Leveraging Periodic as a Quantum PDE Solver

Related references

Leveraging Periodic as a Quantum PDE Solver, to appear,
Joint with **Mariia Sobchuk, Xiaoran Li, Arsalan Motamedi, Grecia Castelazo, Ala Shayeghi**

Gibbs Sampling of Periodic Potentials on a Quantum Computer. arXiv:2210.08104 (2022), and Proceedings of the 41st International Conference on Machine Learning, PMLR 235:36322-36371, 2024
Joint with **Arsalan Motamedi**.

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Chief Technology Officer | 1QBit

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The Need for Structure in Quantum Speedups

Scott Aaronson* Andris Ambainis†

Received October 22, 2012; Revised July 10, 2014; Published August 12, 2014

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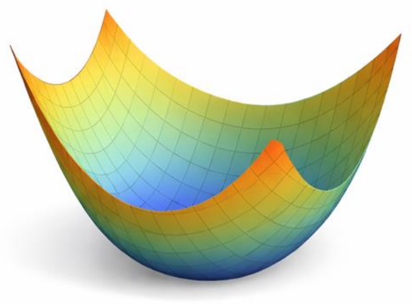
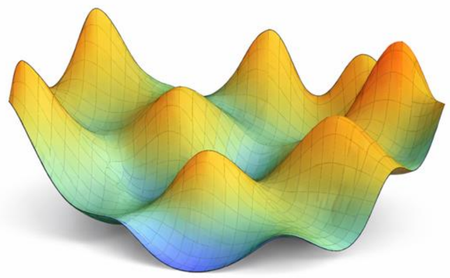
- What about when f is continuous?





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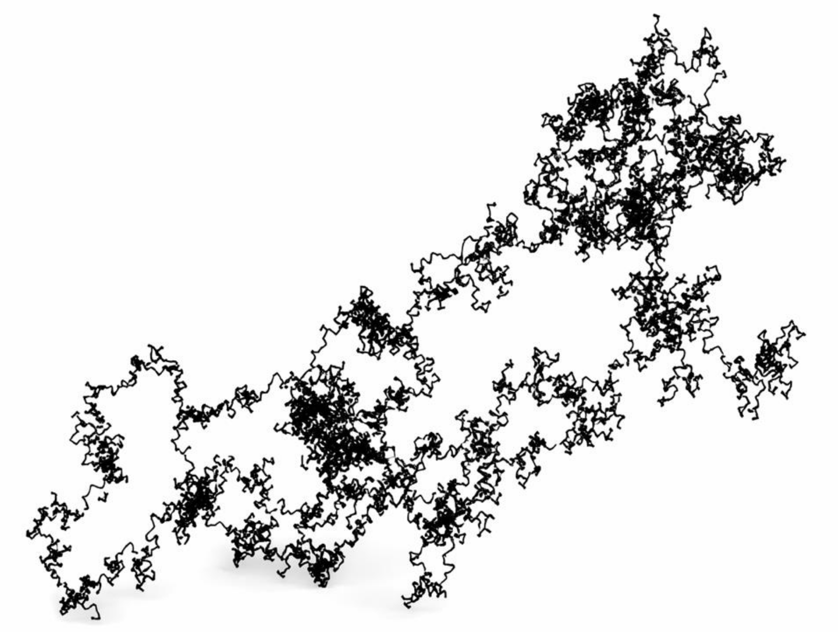

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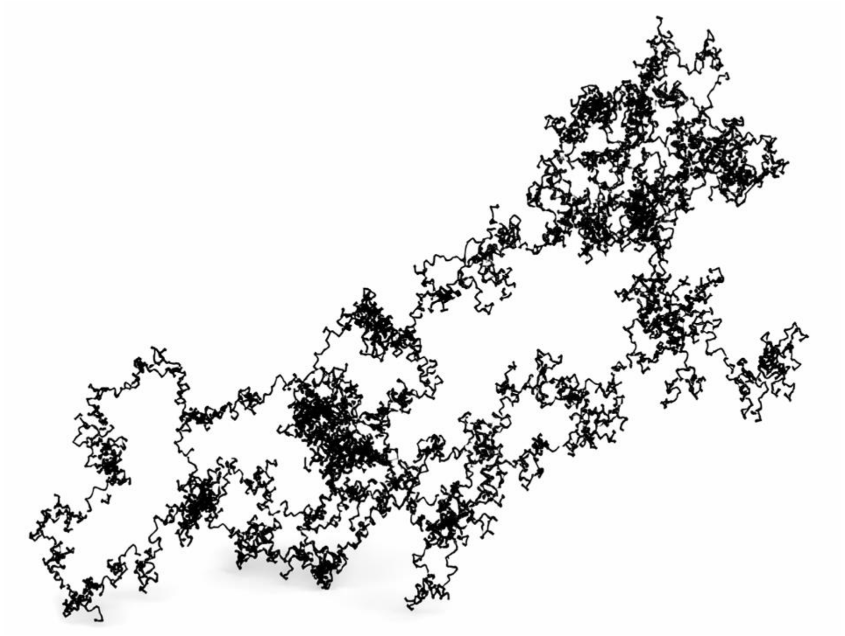

