An optimal quantum sampling regression algorithm for variational eigensolving in the low qubit number regime

2021 Chicago Quantum Exchange Workshop

Pedro Rivero

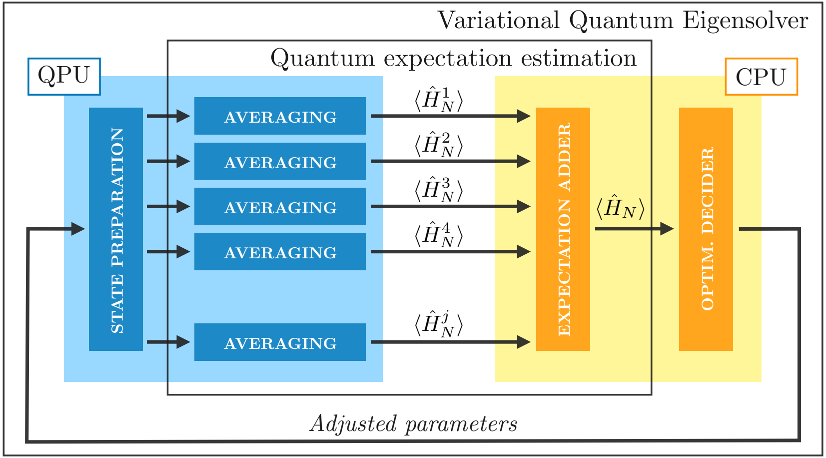
Illinois Institute of Technology
Argonne National Laboratory

`priveroramirez@anl.gov`

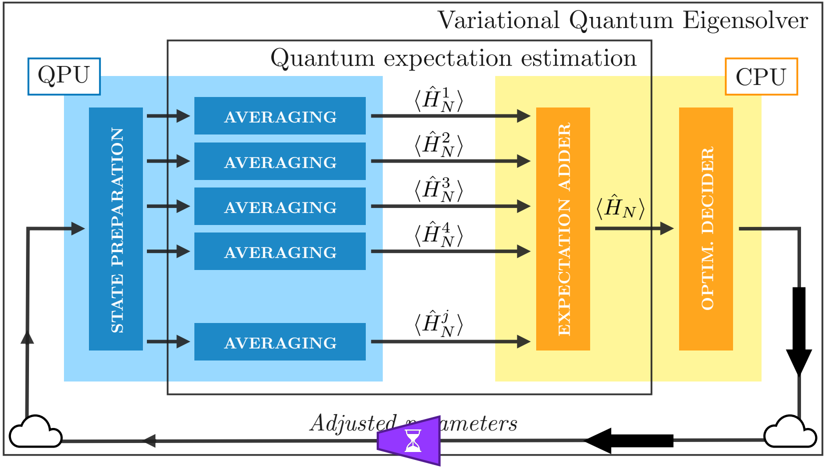
arXiv:2012.02338

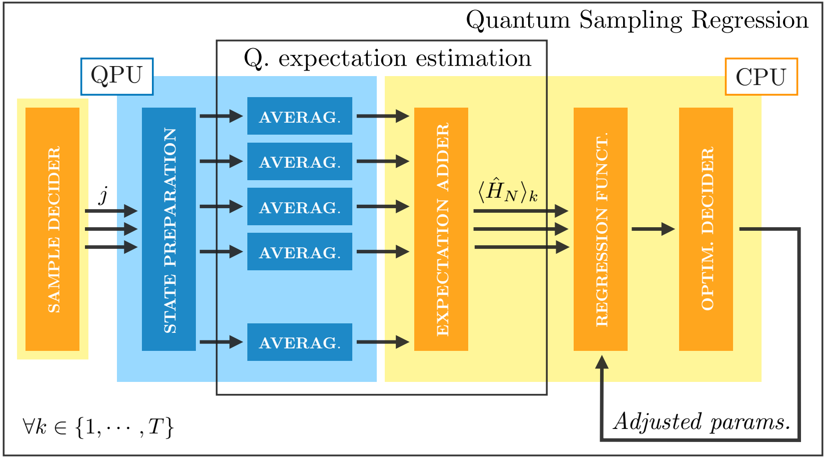
2021-04-20

Variational Quantum Eigensolver (VQE)



Variational Quantum Eigensolver (VQE)

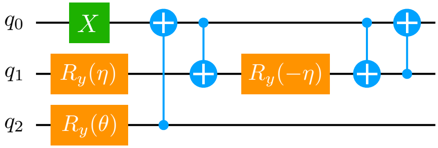




Quantum Sampling Regression
Q. expectation estimation
QPU
CPU
SAMPLE DECIDER
j
STATE PREPARATION
AVERAG.
AVERAG.
AVERAG.
AVERAG.
AVERAG.
EXPECTATION ADDER
$\langle \hat{H}_N \rangle_k$
REGRESSION FUNCT.
OPTIM. DECIDER
$\forall k \in \{1, \cdots, T\}$
Adjusted params.

