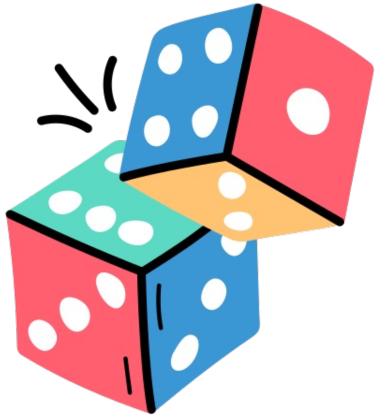
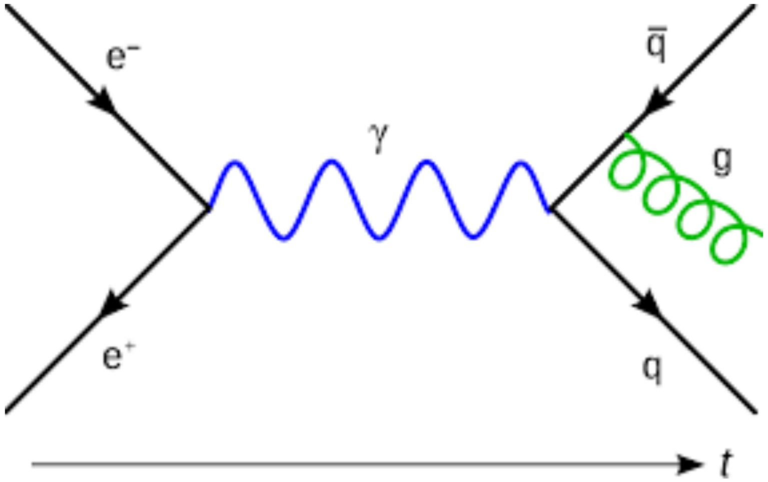
Stochastic quantum simulations for scattering experiments





Oriel Kiss, Michele Grossi and Alessandro Roggero

QTI Lecture, 5th April 2023

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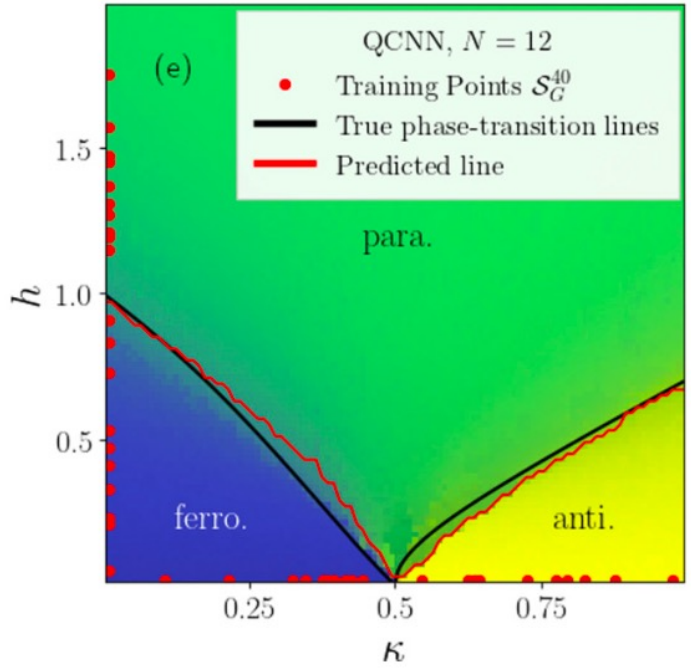
Quantum Simulation

- Use quantum computers to simulate quantum physical systems via evolving the Hamiltonian in time (Schrödinger equation).
- Quantum many-body systems are challenging for classical computers due to the exponential scaling of the Hilbert space.
- Available and useful with only ~100 (partially) error-corrected qubits on intermediate scale quantum devices (ISQ).
- We need better algorithms: smaller depth and lower overhead.

Applications

- Spectrum: compute energies via quantum phase estimation
- Dynamical properties: response functions, density of states, correlators, spin dynamics, etc
- Quantum phase diagram: crititcal points



Monaco, Kiss, et al., Phys. Rev. B 107, L081105 (2023)
Grossi, Kiss, et al, Phys. Rev. E 107, 024113 (2023)

Outline:

1. Stochastic product formula (QDRIFT).

2. Implementation cost reduction with importance sampling.

3. Composite channels: how to reduce the implementation cost?

4. Numerical simulations: lattice effective field theory.

5. Response functions computations from scattering experiments.

Stochastic product formula (QDRIFT)

Deterministic product formulas

Problem: scaling with *L*

Hamiltonian $H = h_1 H_1 + h_2 H_2 + h_3 H_3$

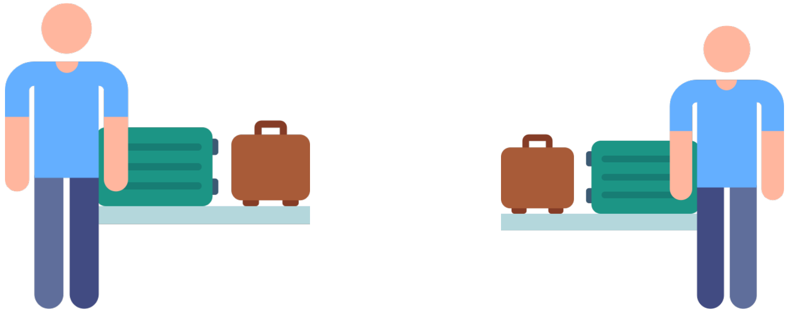
Time evolution e^{-iHt}

First order: apply term sequentially

ρ — $e^{-ith_1H_1}$ — $e^{-ith_2H_2}$ — $e^{-ith_3H_3}$ —

$$\mathcal{U}_1(t) = \prod_{\gamma}^{\rightarrow} e^{-itH_\gamma} = \mathcal{U}(t) + \mathcal{O}(t^2),$$

