QSR algorithm

QC40: Physics of Computation Conference 40th Anniversary

Pedro Rivero — May 6, 2021

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- Quantum Sampling Regression (QSR)
- Algorithmic complexity in the low quit number regime
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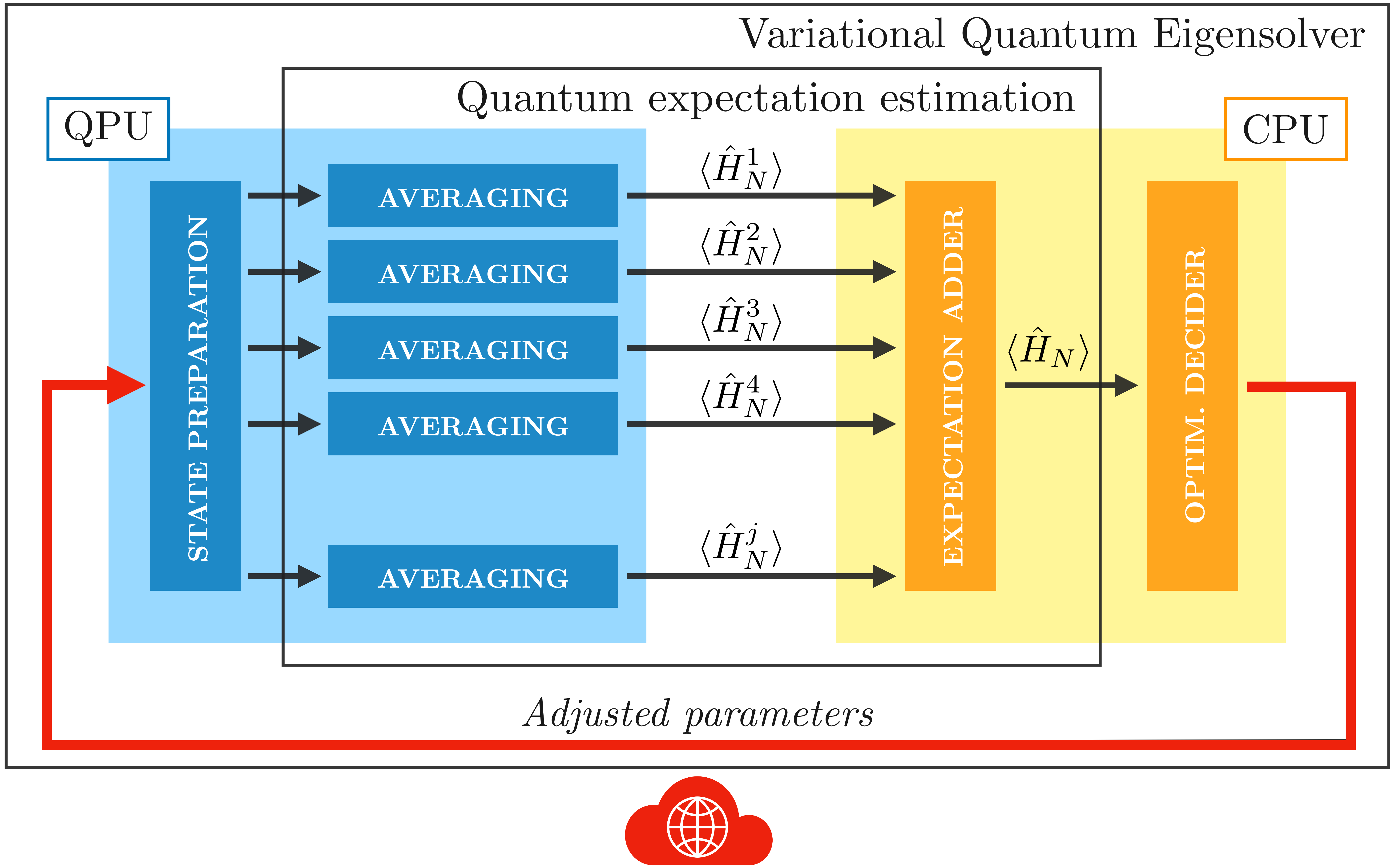
VQE algorithm

Hybrid quantum-classical variational eigensolving



(1) Quantum processor embedded within a classical optimization loop.

(2) On each cycle the QPU gets called several times by the classical optimizer.

(3) **Bottleneck**: establishing an HTTP connection to update the parameters in the quantum circuit.

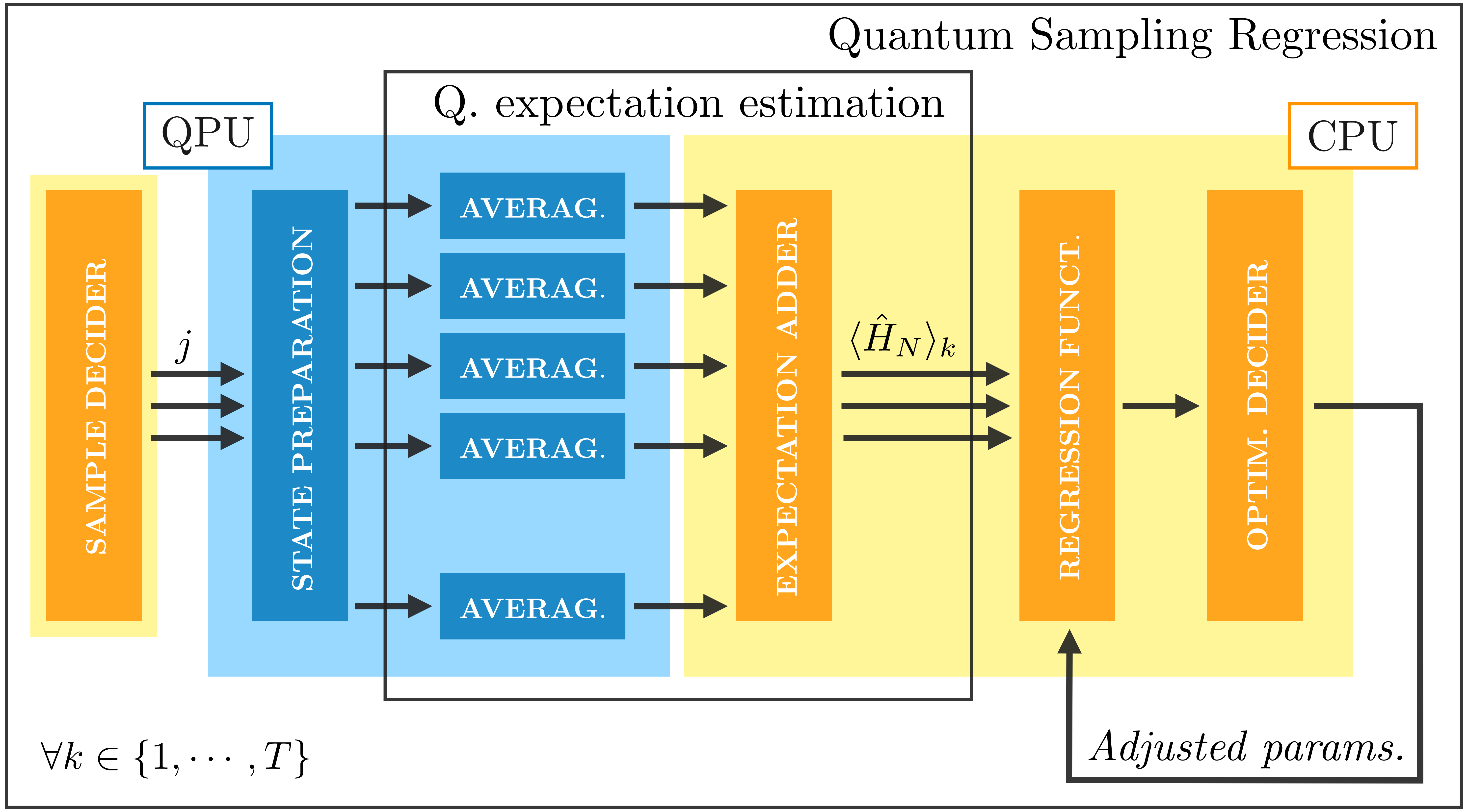
QSR algorithm

Hybrid quantum-classical variational eigensolving

(1) All calls to the QPU are performed together at the beginning.

(2) Target function is reconstructed classically as a **trigonometric series.**

(3) Optimization loop runs isolated in the CPU → **Better convergence**.



