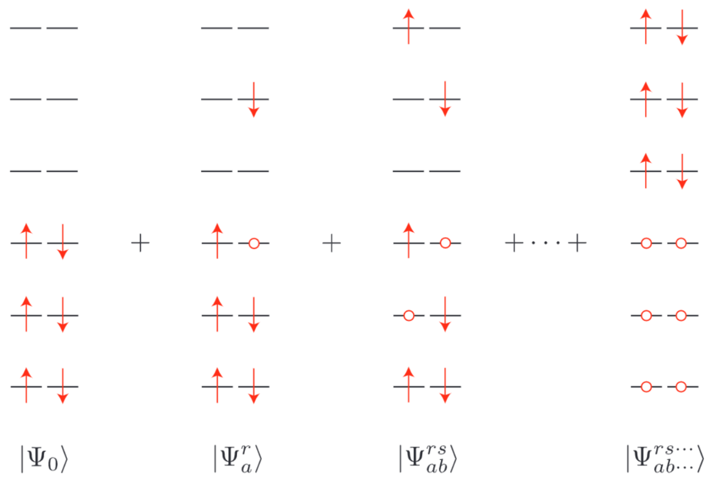
EXACT DIAGONALISATION

- Basis size scales with all possible configurations

$$|\Psi_{FCI}\rangle = c_0|\Psi_0\rangle + \sum_{a}^{occ}\sum_{r}^{virt} c_a^r|\Psi_a^r\rangle + \sum_{a<b}^{occ}\sum_{r<s}^{virt} c_{ab}^{rs}|\Psi_{ab}^{rs}\rangle + \cdots + \sum_{a<b<\cdots}^{occ}\sum_{r<s<\cdots}^{virt} c_{ab\ldots}^{rs\ldots}|\Psi_{ab\ldots}^{rs\ldots}\rangle$$



- Combinatorial scaling Generalised EVP

$$\mathbf{HC} = E\mathbf{SC}$$

Scaling: $\binom{K}{N} = \frac{(K)!}{N!(K-N)!}$

- **Krylov methods offer a way around this scaling**

KRYLOV METHODS

- Kyrlov Basis:
  - Powers of functions of H

$$\{|\psi_0\rangle, f(H)^1|\psi_0\rangle, f(H)^2|\psi_0\rangle, ..., f(H)^K|\psi_0\rangle\}$$

- Weighted linear combination

$$|\psi\rangle = c_0|\psi_0\rangle + c_1 f(H)^1|\psi_0\rangle + c_2 f(H)^2|\psi_0\rangle + \cdots + c_K f(H)^K|\psi_0\rangle$$

- **Smaller GEVP to solve (10 – 100s)**

$$\mathbf{HC} = E\mathbf{SC}$$

KRYLOV METHODS

- Kyrlov GEVP:

$$\mathbf{HC} = E\mathbf{SC}$$

- Hamitonian matrix elements

$$H_{ij} = \langle\psi_0|f(H)^i\hat{H}f(H)^j|\psi_0\rangle$$

- Overlap matrix elements

$$S_{ij} = \langle\psi_0|f(H)^i f(H)^j|\psi_0\rangle$$

- **Complexity shifted to matrix element calculation**

KRYLOV METHODS $f(H)$

Matrix function via SVD: $f(M) = Uf(s)V$

- Real time evolution

$$|\psi_j\rangle = f(H)^j|\psi_0\rangle = e^{-iHjt}|\psi_0\rangle$$

- Imaginary time evolution

$$|\psi_j\rangle = f(H)^j|\psi_0\rangle = e^{-Hjt}|\psi_0\rangle$$

- Cheybshev polynomials (recursive double angle formulas)

$$|\psi_j\rangle = f(H)^j|\psi_0\rangle = T_j(H)|\psi_0\rangle = \cos(j\arccos(H))|\psi_0\rangle$$

- **Lots of open research in this area**

QUANTINUUM

UNITARY KRYLOV

- Real time evolution $$e^{i\mathbf{H}t}\mathbf{C} = e^{i\mathbf{e}t}\mathbf{SC}$$ $$e_n = \frac{\ln(\lambda_n)}{i\Delta t} \pm \frac{2n\pi}{\Delta t}$$

- Hamiltonian matrix elements $$|\psi_j\rangle = f(H)^j|\psi_0\rangle = e^{-iHjt}|\psi_0\rangle$$

$$e_{ij}^{-i\mathbf{H}t} = \langle\psi_0|e^{iHit}e^{-iHt}e^{-iHjt}|\psi_0\rangle = \langle\psi_0|e^{-iH(-i+1+j)t}|\psi_0\rangle$$

- Overlap Matrices

$$S_{ij} = \langle\psi_0|e^{iHit}e^{-iHjt}|\psi_0\rangle = \langle\psi_0|e^{-iH(i+j)t}|\psi_0\rangle$$