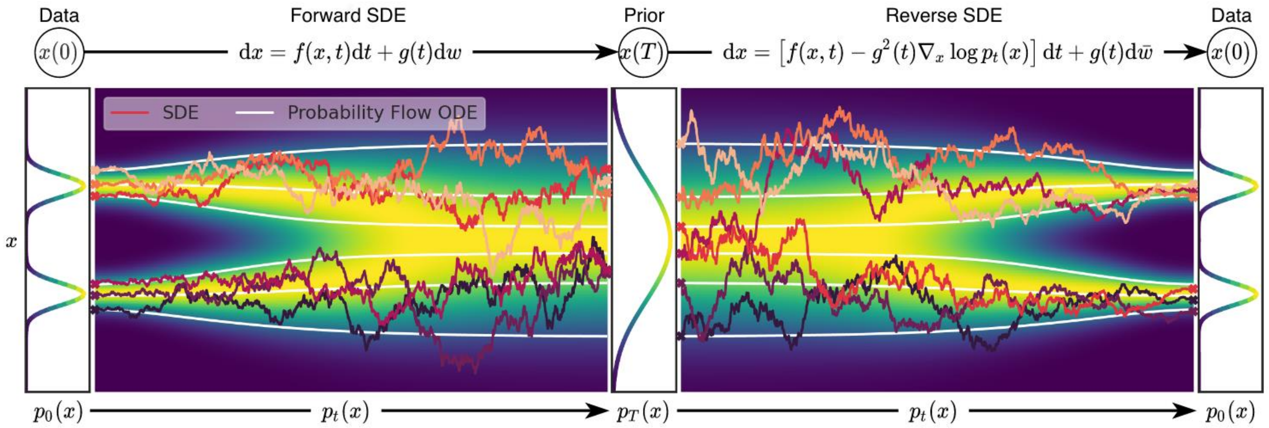

Feynman–Kac formula

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- An SDE

$$dX_t = b(X_t)dt + \sigma(X_t)dW_t$$

corresponds to a PDE with generator:

$$\mathcal{L} = \sum b_j \frac{\partial}{\partial x_j} + \frac{1}{2} \sum \sum_k \sigma_{ik}(x)\sigma_{jk}(x) \frac{\partial^2}{\partial x_i \partial x_j}$$

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- Transition operators $P(t, x, dy) = p(t, x, y)dy$
- Forward and backward Kolmogorov equations:

$$\frac{\partial}{\partial t}p(.,.,y) = \mathcal{L}_x p(.,.,y) \qquad \frac{\partial}{\partial t}p(.,x,.) = \mathcal{L}_y^* p(.,x,.)$$

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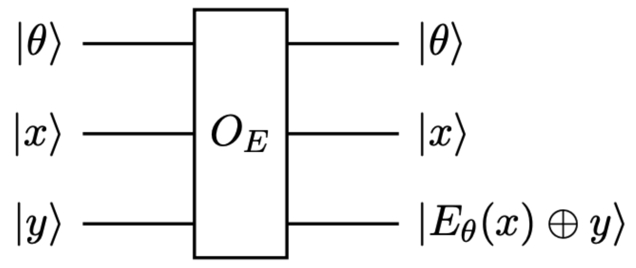

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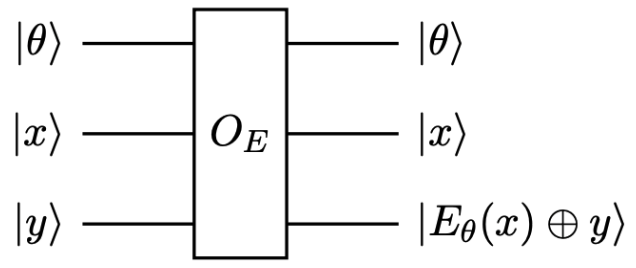

