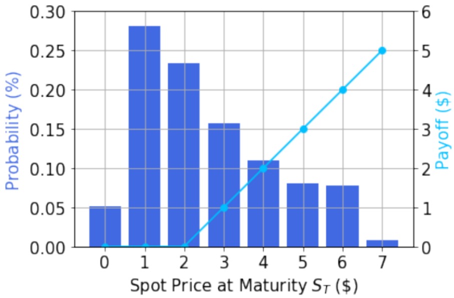
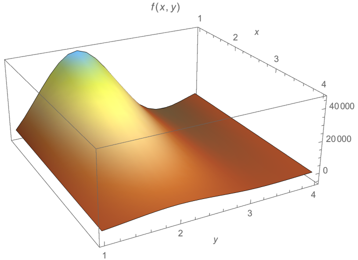
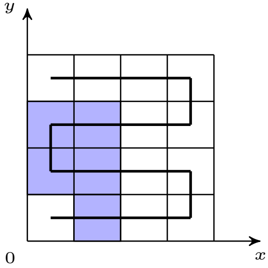


$$I = \int \mathrm{d}x\, f(x) g(x)$$

- In finance:
  - f: probability
  - g: payoff
- In HEP:
  - f: $|\mathcal{M}|^2$
  - g: $\Theta(\Phi - \Phi_c)$

Integration - 2D [$e^+e^- \to \mathbf{q\bar{q}}'W$ with angles fixed]





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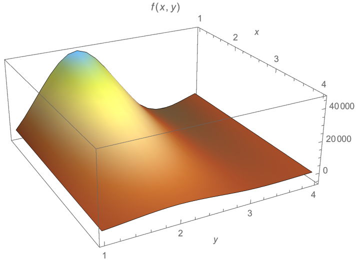
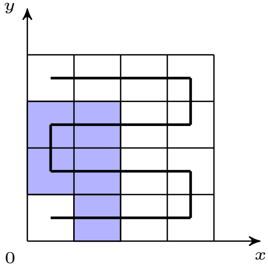




Qubits number	Grid dim.	$\mathcal{S}_1$ σ	$\mathcal{S}_1$ $\delta[\%]$	$\mathcal{S}_2$ σ	$\mathcal{S}_2$ $\delta[\%]$
4	4×4	0.55	0	0.70	-4.1
5	5×5	0.52	-4.92	0.53	-26.6
6	6×6	0.47	-14.1	0.79	9
6	7×7	0.62	-14.4	0.70	-3.0
6	8×8	0.55	0	0.78	7.6

$\mathcal{S}_1$: matching boundary of integration

$\mathcal{S}_2$: no matching boundary of integration

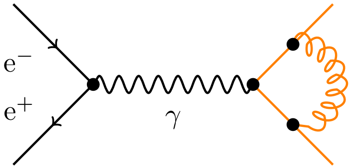
[Agliardi, Grossi, MP, Prati; 2201.01547]

Working but control of uncertainty crucial!

Alternative to loading - [Chawdhry, MP; 2303.04818]

$$\mathcal{M} \sim \sum \mathrm{Tr}\left(T^{a_1} \ldots T^{a_n}\right) \mathcal{K}(1, \ldots, n)$$

- Kinematic part: made of spinors and tensors (and kinematic invariants)
- Colour part: made of SU(3) generators of QCD



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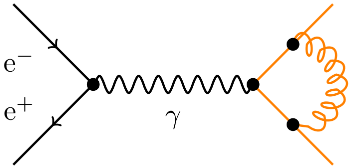

Remarks

- First step towards a full quantum amplitude/Monte Carlo
- Useful for a quantum parton shower

Colour algebra in QCD - crash course

- $[T^a, T^b] = \mathrm{i} f_{abc} T^c$.
- $T^a, T^c, \ldots$: SU(3) generators
- Gell-Mann matrices

$$T^1 = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad T^2 = \frac{1}{2}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad T^3 = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad T^4 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$T^5 = \frac{1}{2}\begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad T^6 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad T^7 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad T^8 = \frac{1}{2\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

Attention! T^a are not unitary!