QSR algorithm

Motivation

FOURIER ANALYSIS

PARAMETRIZATION ANSATZES

Rotations

→

BOUNDED AND PERIODIC DOMAIN

Trigonometric series expansion

→

QUANTUM CIRCUIT TOPOLOGY

Frequency bounds

QSR algorithm

How it works

- Reconstruct the energy landscape classically → Trigonometric series (1D)

$$h(\theta) \triangleq \left\langle \hat{H}_N \right\rangle (\theta) \equiv a_0 + \sum_{k=1}^{S} \left[a_k \cos(k\theta) + b_k \sin(k\theta)\right]$$

- To find the coefficients we have to solve a linear system of the form:

$$Fc = h \quad \rightarrow \quad \boxed{F^\dagger F c = F^\dagger h}$$ **LEAST SQUARES**

- Total number of samples needed is:

$$T = \prod_{j=1}^{n} (2S_j + 1) \leq (2S_{\max} + 1)^n \equiv 2^{sn}$$

$$s \equiv \log_2 (2S_{\max} + 1) \geq \frac{\log_2 T}{n}$$

QSR algorithm

Optimality

NYQUIST-SHANNON SAMPLING THEOREM

If a function $h(\theta)$ contains no angular frequencies higher than ω, it is completely determined by giving its ordinates at a series of points $1/2\omega_S$ apart: $\omega_{sampling} > 2\omega_S$

SIGNAL PROCESSING

Using techniques such as *compressed sensing* we could improve upon this.

ERROR MITIGATION

Increase the total amount of samples, or optimize the spacing between them (i.e. the lattice)

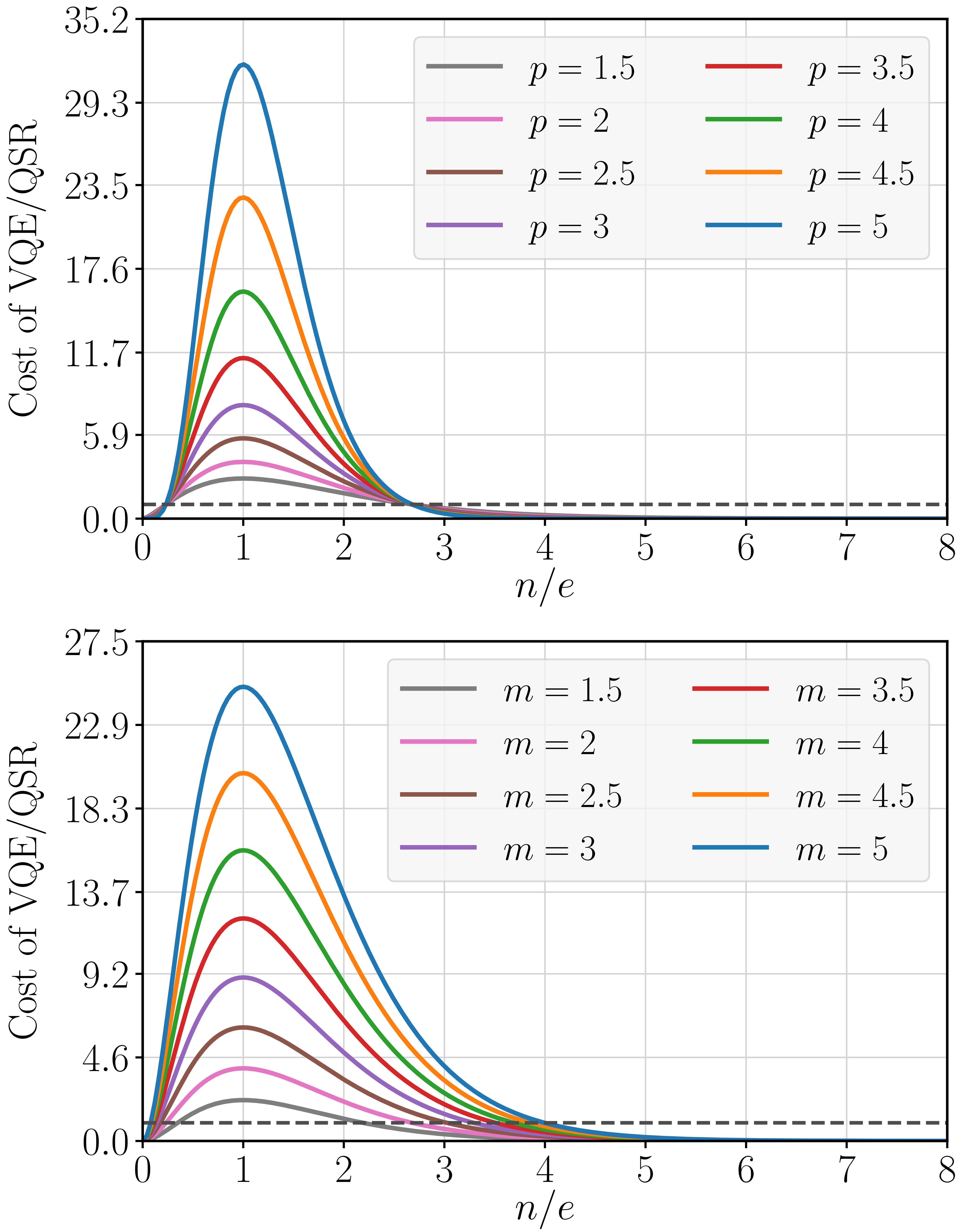
Algorithmic complexity

Low quit number regime model

- Monomial complexity lower bound for VQE → $(mn)^p$
- Samples required by QSR → 2^{sn}
- Resulting complexity model:

$$\frac{\text{VQE}}{\text{QSR}} = \left(mn2^{-n/r}\right)^p$$

$$r \triangleq p/s$$



Algorithmic complexity

Low quit number regime model

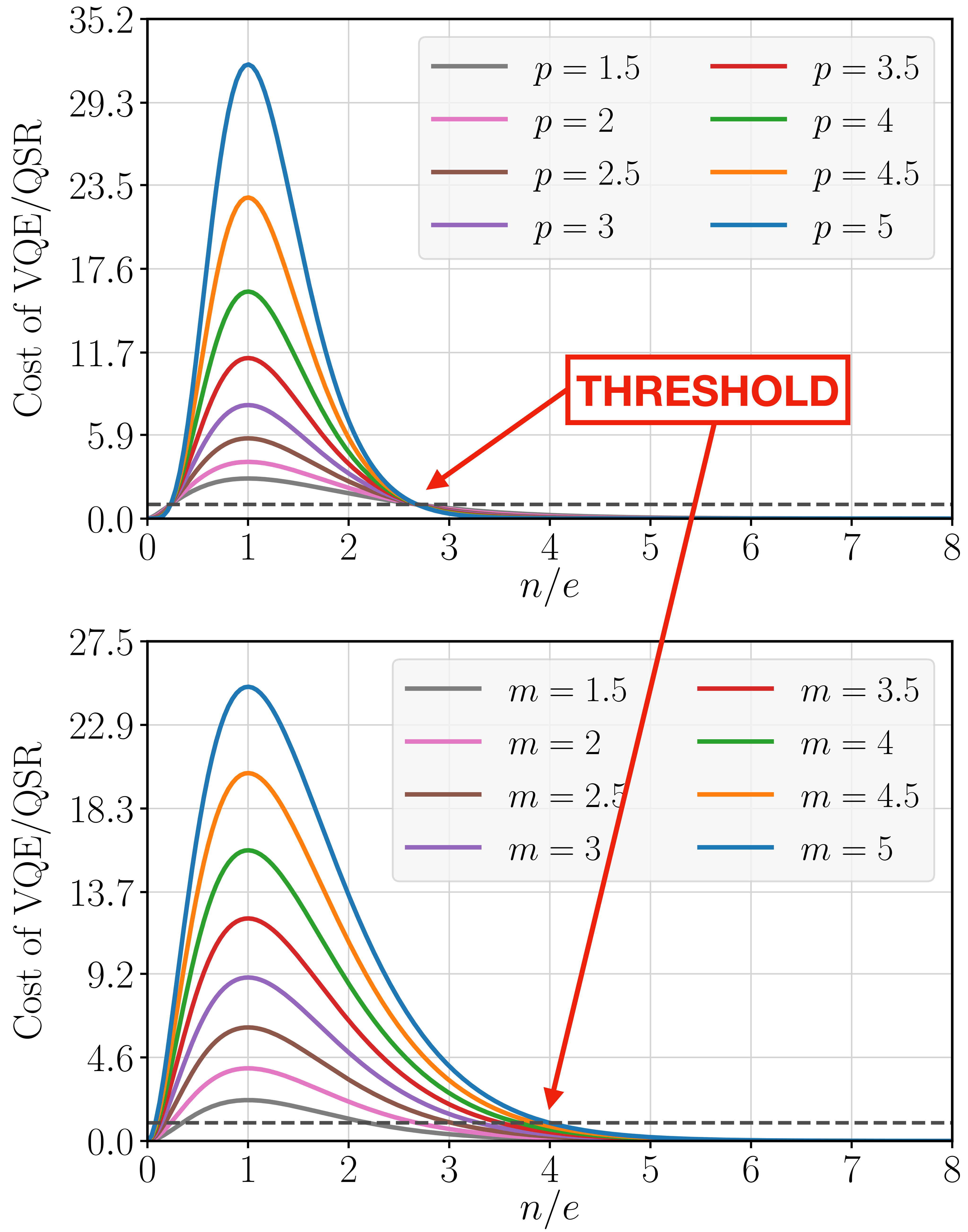
- Cost ratio distribution peak:

$$n^* = \frac{r}{\ln 2}$$

- Condition to outperform VQE:

$$\left.\frac{\text{VQE}}{\text{QSR}}\right|_{n=n^*} > 1 \quad \Rightarrow \quad mn^* > e$$

$$\boxed{\begin{gathered}\frac{\text{VQE}}{\text{QSR}} = \left(mn2^{-n/r}\right)^p \\ r \triangleq p/s\end{gathered}}$$