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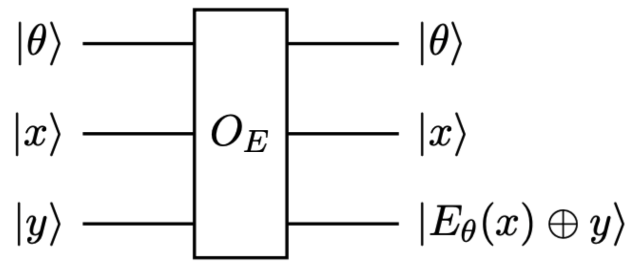

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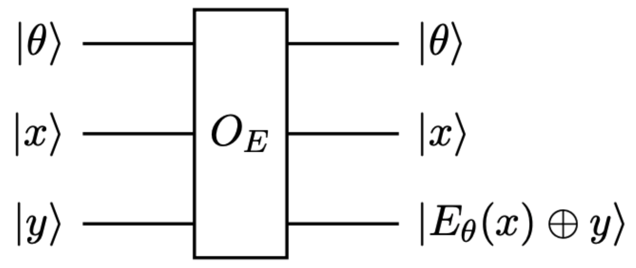

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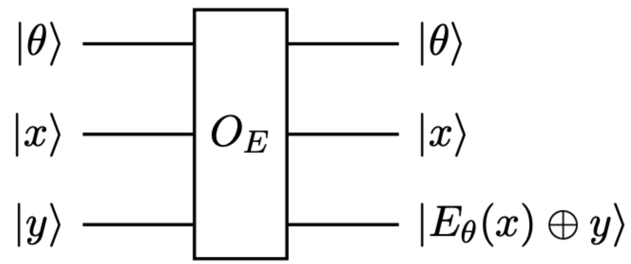

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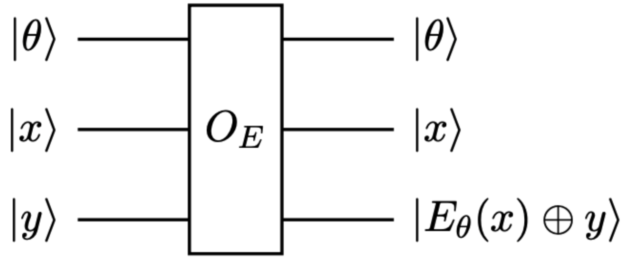

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Why analyticity?

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Critical role of QFT

$$|f_N\rangle := \frac{1}{\sqrt{\langle\!\langle f^2 \rangle\!\rangle_{\Gamma_N}}} \sum_{x \in \Gamma_N} f(x)\,|x\rangle \xrightarrow{F_N^{\otimes d}} |\widetilde{f}_N\rangle := \frac{1}{\sqrt{\langle f^2 \rangle_{\Gamma_N}}} \sum_{\omega \in \Lambda_N} \widetilde{f}_\omega \; |\omega\rangle$$

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$f(x)$	$= \sum_{\omega \in \mathbb{Z}^d} \widehat{f}_\omega\, e^{i\langle \omega, x\rangle}$	Fourier transform / series
$\widehat{f}_\omega$	$= \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} f(x) e^{-i\langle \omega, x\rangle}\, dx = \mathbb{E}_{\mathbb{T}^d}[f(x) e^{-i\langle \omega, x\rangle}]$	Fourier coefficients
$\widetilde{f}_\omega$	$= \mathbb{E}_{\Gamma_N}[f(x) e^{-i\langle \omega, x\rangle}]$	Discrete Fourier coefficients
$\|\widetilde{f}_N\rangle$	$= \frac{1}{\sqrt{N^d}} \sum_{\omega \in \Lambda_N} \widetilde{f}_\omega\, \|\omega\rangle = F_N^{\otimes d}\, \|f_N\rangle$	Discrete / quantum Fourier transform
$\widetilde{f}_\omega$	$= \sum_{m \in \mathbb{Z}^d} \widehat{f}_{\omega + (2N+1)m}$	Aliasing sums