Second order



ρ — $e^{-ith_1H_1/2}$ — $e^{-ith_2H_2/2}$ — $e^{-ith_3H_3/2}$ — $e^{-ith_3H_3/2}$ — $e^{-ith_2H_2/2}$ — $e^{-ith_1H_1/2}$ —

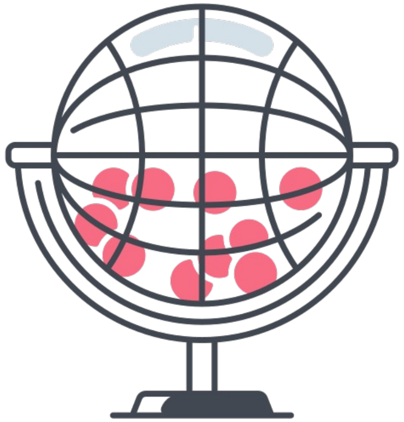
$$\mathcal{U}_2(t) = \prod_{\gamma}^{\rightarrow} e^{-it/2H_\gamma} \prod_{\gamma}^{\leftarrow} e^{-it/2H_\gamma} = \mathcal{U}(t) + \mathcal{O}(t^3),$$

QDRIFT (random compiler)

We evolve terms in the Hamiltonian randomly.

$$\lambda = \sum_{\ell=1}^{L} h_\ell, \tau = \frac{\lambda t}{N}$$

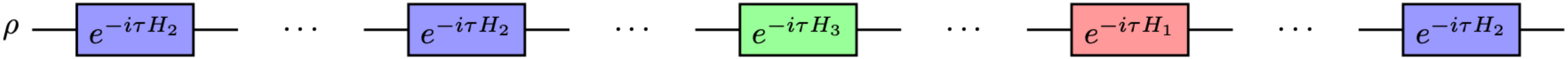
$$H = \sum_{j=1}^{L} h_j H_j$$



$h_1 H_1$
$h_2 H_2$
$h_3 H_3$

$$p(x) = \frac{h_x}{\lambda}$$

$$\tau = \frac{t\lambda}{N}$$



Results: if $\tau = \frac{t\lambda}{N}$, qDrift matches Trotter at first order.

$$N \geq \frac{2t^2\lambda^2}{\epsilon} \quad \text{ensures} \quad \|(\mathbb{E}\mathcal{V})^N - \mathcal{U}\| \leq \frac{\epsilon}{2}.$$

Campbell, PRL **123**, 070503 (2019)

Improvement from Chen, PRX Quantum 2, 040305

How is this working?

Do a Taylor expansion!

QDRIFT

$$\mathcal{E}(t,N)[\rho] = \sum_{j=1}^{L} p_j e^{-i\tau H_j} \rho e^{i\tau H_j} = \sum_{j=1}^{N} p_j (\mathbb{1} + i\tau[H_j,\rho]) + \mathcal{O}(\tau^2) = \mathbb{1} + \frac{it}{N}[H,\rho] + \mathcal{O}\left(\left(\frac{t\lambda}{N}\right)^2\right)$$

EXACT

$$\mathcal{U}(t/N)[\rho] = e^{-iHt/N} \rho e^{iHt/N} = \mathbb{1} + \frac{it}{N}[H,\rho] + \mathcal{O}\left(\left(\frac{t\lambda}{N}\right)^2\right)$$

ERROR

$$\|\mathcal{U}(t) - \mathcal{E}^N(t,N)\|_\diamond = \|\mathcal{U}^N(t/N) - \mathcal{E}^N(t,N)\|_\diamond \le N\|\mathcal{U}(t/N) - \mathcal{E}(t,N)\|_\diamond \le \mathcal{O}\left(\left(\frac{t\lambda}{N}\right)^2\right)$$

Sub-additivity

$$V_{\mathbf{j}}(t) = \prod_{k=1}^{N} e^{-i\tau_{\mathbf{j}_k} H_{\mathbf{j}_k}}. \quad (6)$$

The qDrift channel is then built as the arithmetic average of the M experiments

$$\mathcal{E}(t;N,M)[\rho] = \frac{1}{M}\sum_{m}^{M}\left[V_{\mathbf{j}_m}\rho V_{\mathbf{j}_m}^{\dagger}\right], \quad (7)$$

Implementation cost reduction with importance sampling

Importance sampling for QDRIFT

Kiss et al, arXiv:2212.05952

Idea? Sample from an alternative probability distribution *q(j).*

Why? Computational cost reduction.

How? Considering the implementation cost on hardware.

Importance sampling

$$\mathbb{E}_p[f(x)] = \sum_x q(x)\frac{p(x)}{q(x)} f(x) \equiv \mathbb{E}_q[\omega(x) f(x)],$$

Popular in Monte Carlo for variance reduction.

$$\begin{aligned}\mathcal{E}_q(t)[\rho] &= \sum_j q(j) e^{-i\tau_j H_j} \rho e^{i\tau_j H_j} \\ &\equiv \sum_j q(j) e^{\tau_j \mathcal{L}_j}(\rho) \\ &= \left(1 + \sum_j q(j)\tau_j \mathcal{L}_j + \sum_{n=2}^{\infty}\sum_j q(j)\tau_j^n \mathcal{L}_j^n\right)(\rho)\,. \end{aligned} \quad (14)$$

We match Trotterization at first order if:

$$\tau_j = \frac{th_j}{Nq_j}.$$

What can we show for the IS QDRIFT?