QUANTINUUM

UNITARY KRYLOV

- All the elements of $e^{i\mathbf{H}t}\mathbf{C} = e^{i\mathbf{e}t}\mathbf{SC}$

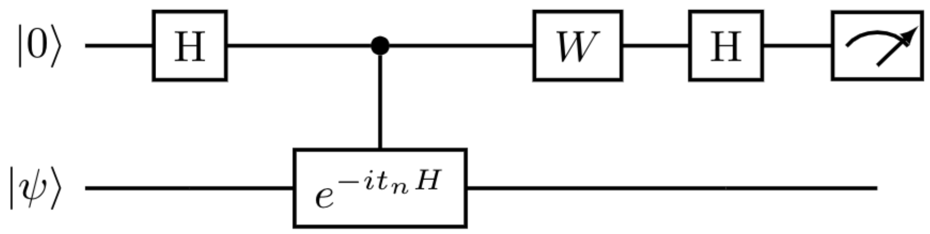
$$S_{ij} = \langle \psi_0 | e^{-iH(i+j)t} | \psi_0 \rangle \qquad e^{-i\mathbf{H}t}_{ij} = \langle \psi_0 | e^{-iH(-i+1+j)t} | \psi_0 \rangle$$

- Generated from a set $\langle \psi_0 | e^{-iHkt} | \psi_0 \rangle$

- Significantly reducing the number of elements compared to the standard krylov

UNITARY QUANTUM KRYLOV

- Calculate $\langle\psi_0|e^{-iHkt}|\psi_0\rangle$ on a quantum computer using the Hadamard test



- In theory a quantum computer would allow us to calculate much larger systems
- Because $|\psi\rangle$ scale linearly with qubit number

KRYLOV METHODS

Matrix function via SVD: $f(M) = Uf(s)V$

- Real time evolution $|\psi_j\rangle = f(H)^j|\psi_0\rangle = e^{-iHjt}|\psi_0\rangle$

- Hamiltonian matrix elements

$$H_{ij} = \langle\psi_0|e^{iHit}\hat{H}e^{-iHjt}|\psi_0\rangle$$

- Overlap Matrices

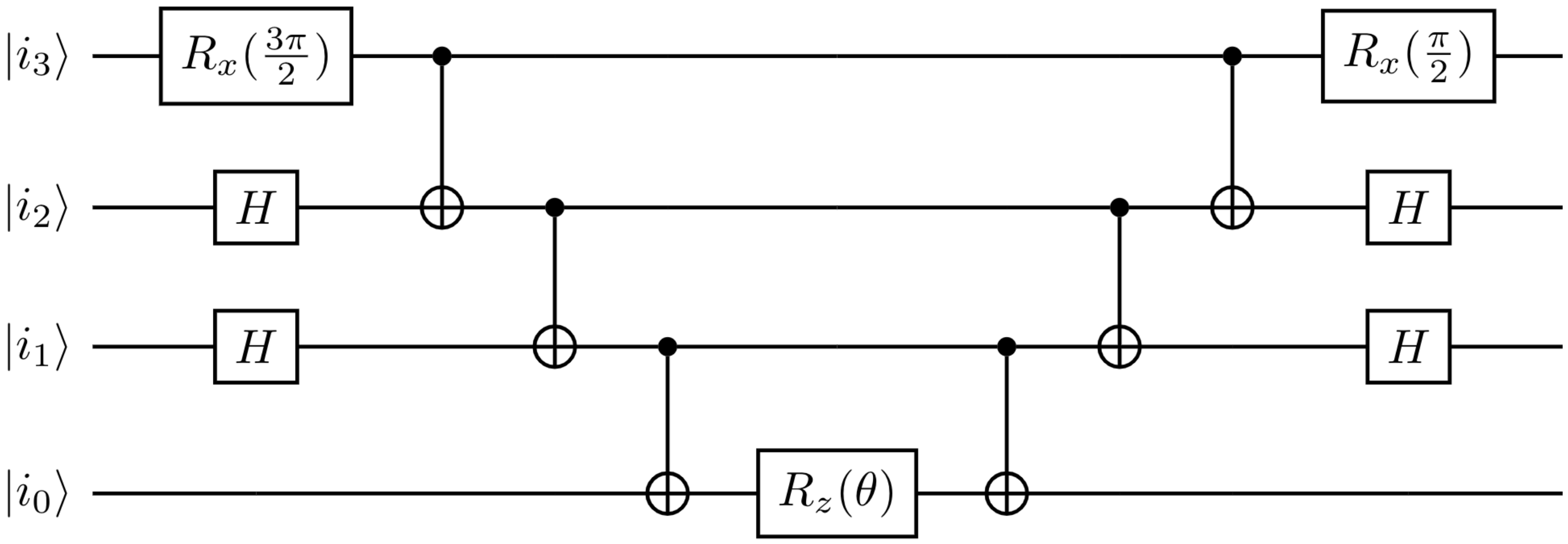
$$S_{ij} = \langle\psi_0|e^{iHit}e^{-iHjt}|\psi_0\rangle = \langle\psi_0|e^{iH(i-j)t}|\psi_0\rangle$$

QUANTINUUM

UCC Quantum Circuit Formulism

- Exponentiated Paulis have a well known quantum circuit representation – PAULI GADGET

$$e^{i\frac{\theta}{2}(\sigma_0^z\otimes\sigma_1^x\otimes\sigma_2^x\otimes\sigma_3^y)}$$



- If not in Z basis need to flip the qubit into the z basis with a rotation