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

APS Prairie Section

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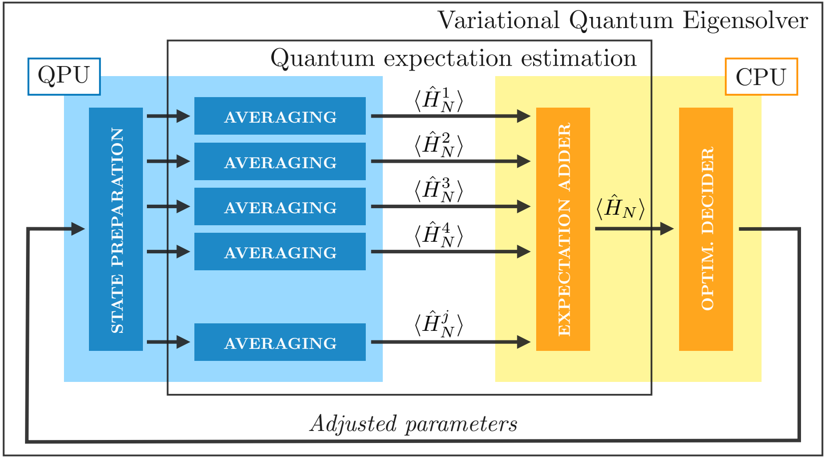
Variational Quantum Eigensolver (VQE)



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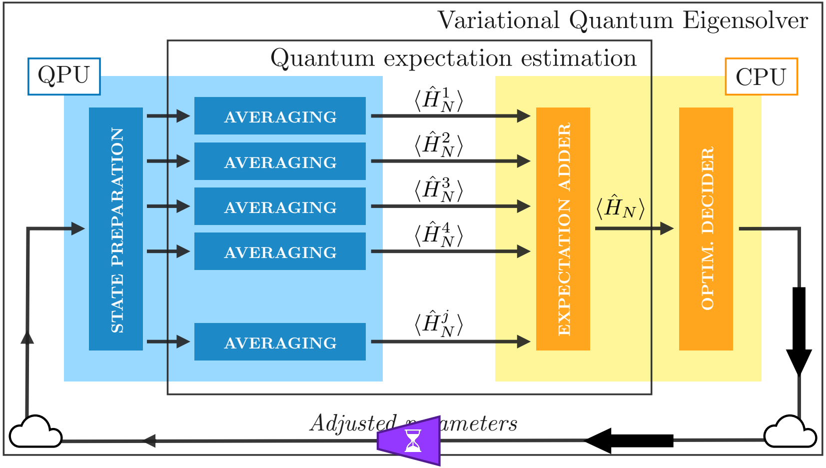
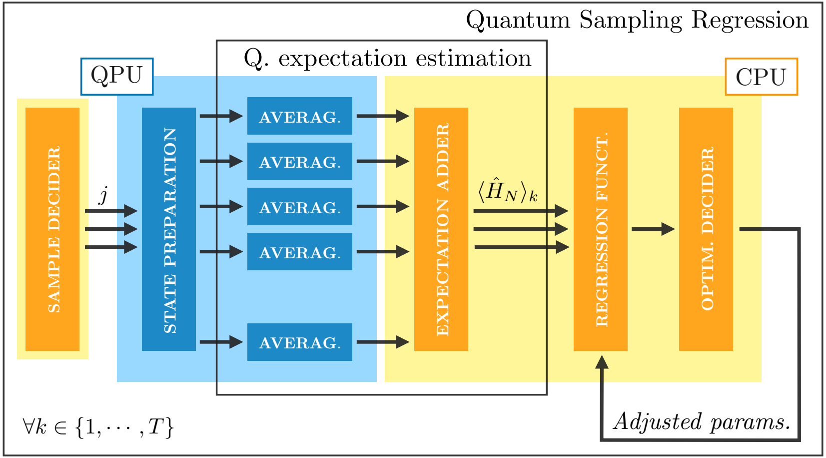
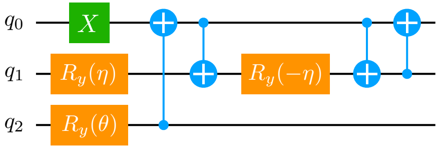


Quantum Sampling Regression (QSR)



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.