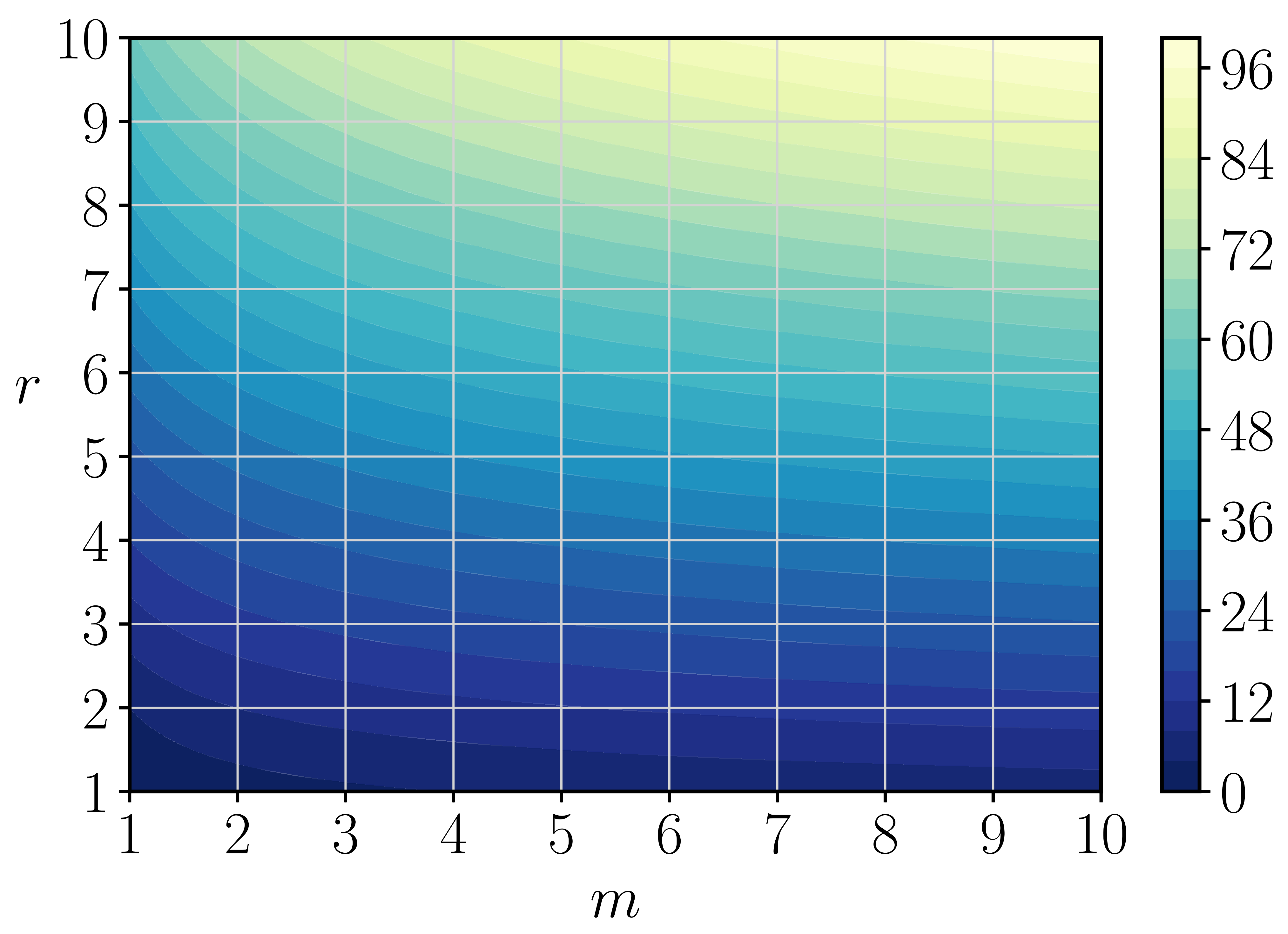


Algorithmic complexity

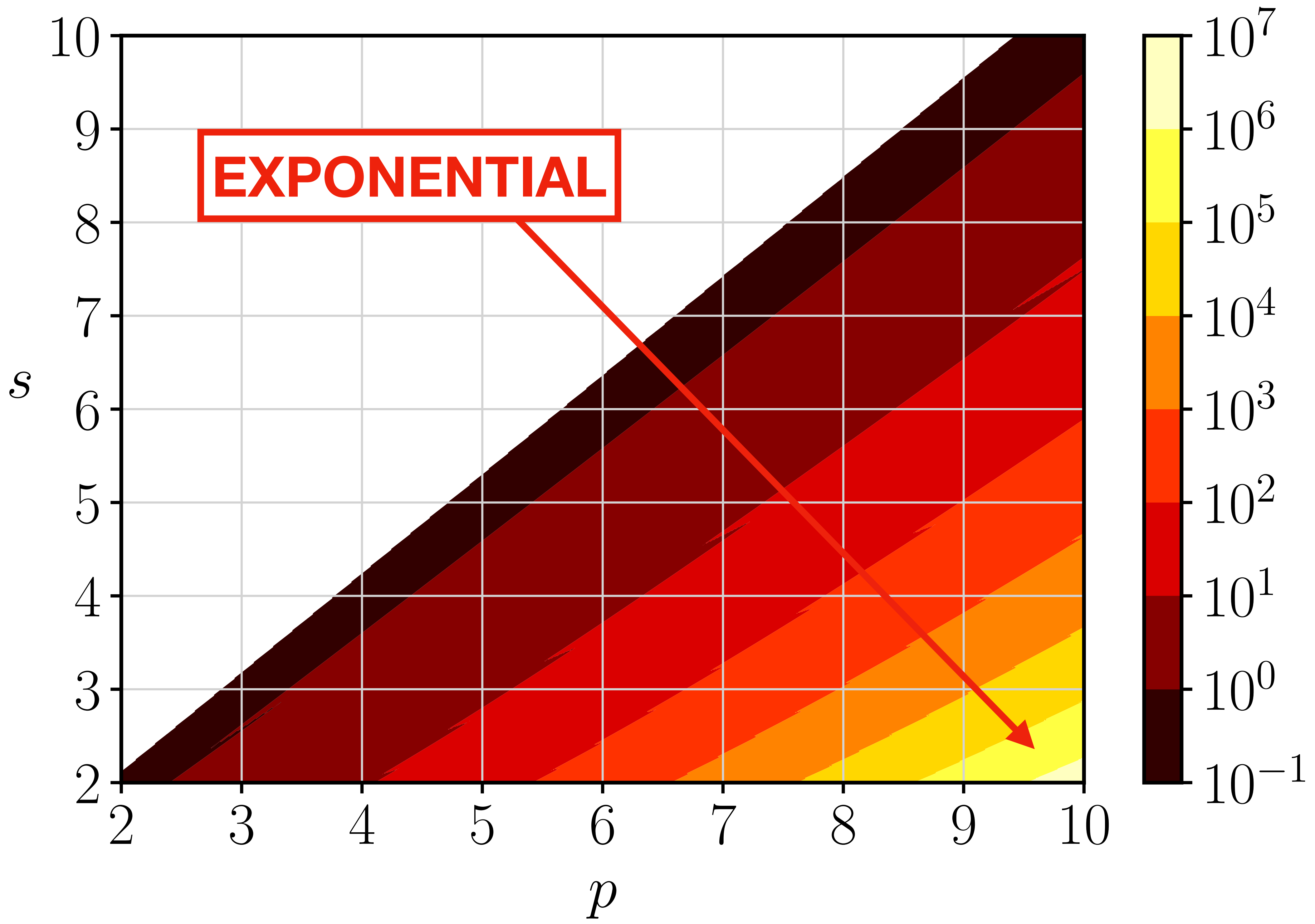
Analytical results

$$a \triangleq \left\lceil -\frac{r}{\ln 2} W_{-1}\left(-\frac{\ln 2}{mr}\right)\right\rceil$$

$$E \triangleq \frac{1}{a}\sum_{n=1}^{a} \frac{\mathrm{VQE}}{\mathrm{QSR}} \approx \frac{1}{as\ln 2}\left(\frac{m}{s\ln 2}\right)^{p}\Gamma(p+1, s\ln 2, as\ln 2)\,.$$



Threshold



Efficiency

Algorithmic complexity

Scale picture

SO FAR...