→ In our example, colour factor: $T^a_{ij} T^a_{ji} = C_F$

Quantum implementation of colour

- Gluon: 8 colours → 3 qubits (2^3)
- Quark: 3 colours → 2 qubits (2^2)

→ Make non-unitary matrices unitary: extend dimension and modify them

$$\overline{T^1} = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \overline{T^2} = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \overline{T^3} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \overline{T^4} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

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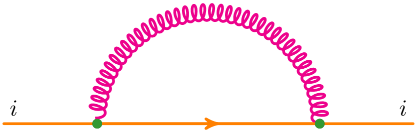
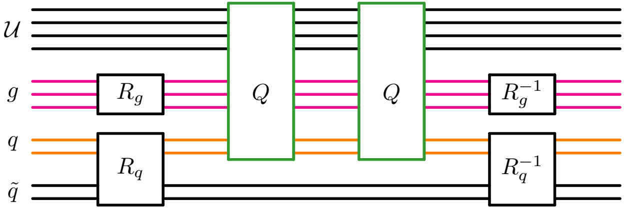
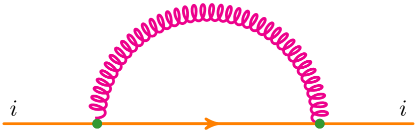
Example

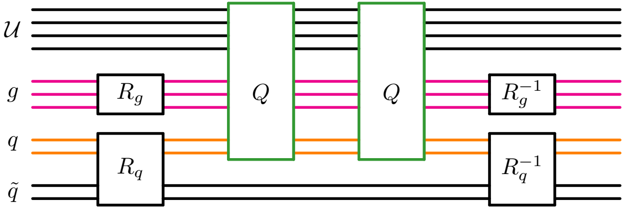




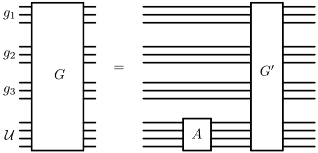
- One-to-one correspondence between Feynman diagram and circuit
- Gates for qqg (Q) and ggg (G) vertices to simulate QCD (colour) interaction

Example

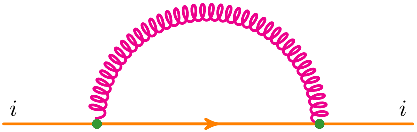


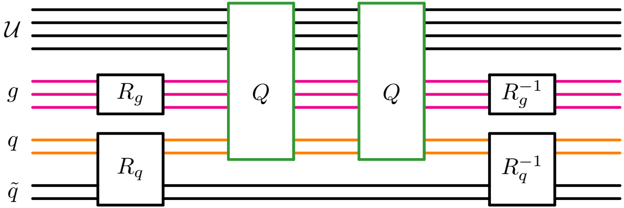


- One-to-one correspondence between Feynman diagram and circuit
- Gates for qqg (Q) and ggg (G) vertices to simulate QCD (colour) interaction



Example





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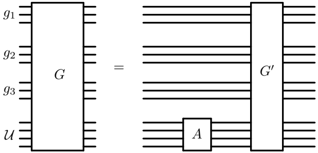
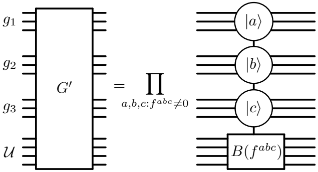
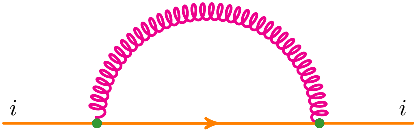
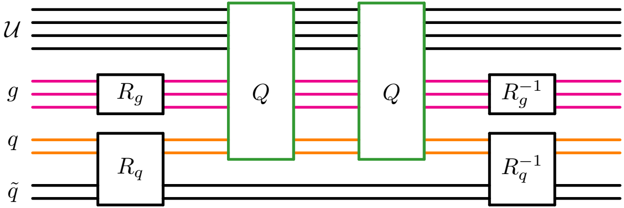
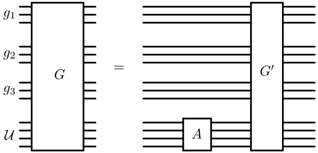


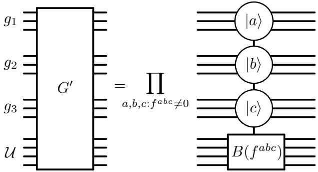


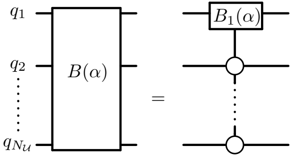




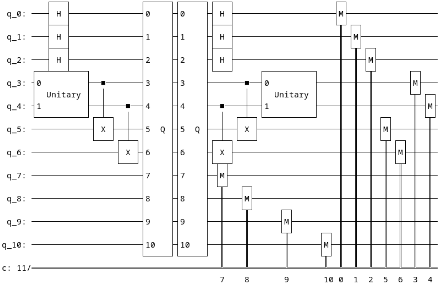
$$\langle\Omega|_{\mathcal{U}} \prod_{i=1}^{N_{ops}} \{B(\alpha_i)A\} |\Omega\rangle_{\mathcal{U}} = \prod_{i=1}^{N_{ops}} \alpha_i$$