Kiss et al, arXiv:2212.05952

Bias error bound

$$\|\mathcal{U}(t)) - \mathcal{E}_q(t; N, 1)\|_\diamond \leq \frac{t^2\lambda^2}{N}\left(1 + \mathbb{E}_p\left[\omega(j)\right]\right).$$

Original QDRIFT:

$$\mathbb{E}_p[\omega(j)] \geq \mathbb{E}_p\left[\frac{p(j)}{p(j)}\right] = \mathbb{E}_p[1] = 1$$

Concentration bound

$$\Pr\left[\left\|\mathcal{E}_q(t; N, M) - \mathbb{E}_q\left[\prod_{k=N}^{1} e^{-i\tau_j H_j}\right]\right\| \geq \epsilon/2\right] \leq 2^{n+1}\exp\left\{-\frac{NM\epsilon^2}{11t^2\lambda^2(1+\max_k \omega(k))^2}\right\}.$$

Price to pay: Increase in the number of samples *N*.

Efficient parallelization because of concentration

To be ε close with probability $(1-\delta)$:

$$NM = 11\frac{t^2\lambda^2}{\epsilon^2}\left(1 + \max_k \omega(k)\right)^2 (n+1)\log\left(\frac{2}{\delta}\right)$$

Computational cost reduction

Kiss et al, arXiv:2212.05952

$$\lambda_c = \sum_l \frac{h_l}{C_l},$$

$$q_c(j) = \frac{h_j}{C_j \lambda_c}.$$

implementation cost of the **generator** ***H_j*.**

- **Number of two-qubit native gates (CNOT).**
- **Connectivity (length of the Pauli string).**
- **Non locality.**

- On **error-corrected** devices: minimize the number of **T gates**.

Theorem:

$$N_{q_c}\mathbb{E}_{q_c}[C] \leq N_p \mathbb{E}_p[C].$$

Monte Carlo iterations

$$q(j) \approx p(j), \text{ while regularising } th_j/(Nq(j)) \approx k\pi.$$

Summary of QDRIFT

- Stochastic channel: good for non-uniform distribution of the coefficients, e.g. chemistry

PRL **123**, 070503 (2019)

- Concentration: N can be kept small.

PRX Quantum 2, 040305 (2021)

- Importance sampling, concentration with NM

Kiss et al, arXiv:2212.05952

- Higher order: qSWIFT = qDRIFT + correction terms

arXiv:2302.14811

Better error scaling

$$d_\diamond\left(\mathcal{U}, \mathcal{E}^{(K)}\right) \in \mathcal{O}\left(\left(\frac{(\lambda t)^2}{N}\right)^K\right).$$

Composite channels:

how to reduce the implementation cost?

Composite channels

Given: a **partition** of the Hamiltonian.

H = A + B

Idea: simulate each terms with a different channel (Trotter & QDRIFT).

Time evolution = Trotter + QDRIFT

Advantages:

- Greater than the sum of the parts.
- Take advantage of the specific properties of each sub-system.
- Cost and error reduction.

$$\left\|\mathcal{I}_H(t) - \widetilde{\mathcal{U}}_H(t/r)^r\right\|_\diamond \leq \frac{t^2}{r}\left(\sum_{i<j} a_i a_j \|[A_i, A_j]\|_\infty + \sum_{ij} a_i b_j \|[A_i, B_j]\|_\infty + \frac{\lambda_B^2(1+\mathbb{E}_p[\omega(j)])}{N_B}\right)$$

Hagan and Wiebe, arXiv: 2206.06409 (2022)

How to choose the partition?

1. **Perturbation theory:** $H = A + \beta B, \beta \ll 1.$ Example: SU(4) lattice gauge theory.

2. **Cost oriented:** A contains the easiest terms while B the most expensive ones.
Example: lattice effective field theory (Hubbard like) potential VS hoping.

3. **Connectivity oriented:** $H = \sum A_i$ where A_i can be simulated with minimal swap over head.

4. **T gate efficient:**

$$tH = \sum_j th_j H_j = \sum_j (k_j \pi) H_j + \sum_j (th_j - k_j \pi) H_j$$
$$= A + B.$$

$$|th_j - k_j \pi| < \epsilon$$

$$k_j \in \mathbb{Q}$$

Numerical simulations:

lattice effective field theory

Scalable model for a nuclei

Pionless EFT on a lattice with MxM sites and A nucleons from N_f different species.

$$H = -t \sum_{f=1}^{N_f} \sum_{\langle i,j \rangle} c_{i,f}^{\dagger} c_{j,f} + 2dtA$$

Kinetic energy (hopping)

$$+ U \sum_{i=1} \sum_{f<f'}^{N_f} n_{i,f} n_{i,f'} + V \sum_{f<f'<f''}^{N_f} \sum_{i=1} n_{i,f} n_{i,f'} n_{i,f''}$$