SIMULATION PROBLEMS

$\{n \sim 50, s \sim 3\} \rightarrow p \geq 14$

OPTIMIZATION PROBLEMS

$\{n \sim 10, s \sim 6\} \rightarrow p \geq 11$

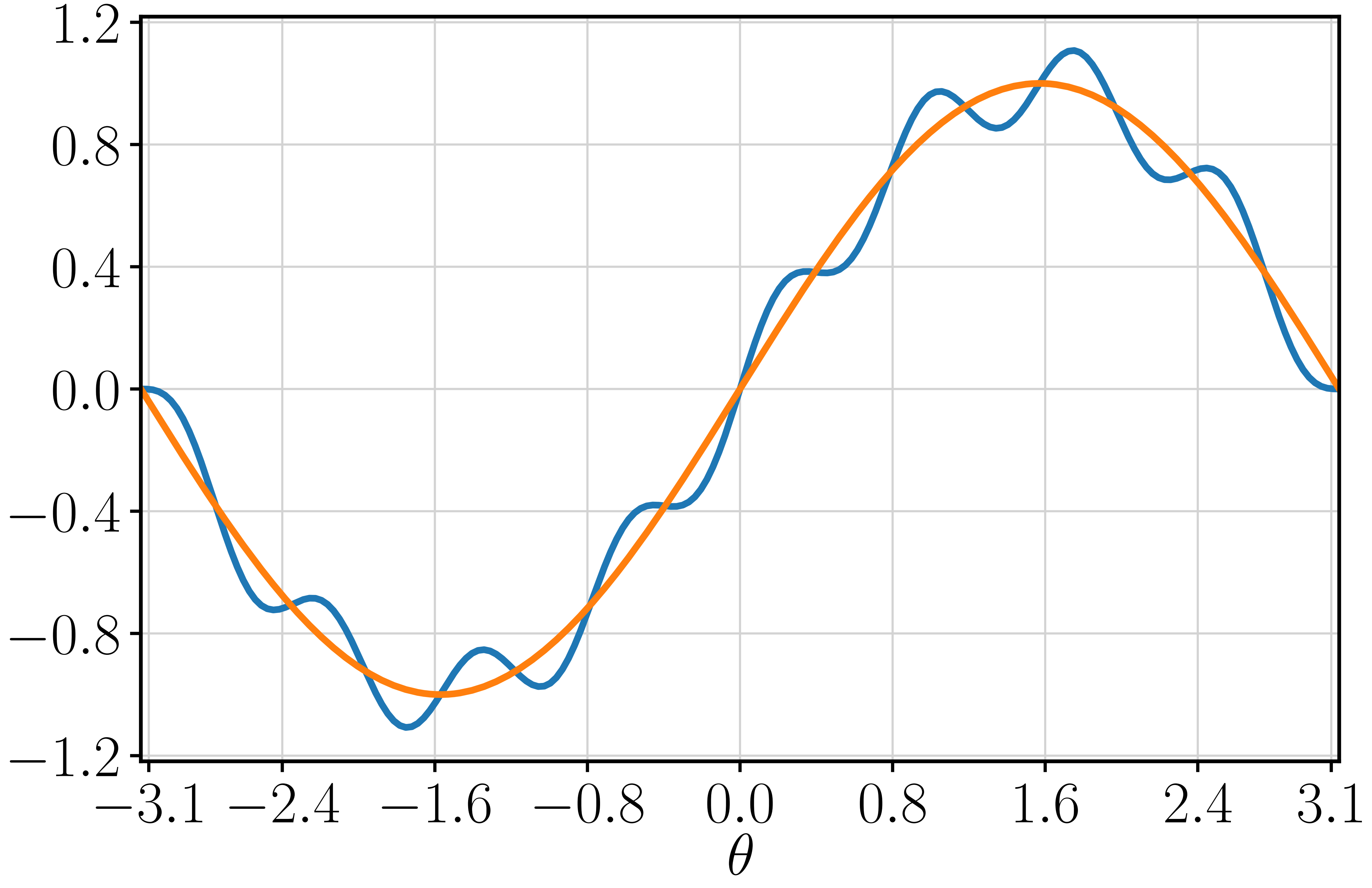
NON-FRONTIER PROBLEMS

$\{n \leq 15, s \leq 4\} \rightarrow p \geq 7 \pm 3$

Applications

Standalone uses

- **Increase precision**
  - Adjust the spacing in the lattice
  - Oversample
- **Undersampling**
  - Boost performance
  - Get rid of local minima
  - Signal processing techniques → Retain precision



Applications

Complementary uses

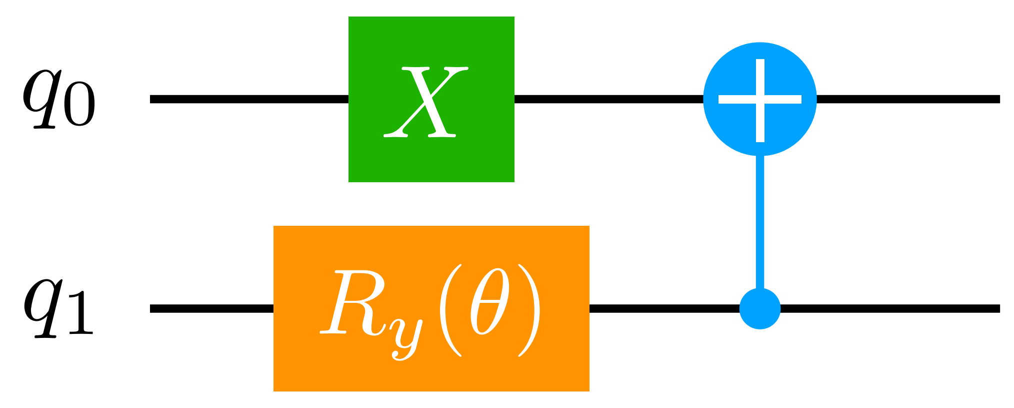
- **Low-resolution start-up supplement to VQE or variants:**
  - Run QSR *undersampling* to obtain an approximate solution
  - Use said approximation as a better initial state for VQE → Alternative to Hartree-Fock
- **Proxy to transition between simulators and real devices:**
  - Improve convergence by removing the stochastic behavior
  - Retain characteristic quantum computational features → Analyze global properties
- **Avoid the exponential matrix formulation in classical computation.**