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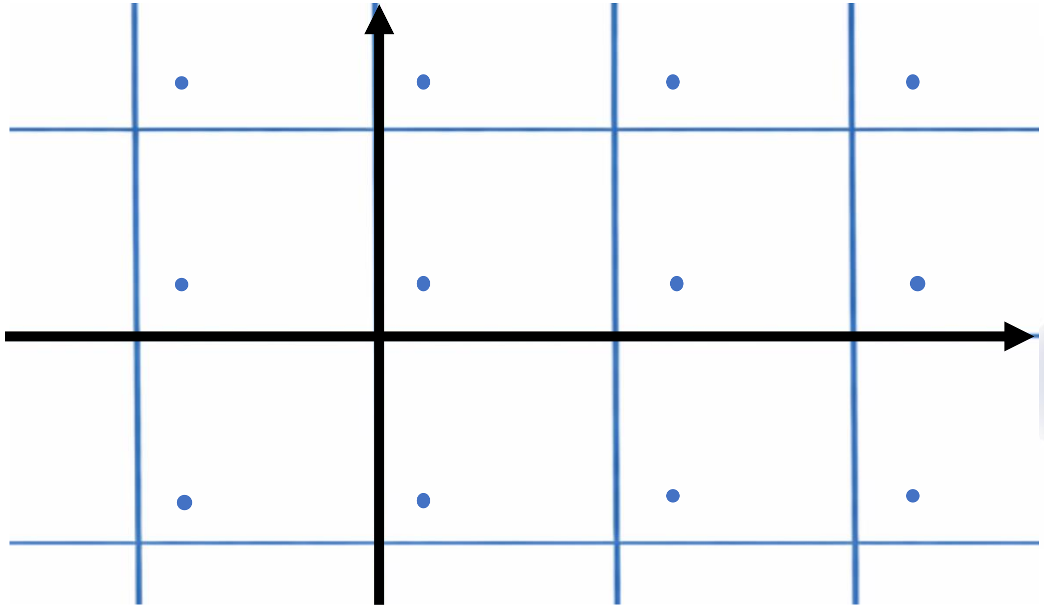
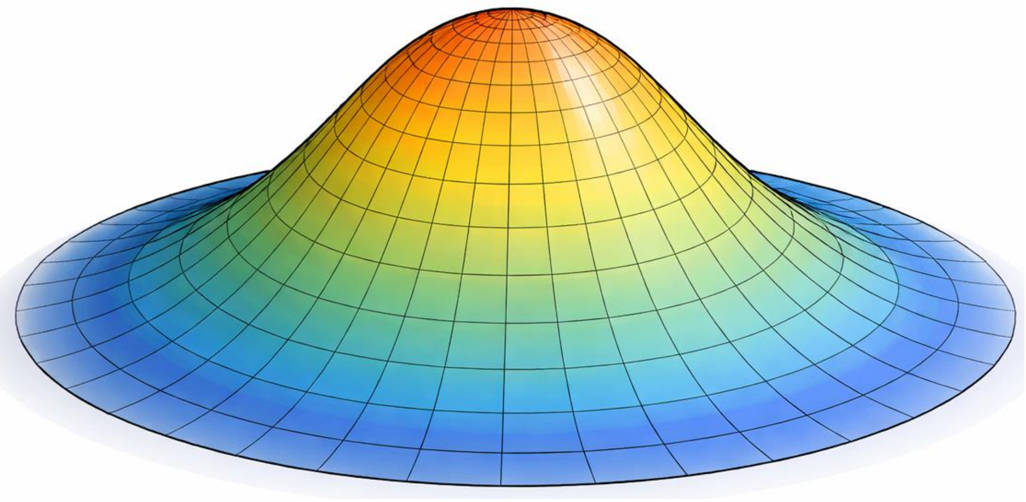




$$\widetilde{f}_\omega = \sum_{m \in \mathbb{Z}^d} \widehat{f}_{\omega+(2N+1)m}$$