Two and three-body on-site interaction

$$+ U \sum_{f=1}^{N_f} n_{1,f} + V \sum_{f<f'}^{N_f} n_{1,f} n_{1,f'}$$

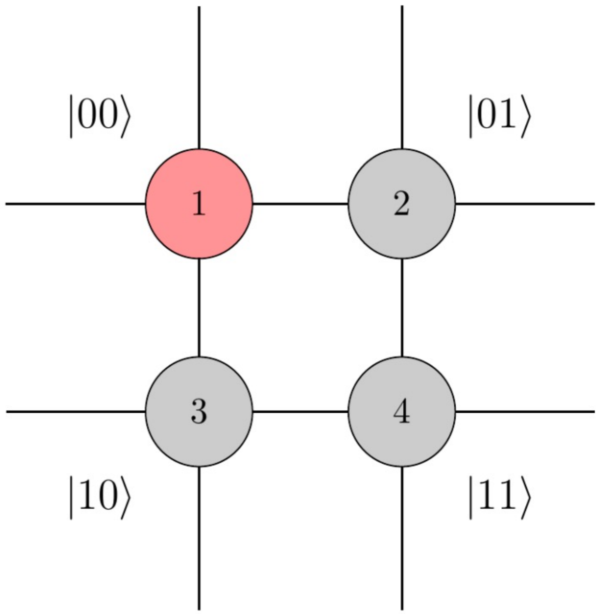
Potential of a frozen nucleon

Roggero et al., Phys. Rev. D **101**, 074038 (2020)

Mapping to qubits:

First quantisation

needs $\log_2(M^2) N_f$ qubits.



Second quantisation (via Jordan-Wigner):

More natural but needs $M^2 N_f$ qubits.

Cost of the different implementations

Assuming a 1423 connectivity

generator	cost	generator	cost
X_k	0.1	Z_1Z_2	6
Z_k	0.1	Z_3Z_4	6
Z_1Z_4	2	$Z_1Z_2Z_3Z_4$	6
Z_2Z_4	2	$Z_1Z_3Z_4$	8
Z_2Z_3	2	$Z_1Z_2Z_3$	8
$Z_1Z_2Z_4$	4	Z_1Z_3	10
$Z_2Z_3Z_4$	4		

Table 1: Implementation cost for the different generators appearing in the two considered Hamiltonians.

Two regimes (A with Trotter, B with QDRIFT):

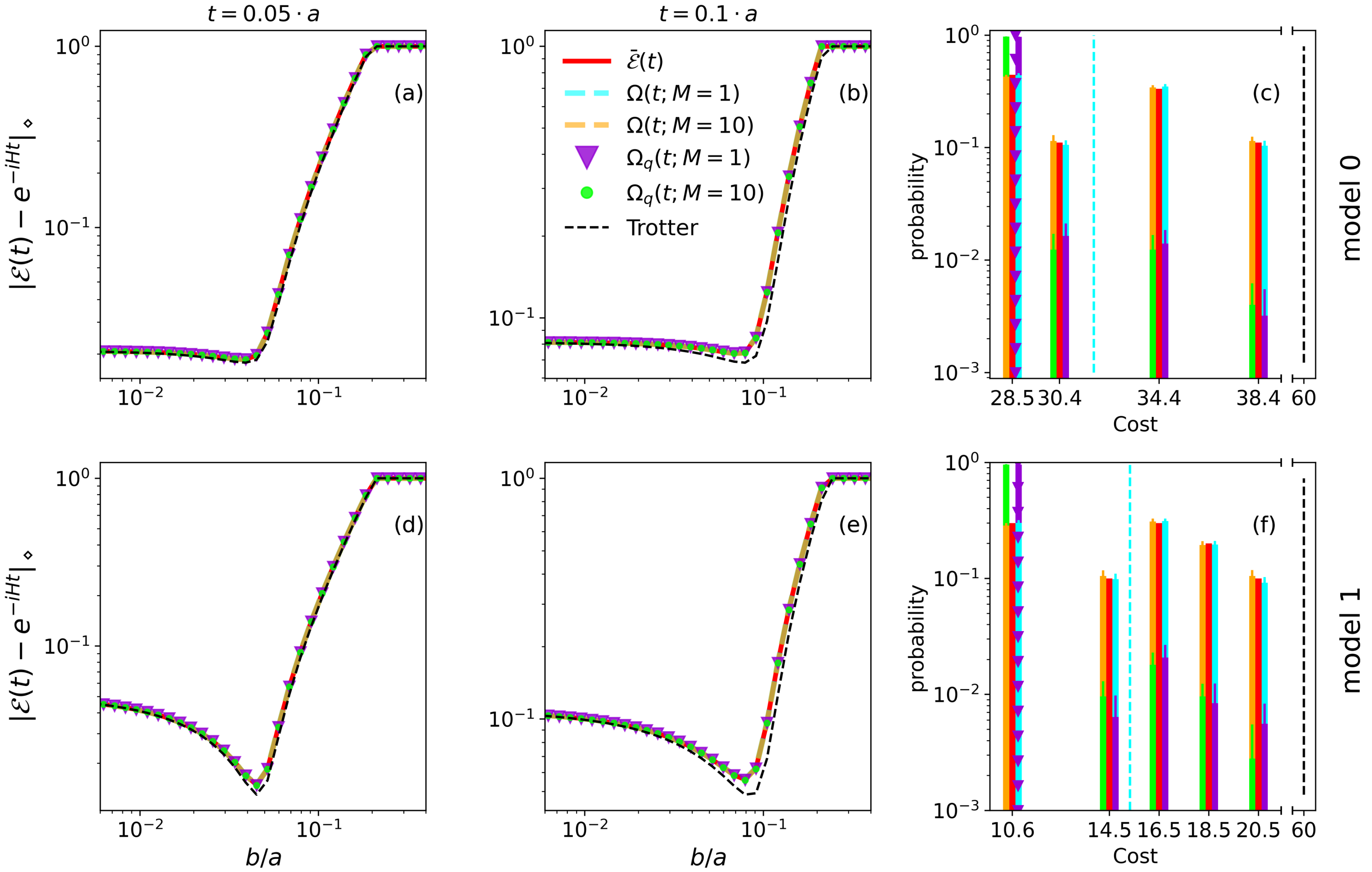
1. ***A*** describes the bulk (U = -4V), while ***B*** is the linear interpolation towards **realistic coefficients**.
2. ***A*** contains the **easy** terms and ***B*** the **expensive** ones.