(real-life) Example



Total counts are: {'00000010101': 226, '00010010011': 342, '00000010110': 225, '00000001101': 696, '00010010010': 362, '00000010001': 872, '00010001101': 2006, '00000001100': 643, '00010001100': 2006, '00010000110': 1051, '00000001111': 638, '00000010010': 904, '00010000010': 1057, '00100010101': 52353, '00010010100': 3342, '00100000101': 6942, '00010000111': 1046, '00000010111': 210, '00100001101': 36223, '00100010111': 51877, '00000001110': 643, '00010010000': 4838, '00000010100': 5421, '00010000100': 1035, '00100000000': 107280, '00010000011': 1075, '00100000111': 6795, '00100001011': 145043, '00100010010': 10275, '00010000000': 65548, '00000000000': 27415, '00010001111': 2031, '00100000110': 7004, '00000001011': 2551, '00100001111': 36471, '00010010111': 8866, '00010000101': 1077, '00100010110': 52220, '00010010110': 9080, '00100010100': 185856, '00100001100': 36173, '00010010101': 8860, '00100010000': 14129, '00100001110': 36925, '00100000100': 6858, '00100010011': 10182, '00100000001': 6950, '00010001110': 2018, '00100000011': 6983, '00000010011': 815, '00010001011': 7957, '00010010001': 340, '00100010001': 10163, '00010000001': 1092, '00100000010': 7010}

→ Trace defined in $|00000000000\rangle = |0_{11}\rangle$ state: $|\psi\rangle = \frac{\mathcal{C}}{\mathcal{N}}|0_{11}\rangle + \ldots$

$$\Rightarrow \frac{27415}{N_{\text{shots}}=1000000} \sim \left(\frac{\mathcal{C}}{\mathcal{N}} = \frac{(N_c{=}3)C_F}{N_c^{n_q=1}(N_c^2-1)^{n_g=1}}\right)^2$$

→ Colour factors encoded in one single state (as needed for QAE)

→ Any colour factor computable

Quantum Monte Carlo in high-energy physics

- Is it possible?
  $\rightarrow$ **Yes.**

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  $\rightarrow$ **In principle, yes. In practice for now, no.**

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  $\rightarrow$ **Yes.**

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- Is it more resource efficient than CPU/GPU?
  $\rightarrow$ **At the moment, not known.**

Road map for quantum Monte Carlo

- Reliable error estimate
  $\rightarrow$ Taking into account binning effects / multi-dimension integrand

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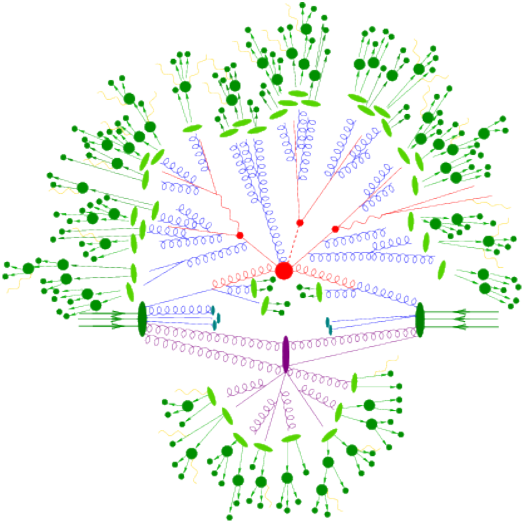
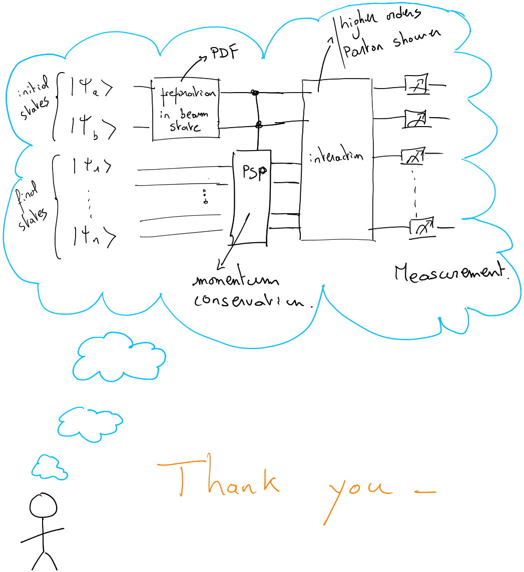
- Can there be quantum advantage for event generation? [Bravo-Prieto et al; 2110.06933]