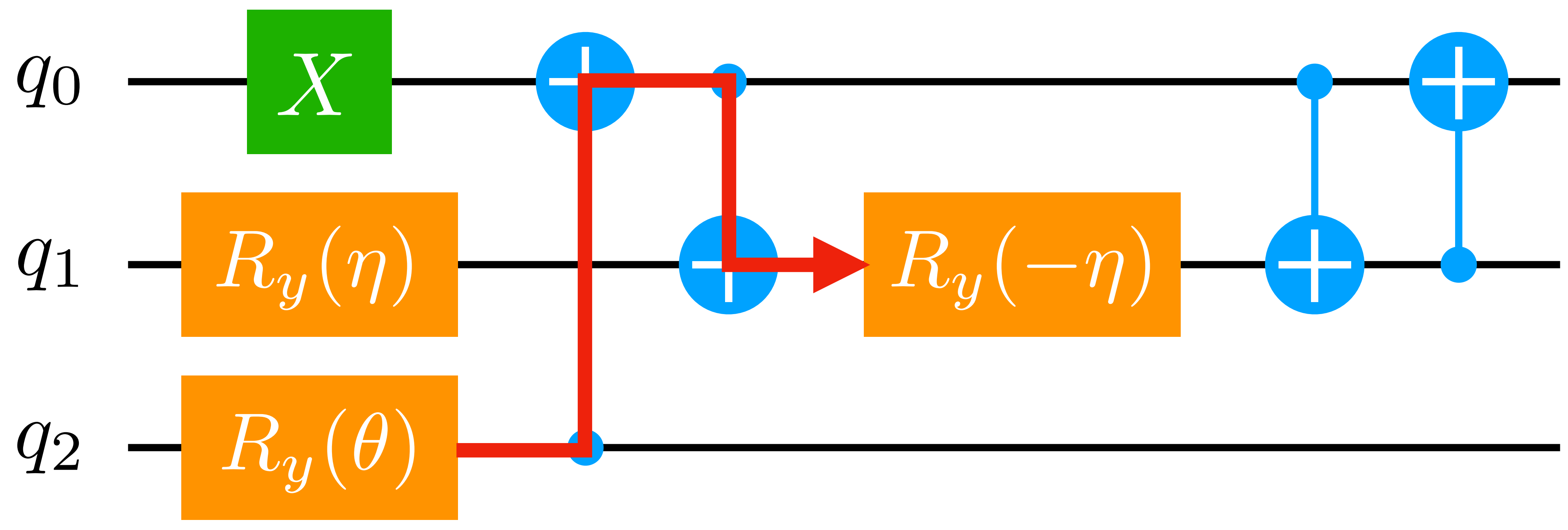
Benchmark

Deuteron binding energy

arXiv:1801.03897

FREQUENCY DOUBLING





$S_\theta = 1$

$\boxed{S_{max} = 1}$

$S_\theta = 1$
$S_\eta = 2$

$\boxed{S_{max} = 2}$

Benchmark

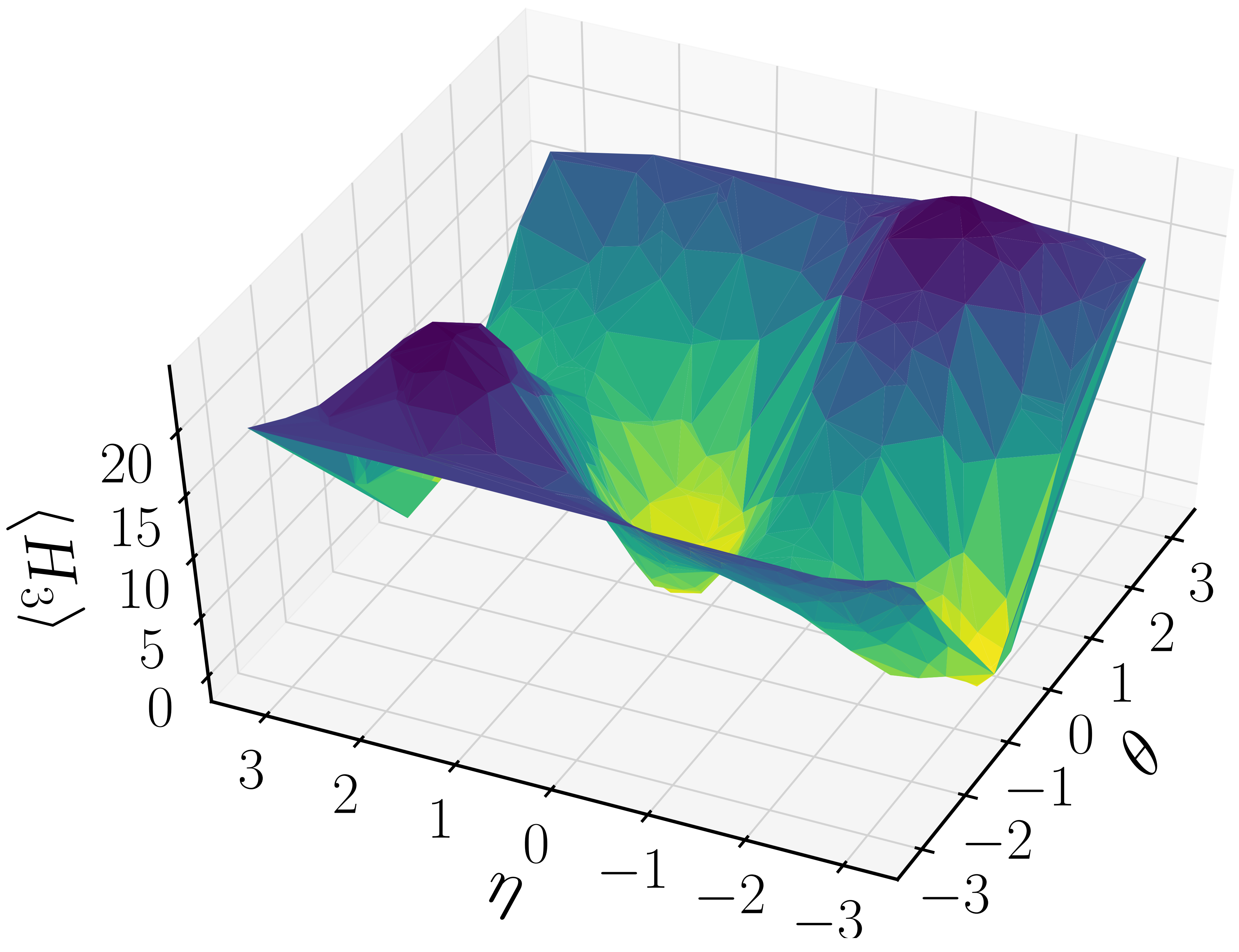
Deuteron binding energy

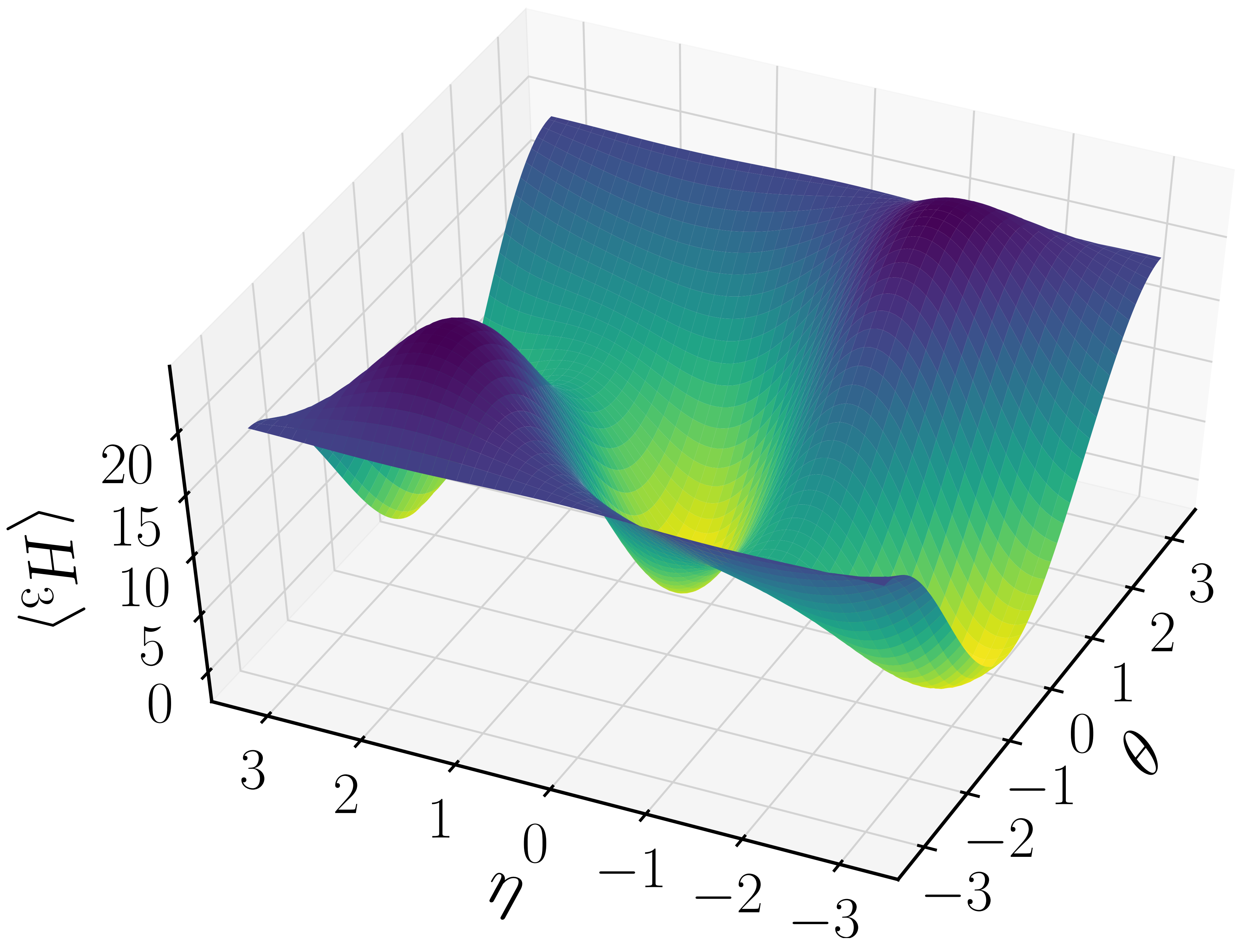
arXiv:1801.03897

IBMQ OURENSE
8192 SHOTS

TABLE I: Comparison between results in [34] reproduced using the VQE and QSR algorithms.

n	Algorithm	Samples	Queries	Error
1	VQE	24	24	3.5%
1	QSR	3	1	1.0%
2	VQE	183	183	0.3%
2	QSR	25	1	0.2%





Conclusions

QSR algorithm

- **QSR is a global approximation technique that gets rid of connection bottlenecks:**
  - For complex enough optimization problems, there is a region in the low quit number regime, where QSR outperforms VQE.
  - QSR knows all the samples needed in advance.
- **QSR behaves well with a larger range of optimizers:**
  - It gets rid of the local stochastic behavior of the target function.
- **QSR enables signal processing techn. to solve optimization problems more efficiently.**
- **QSR can be used in conjunction with other algorithms such as VQE.**