$$A^{(1)} = \sum_{k=1}^{4} X_k + Z_1 + Z_1Z_4 + Z_2Z_3 + Z_2Z_4 + Z_1Z_2Z_4 \tag{63}$$

$$B^{(1)} = \sum_{k=2}^{4} Z_k + Z_1Z_2 + Z_1Z_3 + Z_3Z_4 + Z_1Z_2Z_3 + Z_2Z_3Z_4 + Z_1Z_3Z_4 + Z_1Z_2Z_3Z_4. \tag{64}$$

Numerical Simulation (N=1)

Kiss et al, arXiv:2212.05952

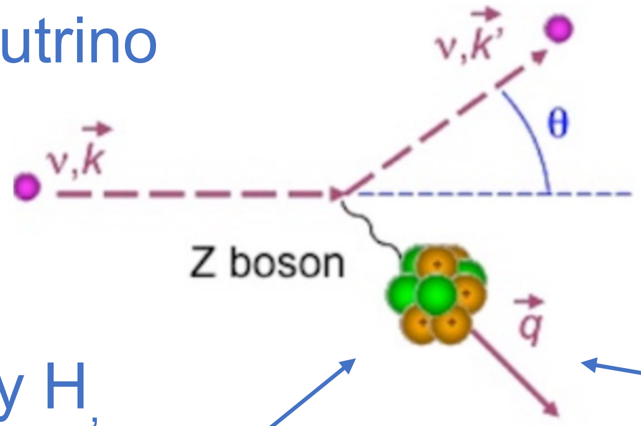


- Cost reduction in the B evolution of factor 10.
- QDRIFT and IS QDRIFT match Trotterization for all values of β.

Response functions computations from scattering experiments

Physical Model

Incoming neutrino



momentum transfer described byO (external probing).

Nuclei described by H in its ground state.

$$H = 4.5 \cdot \mathbb{1} - 2\sum_{i=1}^{4} X_i + 1.75\left(\sum_{i<j<k} Z_iZ_jZ_k + Z_1Z_4 + Z_2Z_3\right)$$

$$\hat{O}(\vec{q}_k) = \sum_{f=1}^{N_f} \rho_f(\vec{q}_i) = \sum_{f=1}^{N_f} e_f \sum_i e^{i\vec{q}_k\cdot\vec{r}_i} n_{i,f},$$

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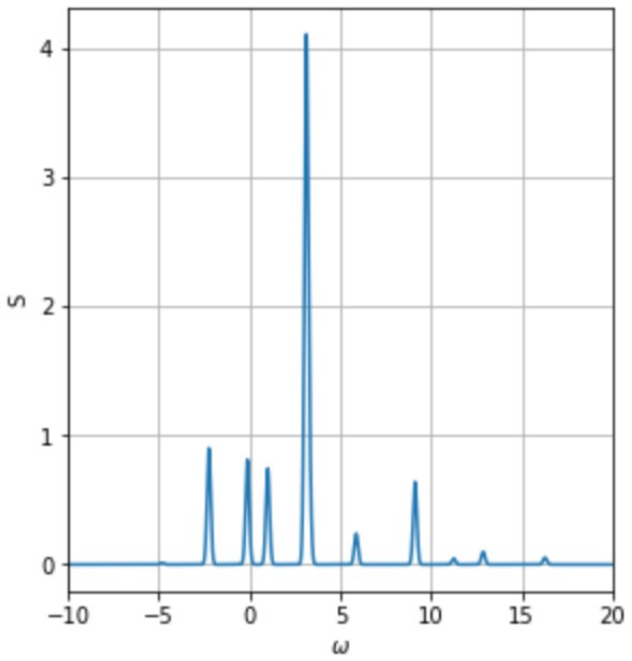
Linear response function

Challenging, since it requires the full spectrum

$$S(\omega, \vec{q}) = \langle \Psi_0 | \hat{O}(\vec{q})^\dagger \delta(\omega - (E_0 - E_f)) \hat{O}(\vec{q}) | \Psi_0 \rangle$$
$$= \sum_f \left| \langle \Psi_0 | \hat{O}(\vec{q}) | f \rangle \right|^2 \delta(\omega - (E_0 - E_f)),$$



Instead: Integral transform with Gaussian Kernel + truncation

$$\Phi_N^\chi(\nu) = \frac{1}{\chi \|H\|} \sum_{n=-N}^{N} g_n^\chi(\nu) \langle \Psi_0 | \hat{O}(\vec{q})^\dagger e^{-in\delta t H} \hat{O}(\vec{q}) | \Psi_0 \rangle ,$$

Groudstate with the Variational Quantum Eigensolver

Hamiltonian moments
Easy with quantum computers!