Quantum Sampling Regression (QSR)

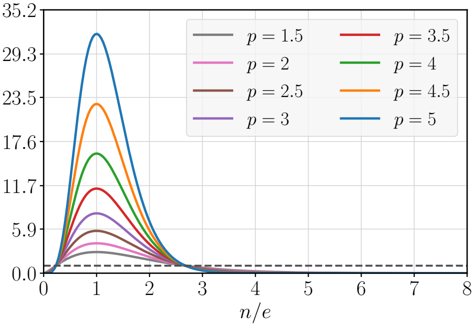
- From the **topology of the quantum circuit** in charge of state preparation, we can infer a frequency bound.
- **Fourier analysis** then allows to fully reconstruct the expectation value function.
- Through the **Nyquist-Shannon sampling theorem** we can show that our sampling technique is optimal.

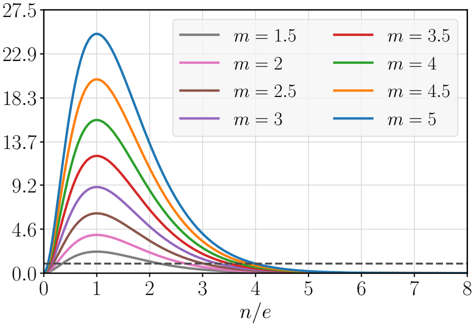


Theorem (Nyquist-Shannon)

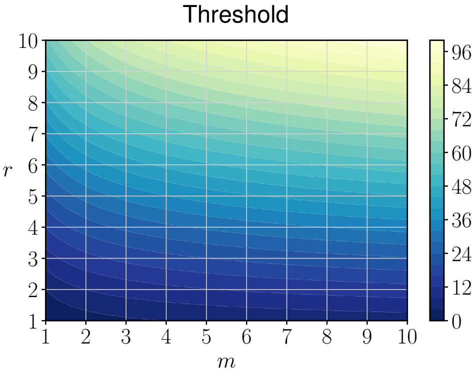
If a function $h(\theta)$ contains no angular frequencies higher than ω_S, it is completely determined by giving its ordinates at a series of points $1/2\omega_S$ apart: $\omega_{\text{sampling}} > 2\omega_S$.

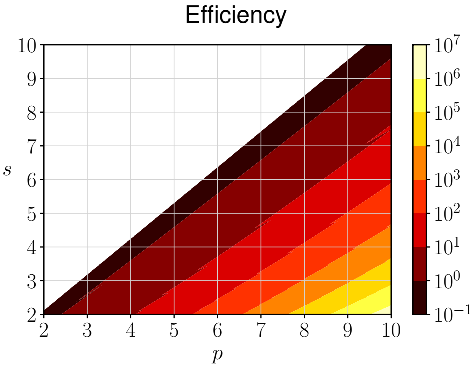
- Algorithmic complexity model: $$\frac{\text{VQE}}{\text{QSR}} = \left(mn2^{-n/r}\right)^{p}$$





Low qubit number regime



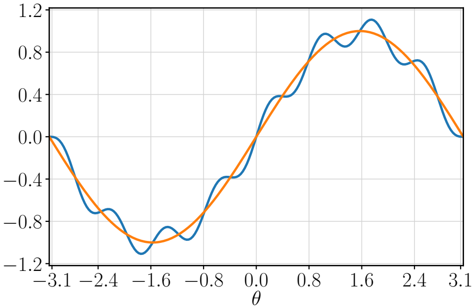


$$a \triangleq \left\lceil -\frac{r}{\ln 2} W_{-1}\left(-\frac{\ln 2}{mr}\right)\right\rceil$$

$$E \approx \frac{1}{as\ln 2}\left(\frac{m}{s\ln 2}\right)^{p} \Gamma(p+1, s\ln 2, as\ln 2)$$

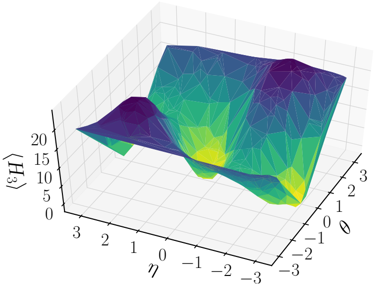
Applications

- **Oversampling** to attain higher precision.
- **Undersampling** to boost performance and get rid of small-wavelength oscillations leading to burdensome local minima.
- VQE low-resolution start-up **supplement**.
- **Proxy** to transition between simulators and real devices.
- Improve convergence by removing the stochastic nature of the quantum expectation value function.
- Avoid the exponential matrix formulation in classical computation.



VQE

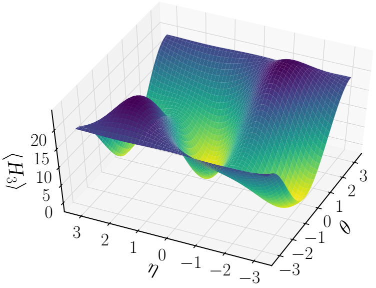
```
DEUTERON BINDING ENERGY:
Minimum 'E3 = -2.0513 (MeV)'
'[theta, eta] = [0.2819, 0.3040] (rad)'
» ERROR = 0.3%
```



183 *samples* → 183 *queries*

QSR

```
DEUTERON BINDING ENERGY:
Minimum 'E3 = -2.0509 (MeV)'
'[theta, eta] = [0.2688, 0.3631] (rad)'
» ERROR = 0.2%
```



25 *samples* → 1 *query*

Thanks

CHICAGO QUANTUM EXCHANGE

NSF

U.S. DEPARTMENT OF ENERGY | Office of Science

Argonne
NATIONAL LABORATORY