higher orders
Parton shower
PDF
initial states
$|\psi_a\rangle$
$|\psi_b\rangle$
preparation in beam state
final states
$|\psi_1\rangle$
$|\psi_n\rangle$
PSP
interaction
momentum conservation.
Measurement.

Thank you –

BACK-UP

Reviews

- [Gray, Terashi; Gray:2022fou] (selected topics)
- [Delgado et al.; 2203.08805] (Snowmass)
- [Klco et al.; 2107.04769] (lattice)

Selected references

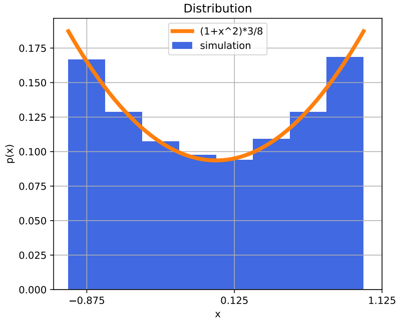
- Amplitude/loop integrals: [Ramirez-Uribe et al.; 2105.08703], [Bepari, Malik, Spannowsky, Williams; 2010.00046], **[Chawdhry, MP; 2303.04818]**
- Parton shower: [Bauer, de Jong, Nachman, Provasoli; 1904.03196], [Bepari, Malik, Spannowsky, Williams; 2010.00046], [Williams, Malik, Spannowsky, Bepari; 2109.13975], [Chigusa, Yamazaki; 2204.12500], [Gustafson, Prestel, Spannowsky, Williams; 2207.10694], [Bauer, Chigusa, Yamazaki; 2310.19881]
- Machine learning: [Filipek et al; 2105.04582], [Bravo-Prieto et al; 2110.06933], [Alvi, Bauer, Nachman; 2206.08391]
- Others: [Ciavarella; 2007.04447], [Perez-Salinas, Cruz-Martinez, Alhajri, Carrazza: 2011.13934], [Bauer, Freytsis, Nachman; 2102.05044], [Martenez de Lejarza, Cieri, Rodrigo; 2204.06496], **[Agliardi, Grossi, MP, Prati; 2201.01547]**, [Martenez de Lejarza et al.; 2401.03023], [Cruz-Martinez, Robbiati, Carrazza; 2308.05657]

Loading of distribution / encoding into qubits

Encoding the distribution to be integrated into qubits

- Exact loading [Shende, Bullock, Markov, quant-ph/0406176] (resource intensive)
- Using quantum machine learning (qGAN) [Zoufal, Lucchi, Woerner; 1904.00043] (not exact)

- Example: Exact loading - $1 + x^2$



→ 3 qubits: $2^3 = 8$ bins

Quantum Amplitude Estimate (QAE)

[Brassard, Hoyer, Mosca, Tapp; Quantum Amplitude Amplification and Estimation]

$$\mathcal{A}|0\rangle = \sqrt{1-a}|\Psi_0\rangle + \sqrt{a}|\Psi_1\rangle$$

QAE estimates a with high probability such that the estimation error scales as $\mathcal{O}(1/M)$ [as opposed to $\mathcal{O}(1/\sqrt{M})$]

M: number of applications of $\mathcal{A}$

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→ What the (orignal) algorithm provides:

- An estimate: $\tilde{a} = \sin^2(\tilde{\theta}_a)$
  with $\tilde{\theta}_a = y\pi/M$, $y \in \{0, ..., M-1\}$, and $M = 2^n$
- A success probability (that can be increased by repeating the algorithm)
- A bound: $|a - \tilde{a}| \leq \mathcal{O}\left(1/M\right)$

Applications

- **$e^+e^- \to q\bar{q}$** (in QED)

$$\sigma \sim \int_{-1}^{1}\int_{0}^{2\pi} \mathrm{d}\cos\theta \mathrm{d}\phi \left(1+\cos^2\theta\right)$$