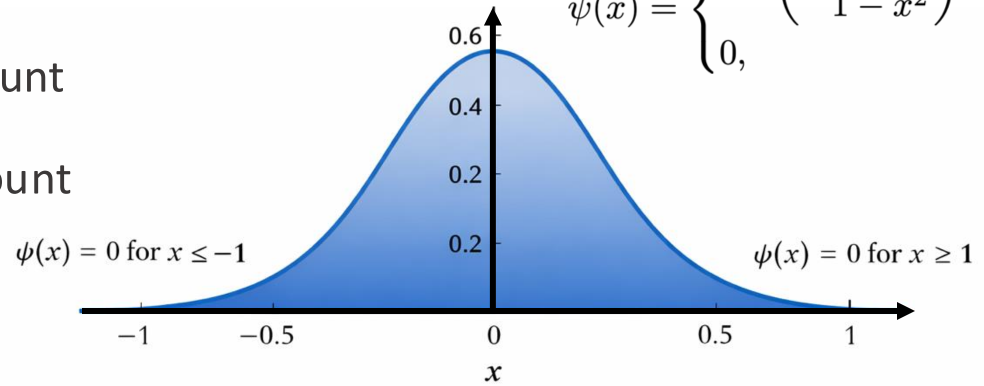
Aliasing sums

More smoothness = Faster decay of spectrum

Regularity class	Decay rate of Fourier coefficients ($\lvert\widehat{f}_\omega\rvert$)	Taildedness at cutoff N (truncation error, E_N)	Cutoff N to guarantee target precision ε
p-smooth ($\mathcal{C}^p$)	$C\lVert\omega\rVert_\infty^{-p}$	$C\sqrt{\frac{d}{d-2p}}N^{-p+d/2}$	$\left(\frac{C}{\varepsilon}\right)^{1/(p-d/2)}$
(p,q)-Hölder ($\mathcal{C}^{p,q}$)	$C\lVert\omega\rVert_\infty^{-p-q}$	$C\sqrt{\frac{d}{d-2p-2q}}N^{-p-q+d/2}$	$\left(\frac{C}{\varepsilon}\right)^{1/(p+q-d/2)}$
smooth ($\mathcal{C}^\infty$)	sub-polynomial	sub-polynomial	super-logarithmic
s-Gevrey ($\mathcal{G}^s$ for $s>1$)	$Ce^{-r\lVert\omega\rVert_\infty^{1/s}}$	$C\sqrt{\frac{ds}{r}N^{d-1/s}}\,e^{-rN^{1/s}}$	$\left(\frac{1}{2r}\log\frac{C^2ds}{r\varepsilon}\right)^s$
Analytic ($\mathcal{C}^\omega=\mathcal{G}^1$)	$Ce^{-r\lVert\omega\rVert_\infty}$	$C\sqrt{\frac{d}{r}N^{d-1}}\,e^{-rN}$	$\frac{1}{2r}\log\frac{C^2d}{r\varepsilon}$

- Faster decay of the Fourier coefficients ⇒ Less aliasing effects
- Only continuity ⇒ No guaranteed bound on qubit count
- Only p-smoothness ⇒ Polynomially growing qubit count
- Analytic functions have the fastest decay.

$$\psi(x)=\begin{cases}\exp\left(-\frac{1}{1-x^2}\right), & |x|<1,\\ 0, & |x|\geq 1.\end{cases}$$



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Example: Solving general linear PDEs

$$\sum_{\alpha \in \mathcal{J}} g_\alpha(x) D^\alpha u(x) = \eta(x)$$

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- We wish to perform: $D^\alpha f = \mathcal{F}^{-1} \operatorname{diag} \left\{ (i\omega)^\alpha : \omega \in \mathbb{Z}^d \right\} \mathcal{F}(f)$

- But we only can do: $\widetilde{D}^\alpha = (F_N^{\otimes d})^{-1} \operatorname{diag} \left(\left\{ \prod_{j=1}^{d} (i\omega_j)^{\alpha_j} \right\}_{\omega \in \Lambda_N} \right) F_N^{\otimes d}$