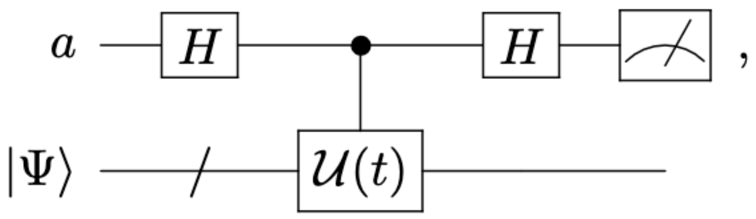
arXiv:2211.00790

Estimating expectation values

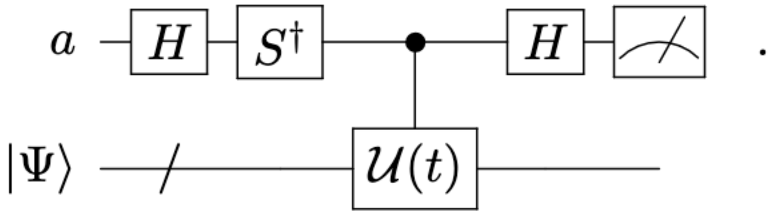
$$g(t) = \langle \Psi_0 | \hat{O}(\vec{q})^\dagger e^{-itH} \hat{O}(\vec{q}) | \Psi_0 \rangle,$$

Hadamard test
(phase kickback)

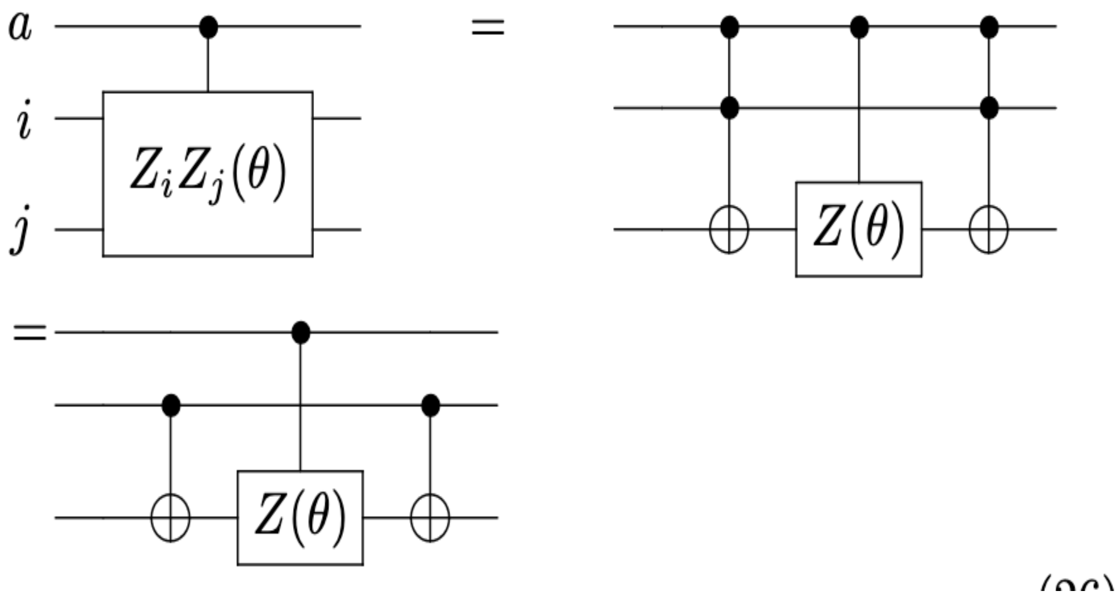
Real



Imag.



In practice, control operations are expensive!



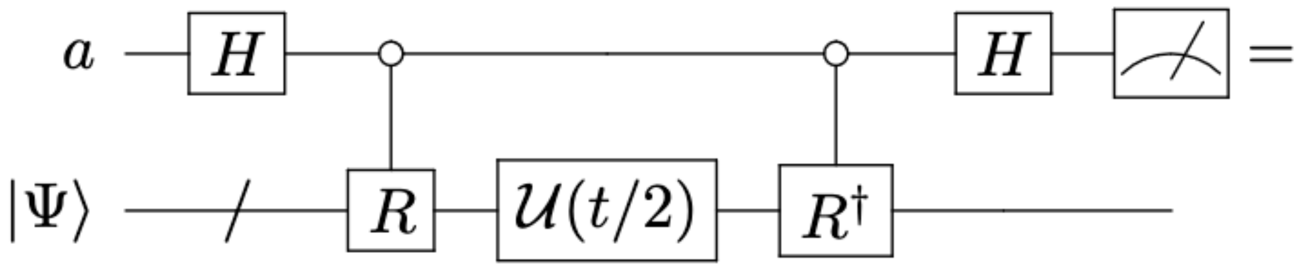
Control Reversal Gates
How to avoid the control operation?

R anti commutes with H: {H,R} = 0
Use R to toggle the flow of time

$$R\exp\{-iHt\}R^\dagger = R\sum_n \frac{(-itH)^n}{n!}R^\dagger =$$

$$\sum_n \frac{(itH)^n}{n!}RR^\dagger = \exp\{itH\},$$

Hadamard test with control reversal gates



Caveats:

- we may need to split the Hamiltonian, and/or insert the CRG between each Trotter steps!
- **We were able to avoid this here!**
- Require **even order product** formula.