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Thanks

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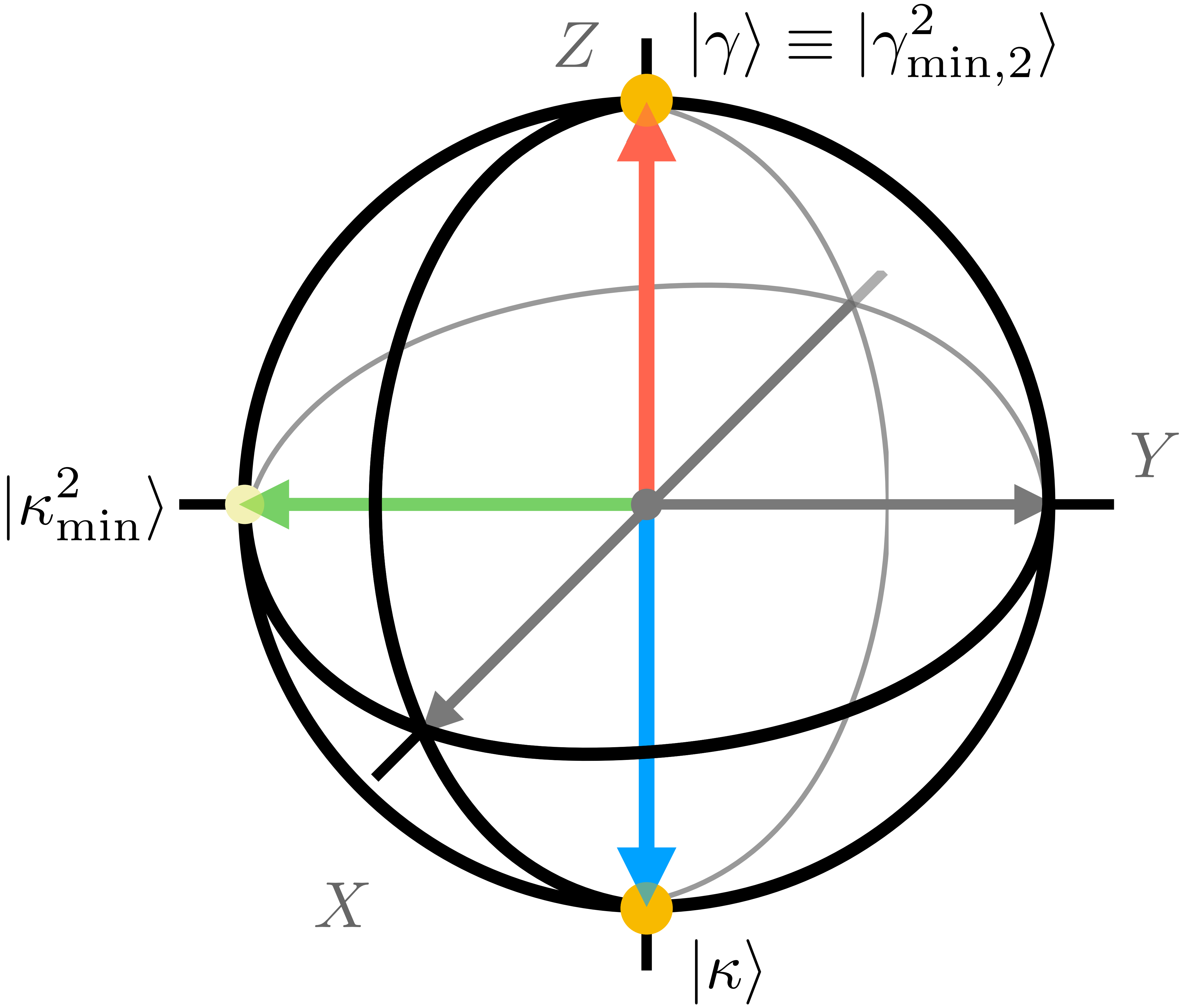
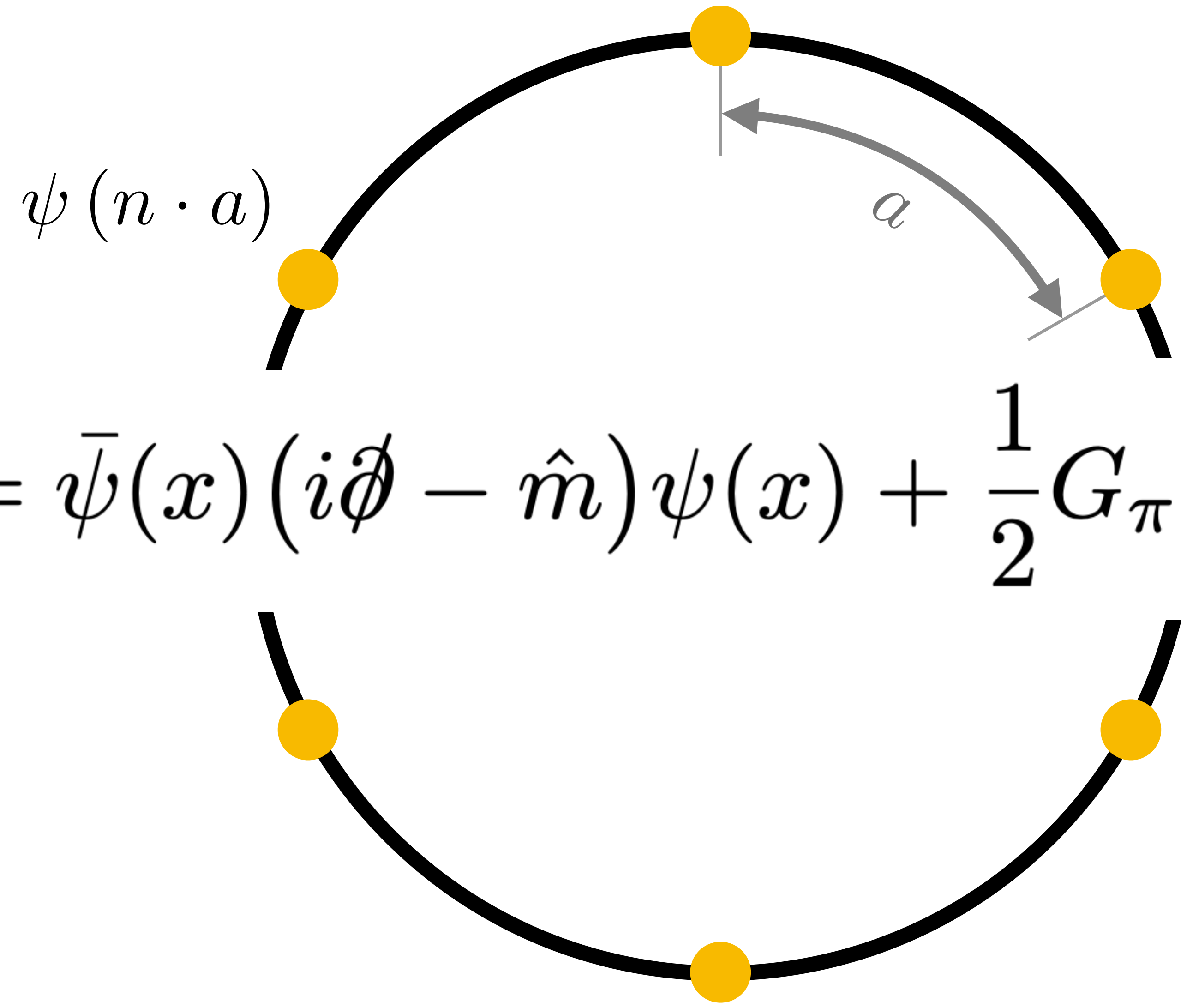
NJL model