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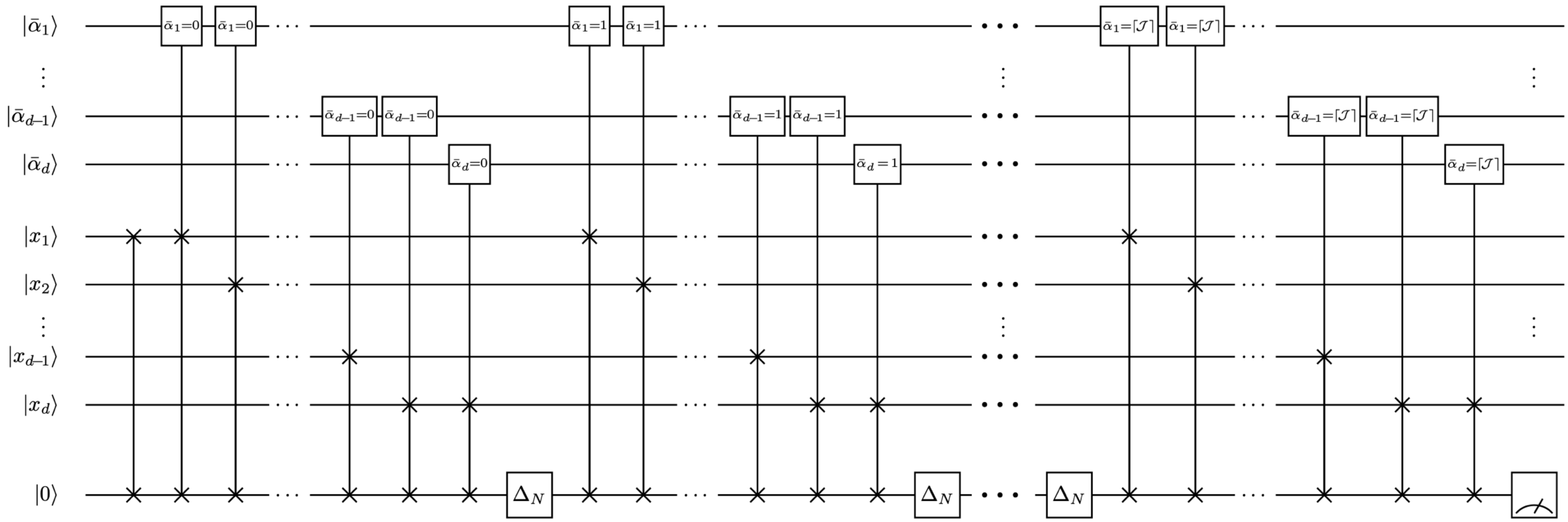
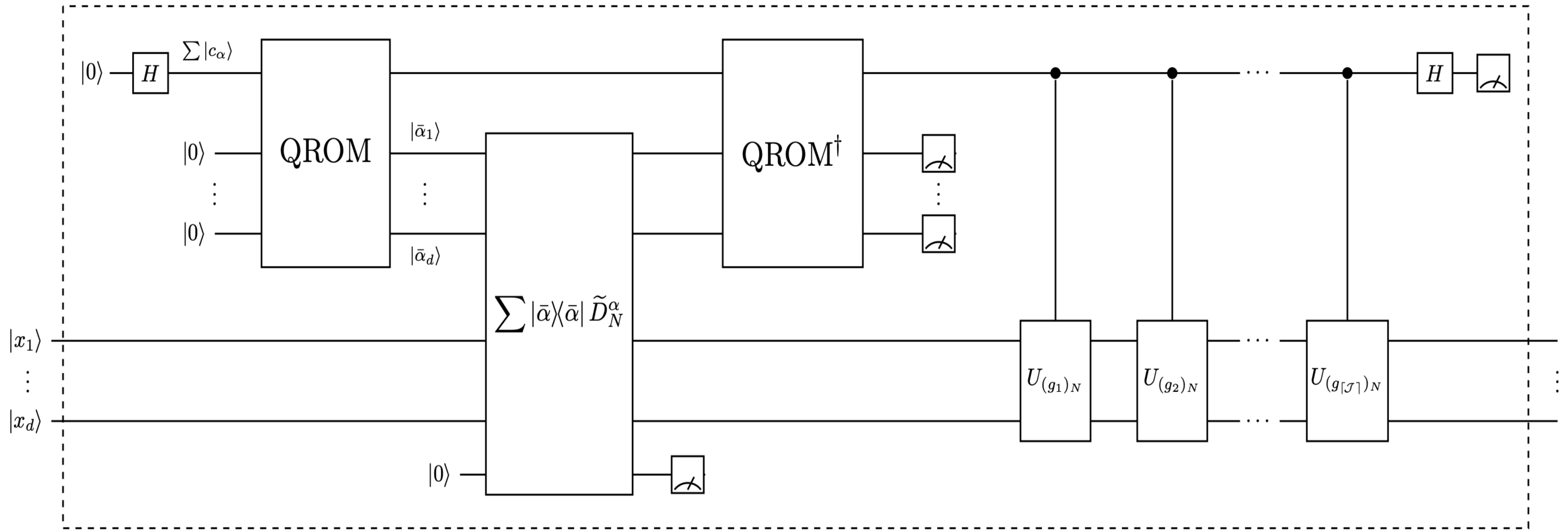
Block encoding of the approximate differentials



$$\Delta_N = F_N^{-1}\,\mathrm{diag}\{(i\omega)_{\omega\in\{-N,\cdots,N\}}\}F_N$$

$O(\log N \log\log N)$ elementary gates
$O(\log N)$ qubits

Block encoding of $\mathbb{L}_N$



$\mathbb{L}_N$

End-to-end resource count

$$\left\| \widetilde{D}_N^{\alpha} f_N - (D^{\alpha} f)_N \right\|_2 \lesssim 2^d N^{|\alpha| + d/2} E_N$$

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- Total gate count: $\widetilde{\mathcal{O}}\left(\frac{\lceil g\rceil(|\mathcal{J}| + \lceil\mathcal{J}\rceil)}{\sigma_{\min}^2 \|u_N\|} s^{\lceil\mathcal{J}\rceil s} d^{\lceil\mathcal{J}\rceil s+1}\left(d\log\left(\frac{1}{\sigma_{\min}\|u_N\|\varepsilon}\right)\right)^{\lceil\mathcal{J}\rceil s+1}\right)$
- Total qubit count: $\mathcal{O}(d(\log N + \log\lceil\mathcal{J}\rceil))$