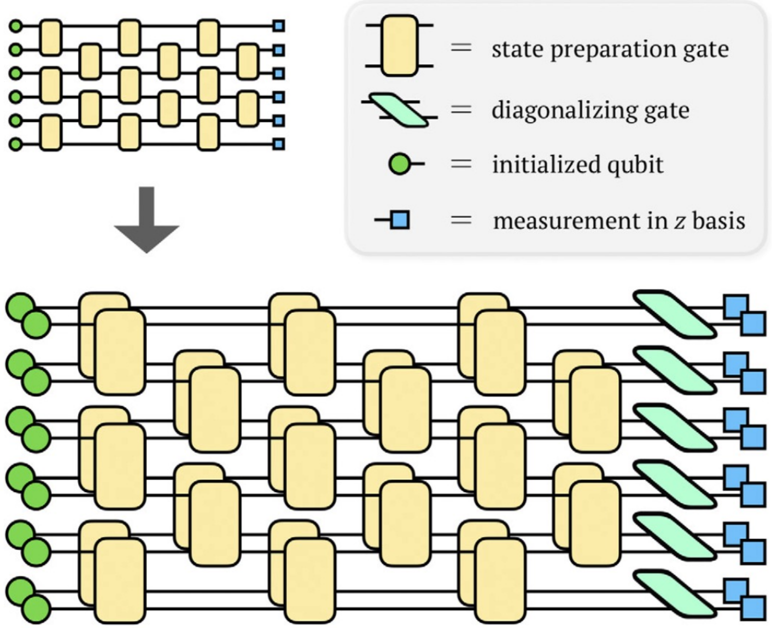
Error mitigation: Virtual Distillation

- requires connectivity between every copy.
- The diagonalising gate can be challenging to implement in general.

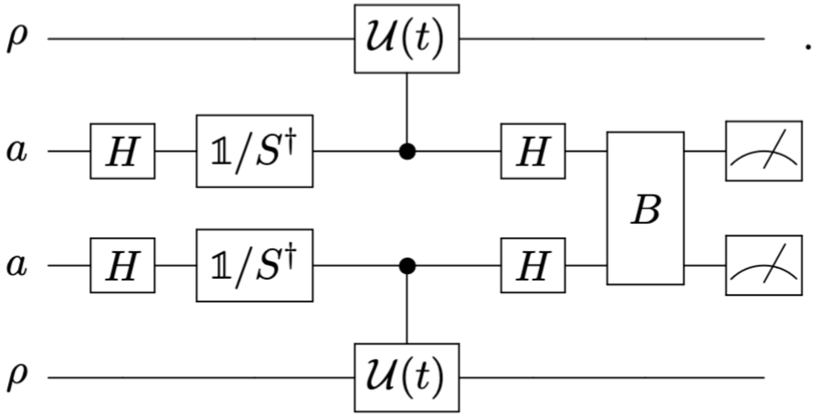
Uses multiple copies to suppress the non-dominating components.

$$\rho^M = \left(\sum_i p_i |i\rangle\langle i|\right)^M = \sum_i p_i^M |i\rangle\langle i|,$$

$$\langle O\rangle_{\mathrm{VD}} \equiv \frac{\mathrm{Tr}(O\rho^M)}{\mathrm{Tr}(\rho^M)}.$$



we only need to connect the ancilla.



Huggins, et al., Phys. Rev. X 11, 041036 (2021)

Error mitigation: Self-verification

Assuming depolarising noise

$$\rho_1 = (1-p)|\Psi_1\rangle\langle\Psi_1| + \frac{p}{2^n}\mathbb{1}. \qquad (38)$$

The expectation value of a Pauli operator P can then be computed as

$$\mathrm{Tr}(P\rho_1) = (1-p)\langle\Psi_1|P|\Psi_1\rangle\,, \qquad (39)$$

We could correct if we knew *p*!

O'Brien, PRX Quantum 2, 020317 (2021)

Idea: compute p using a known circuit.

We **prepare**, then **un-prepare** the targeted state (two Trotter steps).

$$|\Psi_2\rangle = A^\dagger A B\,|0\rangle$$

$$\mathrm{Tr}(Q\rho_2) = (1-p)\langle\Psi_2|Q|\Psi_2\rangle + p\frac{\mathrm{Tr}(Q)}{2^n}\,,$$

And use this value for the correction

$$\langle\Psi|\mathcal{U}(2t)|\Psi\rangle_{\mathrm{SV}} = \frac{\langle 0|B^\dagger\mathcal{U}(2t)B|0\rangle}{\langle 0|B^\dagger\mathcal{U}(t)\mathcal{U}(-t)B|0\rangle},$$

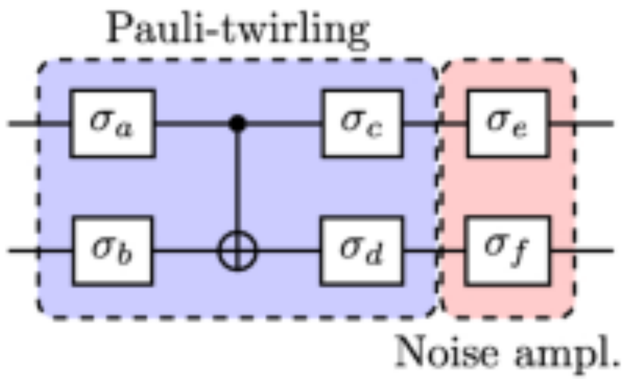
How to make the noise more depolarising?

Use Pauli Twirling!

Turn a noisy operator into a Pauli channel, via gate conjugation.

$$\mathcal{T}_W(\overline{M}) = \frac{1}{|W|} \sum_{w \in W} \overline{wMw^\dagger}\,.$$

In practice: sample!



(a) Pauli-twirling and noise amplification.

σ_a	$\mathbb{1}$	$\mathbb{1}$	$\mathbb{1}$	$\mathbb{1}$	σ_x	σ_x	σ_x	σ_x	σ_y	σ_y	σ_y	σ_y	σ_z	σ_z	σ_z	σ_z
σ_b	$\mathbb{1}$	σ_x	σ_y	σ_z	$\mathbb{1}$	σ_x	σ_y	σ_z	$\mathbb{1}$	σ_x	σ_y	σ_z	$\mathbb{1}$	σ_x	σ_y	σ_z
σ_c	$\mathbb{1}$	$\mathbb{1}$	σ_z	σ_z	σ_x	σ_x	σ_y	σ_y	σ_y	σ_y	σ_x	σ_x	σ_z	σ_z	$\mathbb{1}$	$\mathbb{1}$
σ_d	$\mathbb{1}$	σ_x	σ_y	σ_z	σ_x	$\mathbb{1}$	σ_z	σ_y	σ_x	$\mathbb{1}$	σ_z	σ_y	$\mathbb{1}$	σ_x	σ_y	σ_z

(b) Valid combinations for Pauli-twirling of the CX gate.