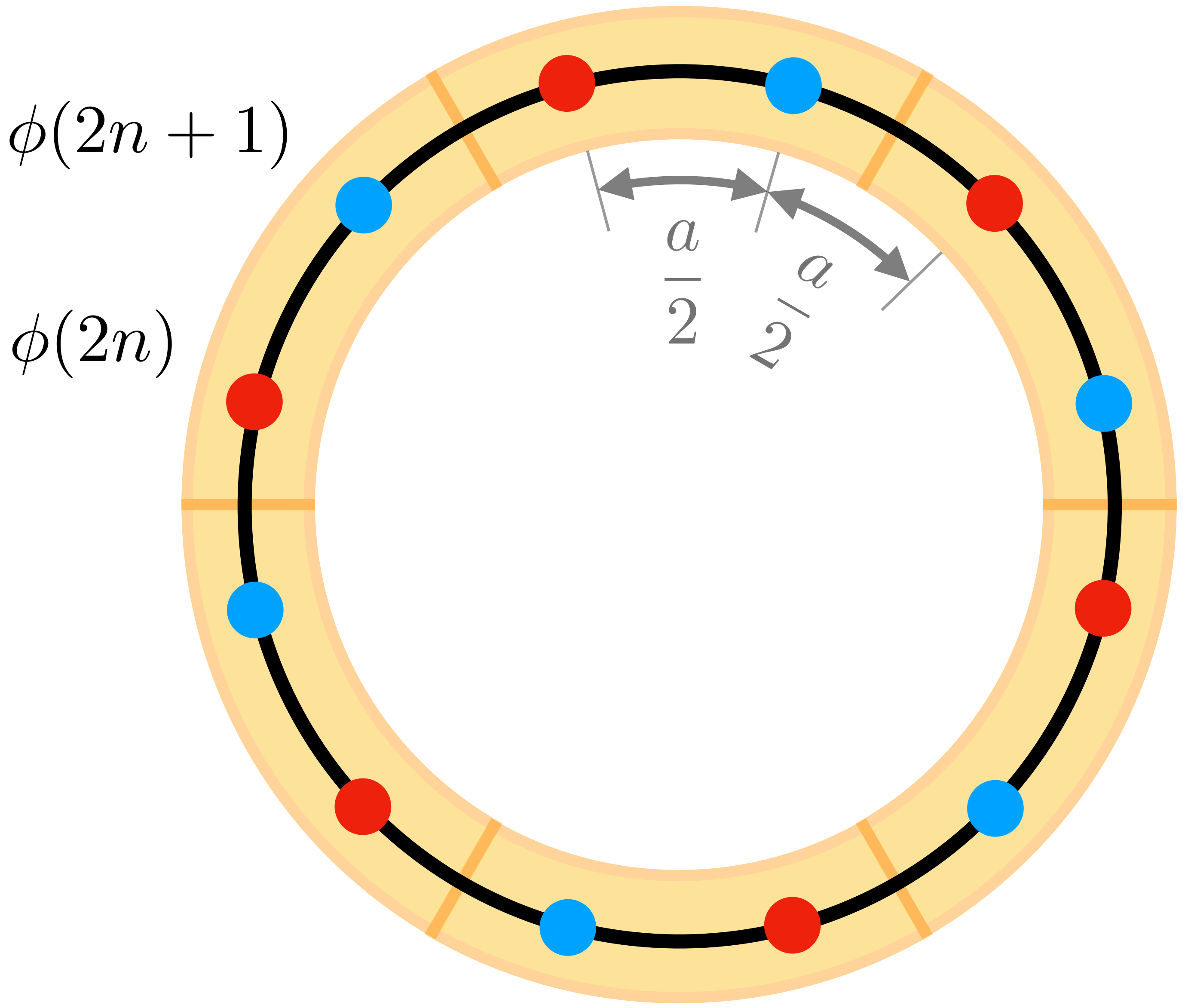
Discretization and parametrization



Symmetry-base parametrization ansatz



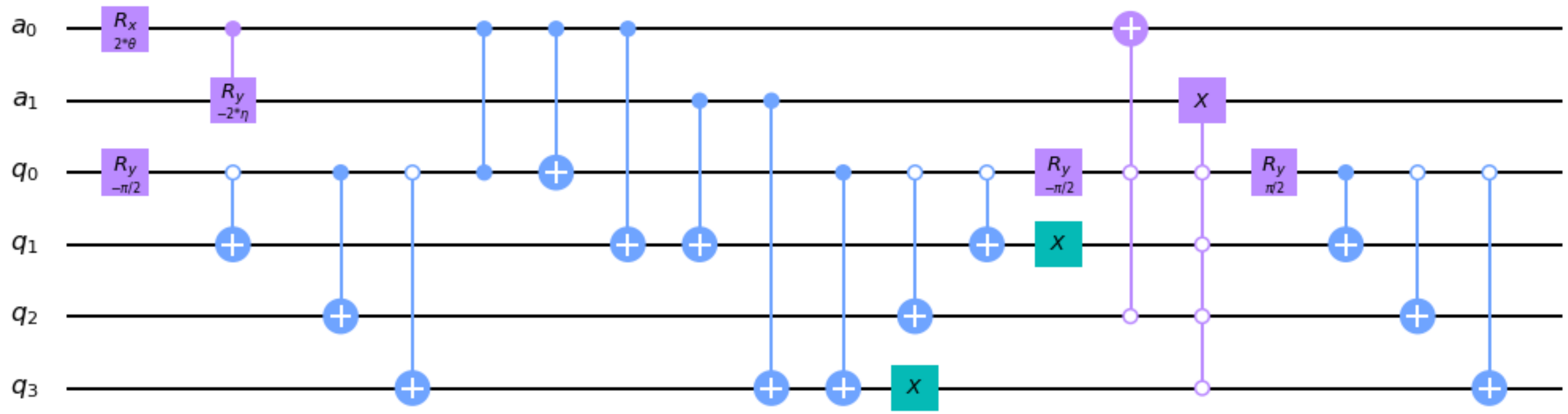
$$\mathcal{L}(x) = \bar{\psi}(x)\big(i\partial\!\!\!/ - \hat{m}\big)\psi(x) + \frac{1}{2}G_\pi\big[\bar{\psi}(x)\psi(x)\big]^2$$