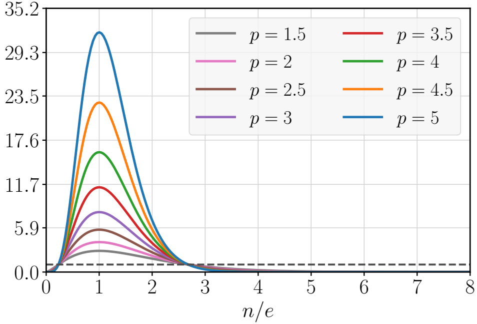


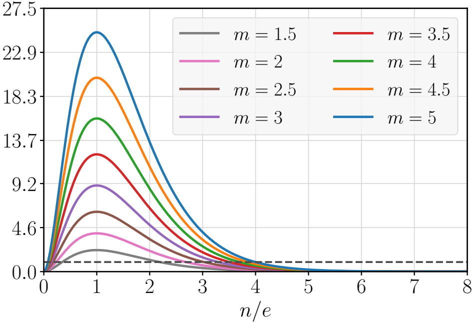
Theorem (Nyquist-Shannon)

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: $\omega_{\text{sampling}} > 2\omega_S$.

Low qubit number regime

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



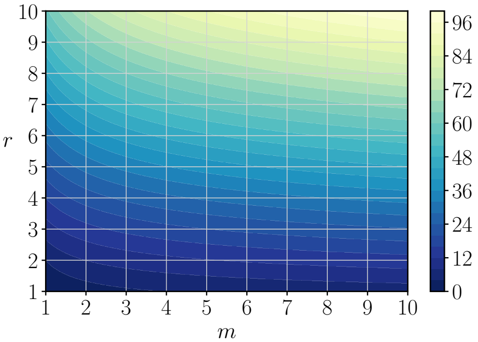


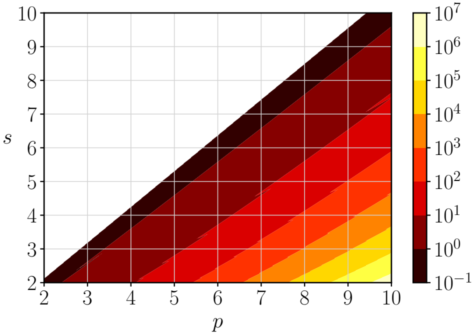
Low qubit number regime

VQE algorithm
QSR algorithm
Complexity
Applications
Banchmarking

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

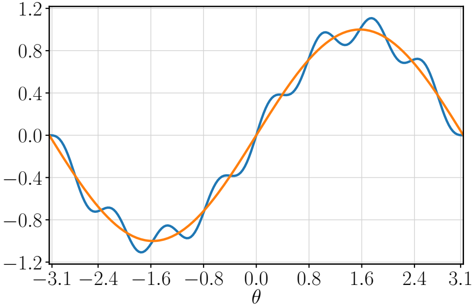
$$E \approx \frac{1}{as\ln 2}\left(\frac{m}{s\ln 2}\right)^{p} \Gamma(p+1, s\ln 2, as\ln 2)$$





Applications

- Reducing the amount of queries that need to be sent to a given quantum processor in order to carry out the optimization process.
- **Oversampling** to attain higher precision.
- **Undersampling** to boost performance get rid of unnecessary small-wavelength oscillations leading to burdensome local minima.
- Low-resolution start-up supplement of VQE.



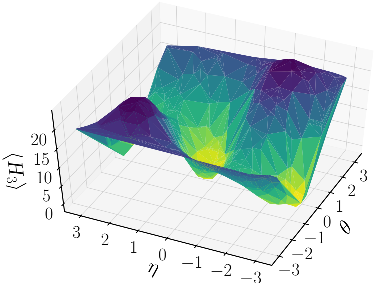
Applications

- Improve convergence by removing the stochastic nature of the quantum expectation value function, stemming out of our flawed sampling process (i.e. we have neither infinite precision nor time to calculate the exact expectation values)
- **Proxy** to transition between simulators and real devices running VQE while analyzing global properties such as error propagation in the expectation value function.
- Fully exploit the power of our ansatz classically, avoiding the usual exponential matrix formulation of quantum mechanics.

Banchmarking (arXiv:1801.03897)

VQE

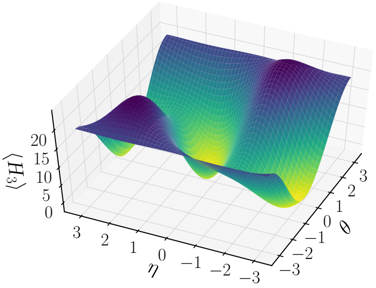
```
GROUND-STATE ENERGY:
Minimum 'E3 = -2.0513 (MeV)'
'[theta, eta] = [0.2819, 0.3040] (rad)'
» ERROR = 0.3%
```



183 *samples* $\rightarrow \sim$ 60 *queries (?)*

QSR

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



25 *samples* $\rightarrow$ 1 *query*

Thanks

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