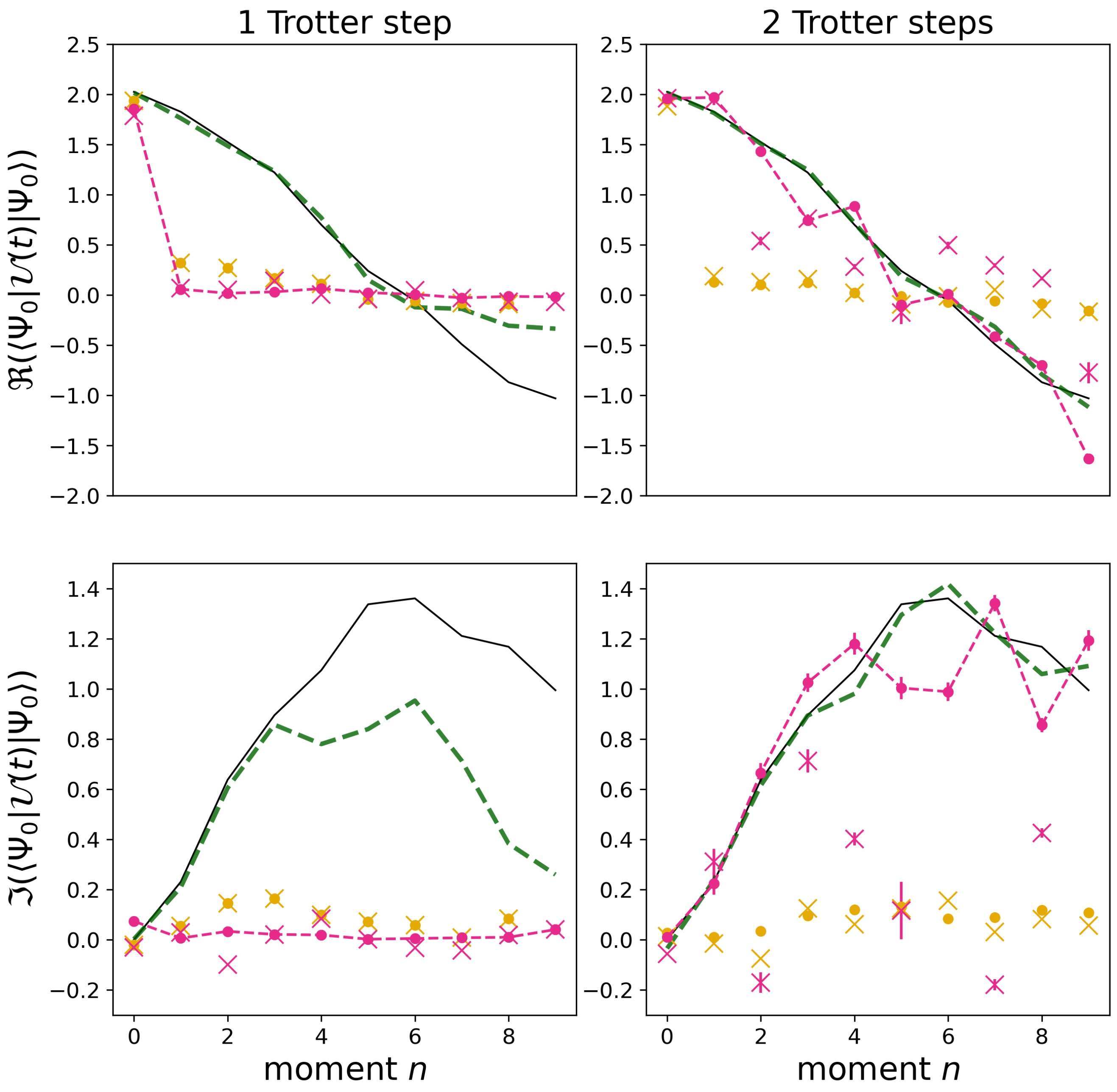
Fuchs, et al., *Eur. Phys. J. Plus* **135**, 353 (2020)

Results on superconducting quantum hardware

	linear connectivity	full connectivity
one Trotter step	38	27
two Trotter steps	68	49

Number of CNOTs

- **VD does not improve the results (noise too important)**
- **Pauli twirling alone is not helpful.**
- **Self Verification works well in conjunction with Pauli Twirling.**

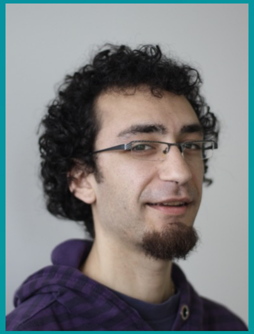


Conclusions

- **QDRIFT** generates random product formulas whose size **does not depend** on the number of terms and concentrates fast (small variance).
- **Importance sampling** can be used to **reduce the actual implementation cost** on hardware (guaranteed cost reduction with the same accuracy).
- **Composite channels** use different techniques to simulate different parts of the Hamiltonian (use the best one in each case!)
- **Response functions** can be estimated from expectation values!
- **Self-verification** and **twirling** are working well together.

Thank you for your attention!

Important sampled QDRIFT
arXiv:2212.05952



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