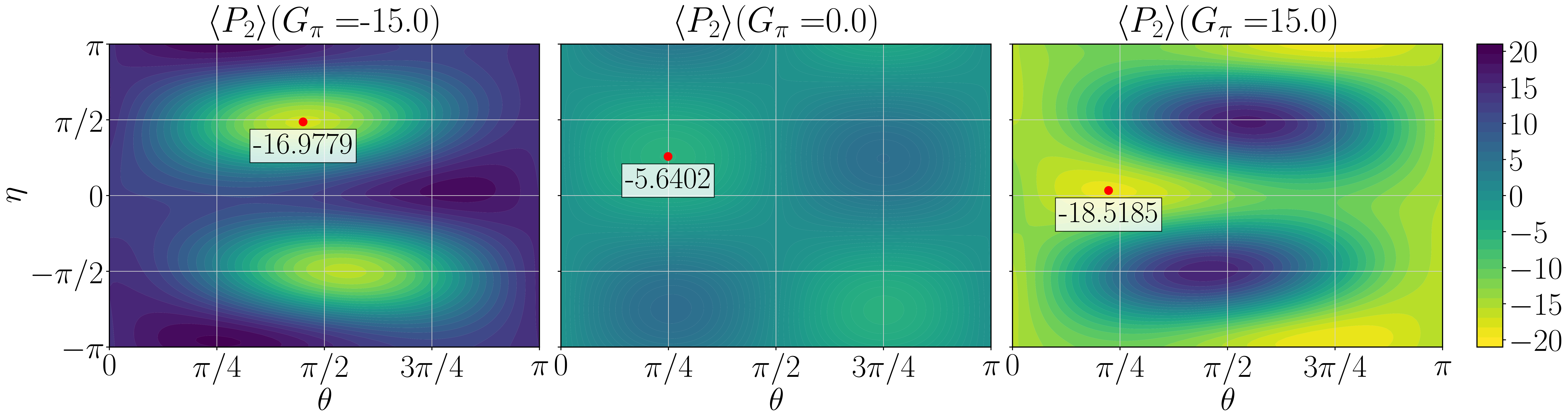


Staggered fermion lattice

NJL model

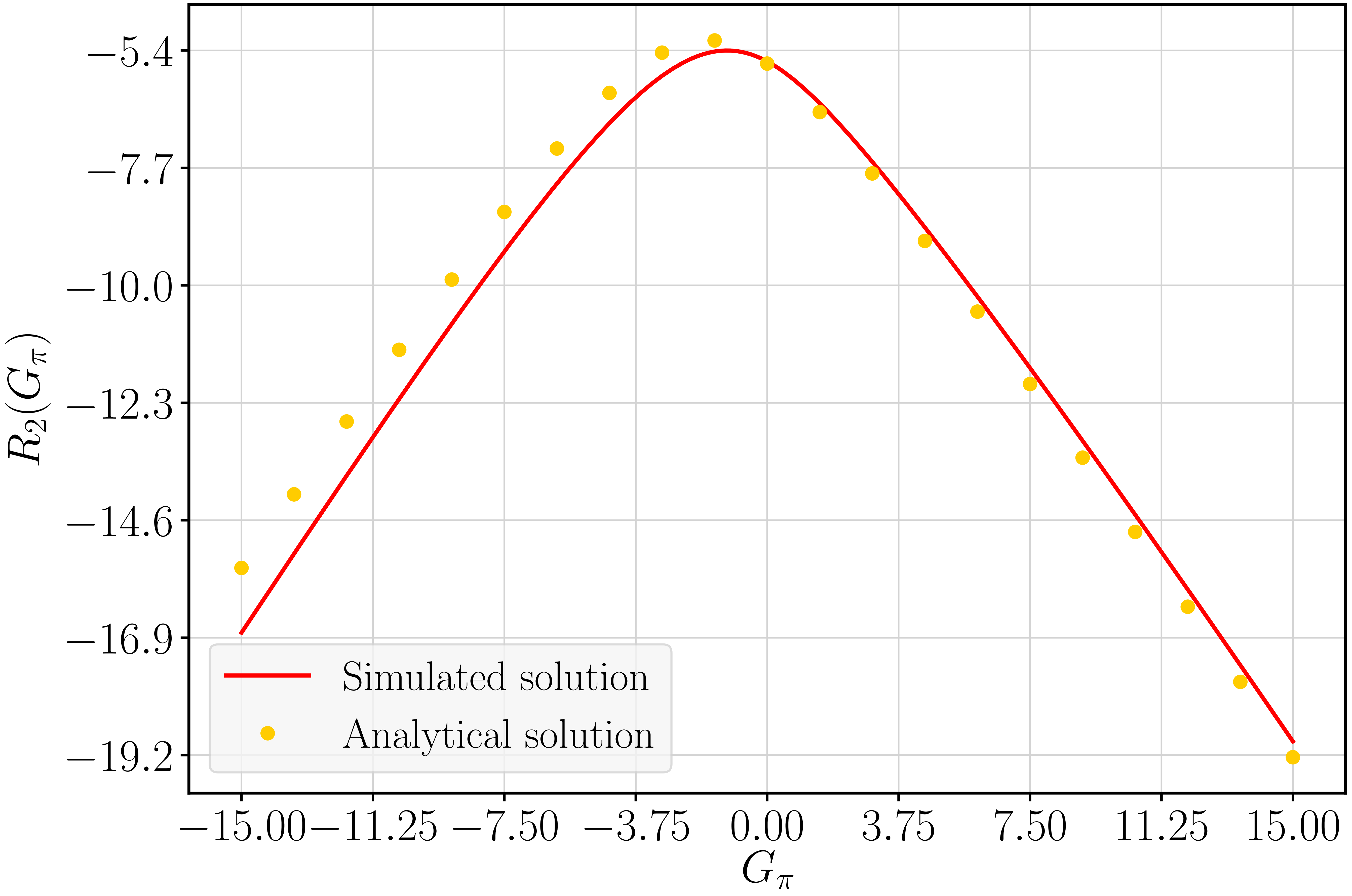
Quantum circuit

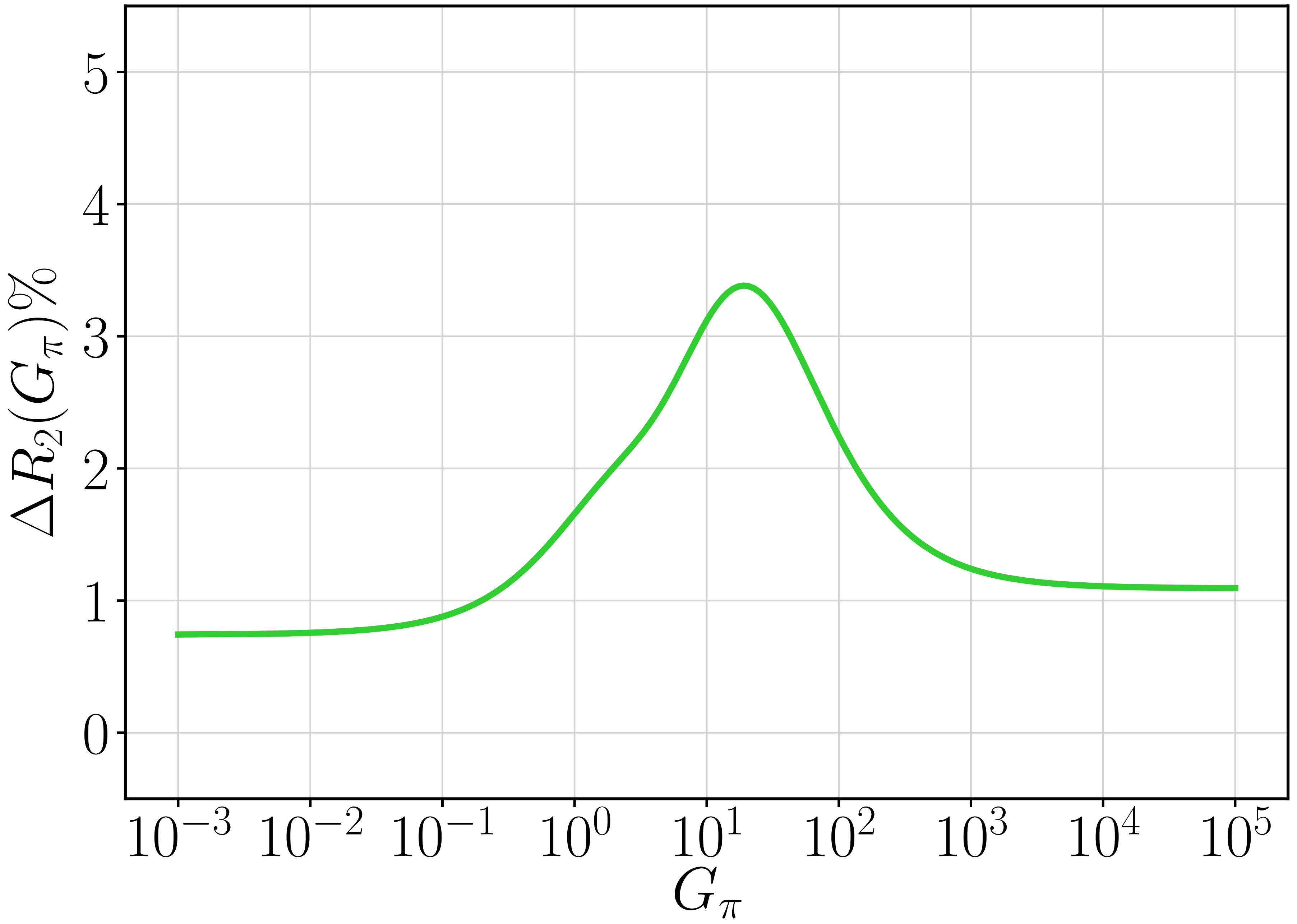


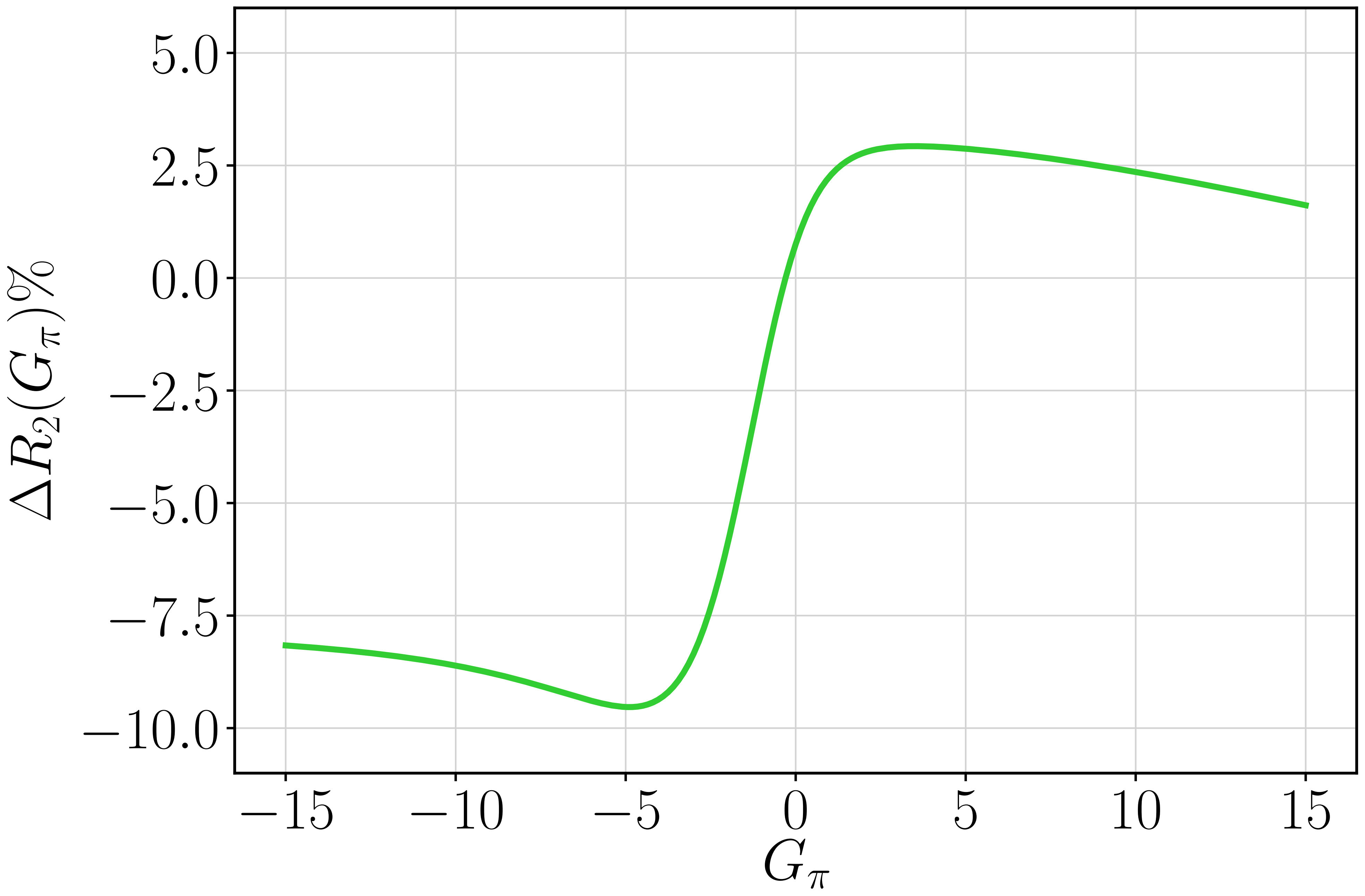


NJL model

Results







NJL model

Results