- **$e^+e^- \to q\bar{q}'W$**

$$\begin{aligned}\sigma &\sim \int_{M_W^2}^{s}\int_{0}^{s_1^{\mathrm{Max}}}\int_{-1}^{1}\int_{0}^{2\pi}\int_{0}^{2\pi} \mathrm{d}\Phi_3 \left|\mathcal{M}_{e^+e^-\to q\bar{q}'W}\right|^2 \\ &\sim \int_{M_W^2}^{s}\int_{0}^{s_1^{\mathrm{Max}}} \mathrm{d}\tilde{\Phi}_3 \left|\mathcal{M}'\right|^2\end{aligned}$$

with $\mathcal{M}' = \mathcal{M}_{e^+e^-\to q\bar{q}'W}\left(\cos\theta_1 = 0,\ \phi_1 = \pi/2,\ \phi_2 = \pi/2\right)$.

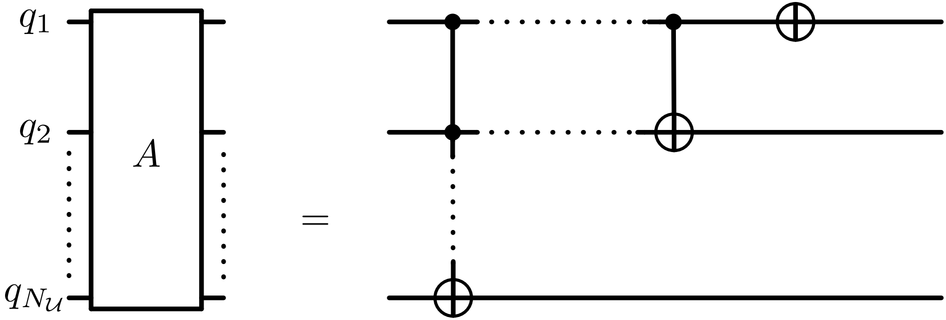
Integration - $1 + x^2$

- Matching boundary of integration (3 qubits $\Rightarrow 2^3$ bins)

Domain	low stat.		high stat.		very high stat.		exact	
	σ	$\delta[\%]$	σ	$\delta[\%]$	σ	$\delta[\%]$	σ	$\delta[\%]$
$[-0.75; 0]$	0.345	-3.31	0.332	0.706	0.334	0.0331	0.334	-8.31×10^{-3}
$[-0.5; 0]$	0.215	-5.86	0.201	1.15	0.203	0.0986	0.203	-0.0161
$[-0.25; 0]$	0.112	-17.1	0.0939	1.87	0.0960	-0.284	0.0957	-0.0389

- Non-matching boundary of integration

Qubits number	$[-0.7; 0.6]$				$[-0.625; 0.375]$			
	high stat.		exact		high stat.		exact	
	σ	$\delta[\%]$	σ	$\delta[\%]$	σ	$\delta[\%]$	σ	$\delta[\%]$
3	0.402	-28.0	0.406	-27.1	0.296	-28.1	0.299	-27.5
4	0.463	-17.0	0.468	-16.0	0.408	-1.07	0.412	5.96×10^{-3}
5	0.527	-5.46	0.532	-4.62	0.408	-1.07	0.412	5.96×10^{-3}
6	0.542	-2.76	0.547	-1.81	0.408	-1.07	0.412	5.96×10^{-3}


q_1
q_2
$q_{N_\mathcal{U}}$
A
=

$$B_1(\alpha) = \begin{pmatrix} \sqrt{1-|\alpha|^2} & \alpha \\ -\alpha & \sqrt{1-|\alpha|^2} \end{pmatrix} \tag{1}$$

$$B(\alpha)A\,|k\rangle = \begin{cases} \alpha\,|0\rangle + \sqrt{1-|\alpha|^2}\,|1\rangle & \text{if } k = 0 \\ |k+1\rangle & \text{if } 0 < k < 2^{N_{\mathcal{U}}} - 1 \\ \sqrt{1-|\alpha|^2}\,|0\rangle - \alpha\,|1\rangle & \text{if } k = 2^{N_{\mathcal{U}}} - 1 \end{cases} \tag{2}$$

$$\langle\Omega|_{\mathcal{U}} B(\alpha)A|\Omega\rangle_{\mathcal{U}} = \alpha \tag{3}$$

$$\langle\Omega|_{\mathcal{U}} \prod_{i=1}^{N_{ops}} \{B(\alpha_i)A\}\,|\Omega\rangle_{\mathcal{U}} = \prod_{i=1}^{N_{ops}} \alpha_i \tag{4}$$