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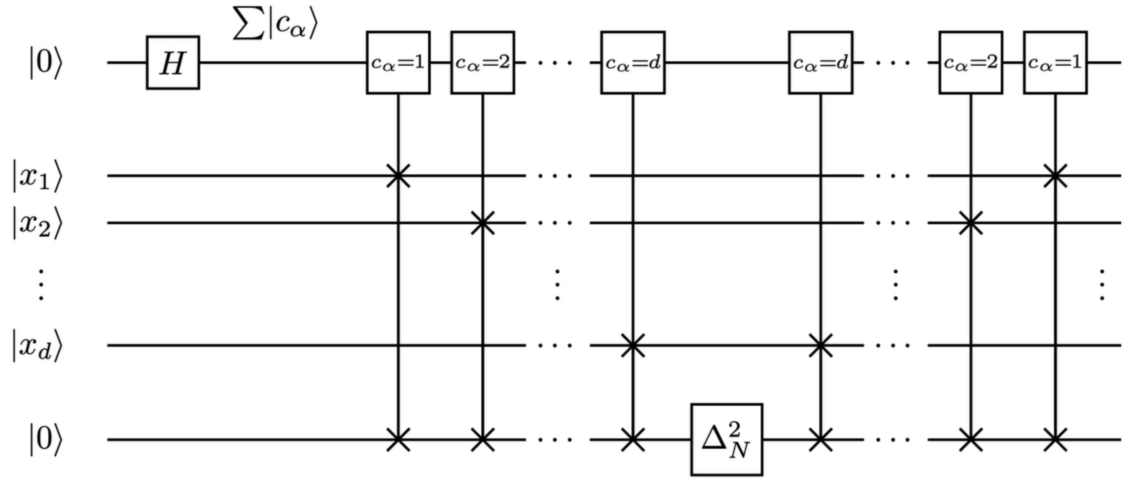
- Simpler block encoding for the Laplacian



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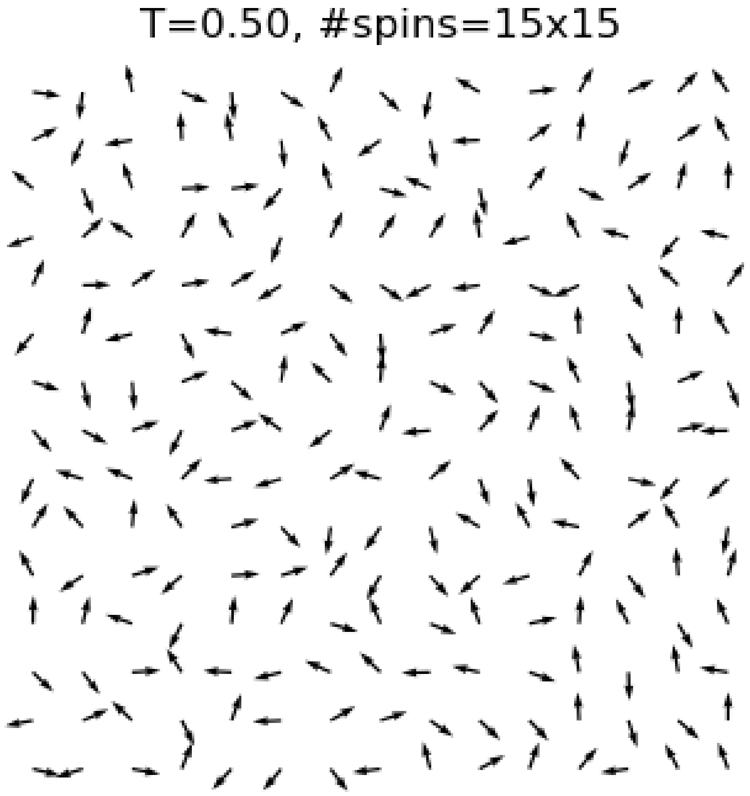
- Note: Classical runtime is $O\big((1/\epsilon)^{3M}\big)$.

Application 2: The classical XY model

- XY Hamiltonian

$$H(\mathbf{s}) = -\sum_{i \neq j} J_{ij}\ \mathbf{s}_i \cdot \mathbf{s}_j - \sum_j \mathbf{h}_j \cdot \mathbf{s}_j$$

$$= -\sum_{i \neq j} J_{ij}\ \cos(\theta_i - \theta_j) - \sum_j h_j \cos\theta_j$$



https://shilingliang.com/XY-MODEL/

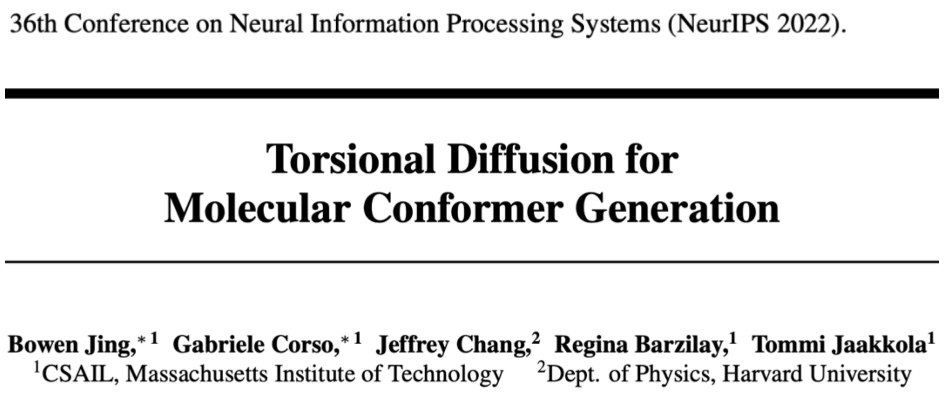
- Generalizations:
  - Heisenberg model
  - The n-vector model
  - Higgs sector of the standard model
- Other applications:
  - U(1) symmetric quantum field theories and gauge theories
  - Translationally invariant problems in condensed matter physics

Application 3: Molecular dynamics

Force field as a function of torsion angles:

$$U = \sum_{\text{bonds}} \frac{1}{2} k_b (r - r_0)^2 + \sum_{\text{angles}} \frac{1}{2} k_a (\theta - \theta_0)^2 + \sum_{\text{torsions}} \frac{V_n}{2} [1 + \cos(n\phi - \delta)]$$

$$+ \sum_{\text{improper}} V_{imp} + \sum_{\text{LJ}} 4\epsilon_{ij} \left(\frac{\sigma_{ij}^{12}}{r_{ij}^{12}} - \frac{\sigma_{ij}^{6}}{r_{ij}^{6}} \right) + \sum_{\text{elec}} \frac{q_i q_j}{r_{ij}},$$


36th Conference on Neural Information Processing Systems (NeurIPS 2022).

Torsional Diffusion for Molecular Conformer Generation

Bowen Jing,*[1] Gabriele Corso,*[1] Jeffrey Chang,[2] Regina Barzilay,[1] Tommi Jaakkola[1]
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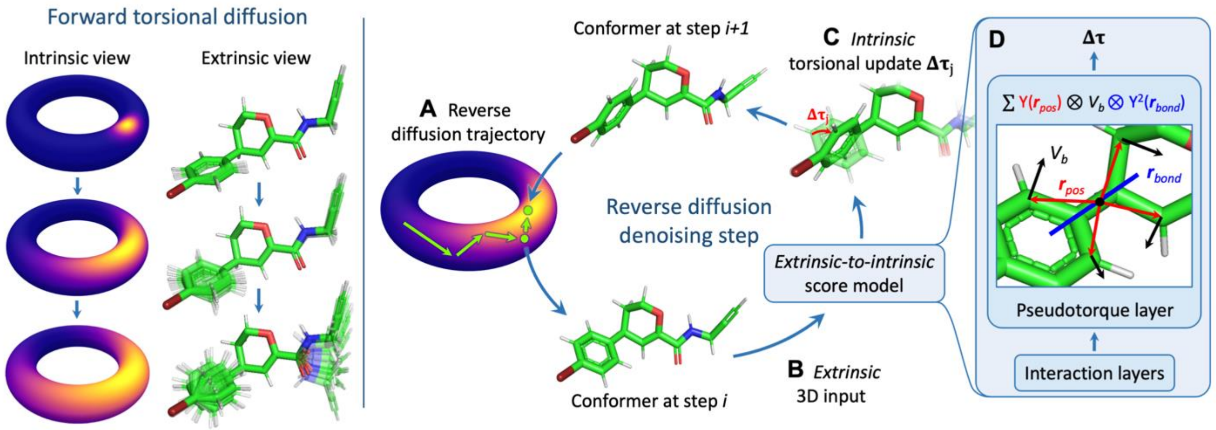

Conclusions

- The hardness of preparing continuous functions on a quantum computer is related to the degree of smoothness of them.

- Quantum ODE/PDE solvers can have interesting applications at the 10s to 100s of logical qubits.

- Quantum simulation using DFT pipelines is an interesting alternative to the common approach of mapping occupancy algebras to the spaces of qubit-based states.

- Potential applications include material science, condensed matter physics, and molecular dynamics simulations.

Thank you for your attention!

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