QUANTUM SIMULATION ALGORITHMS FOR MANY FERMION SYSTEMS IN FIRST QUANTIZATION

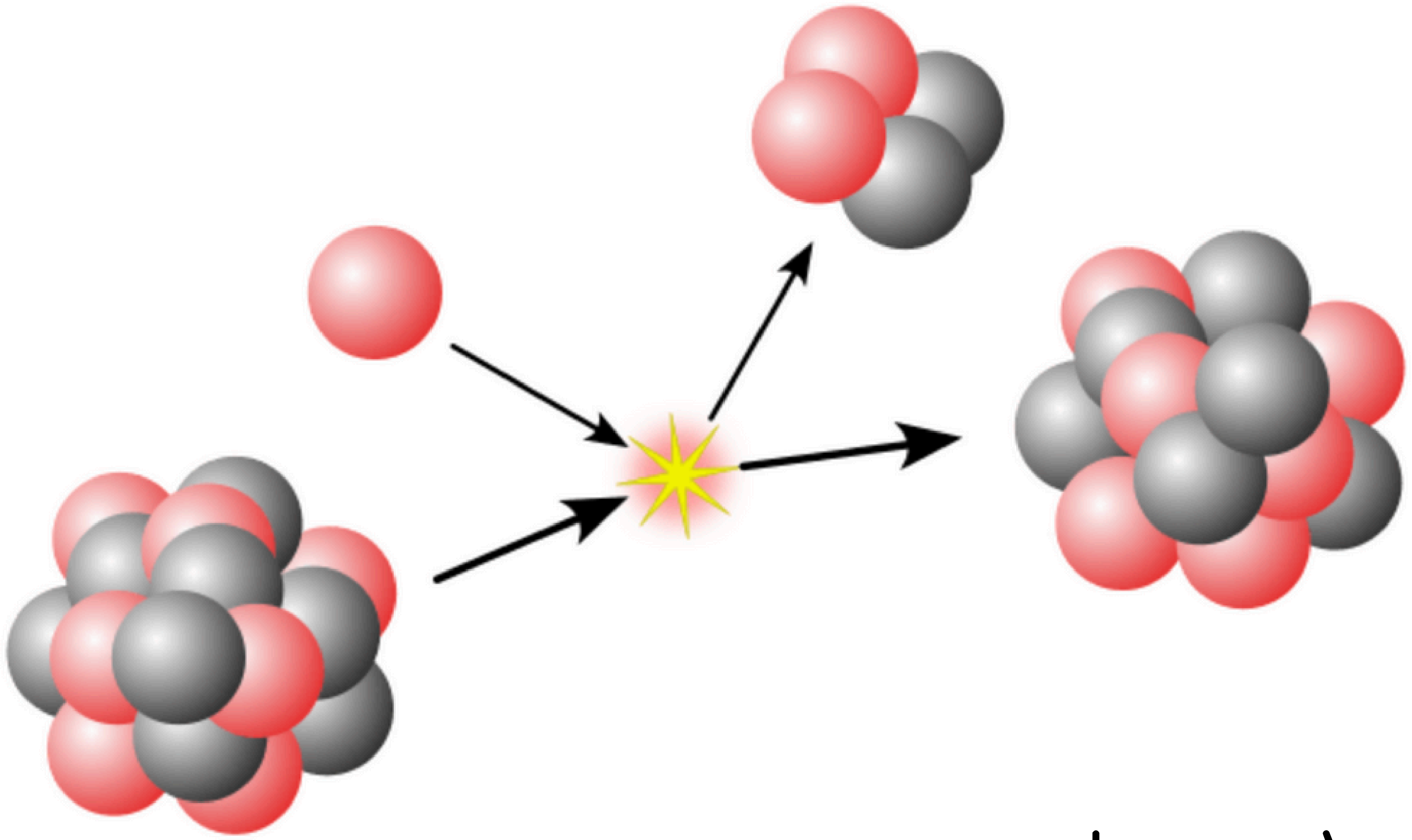
LUCA SPAGNOLI

UNIVERSITY OF TRENTO

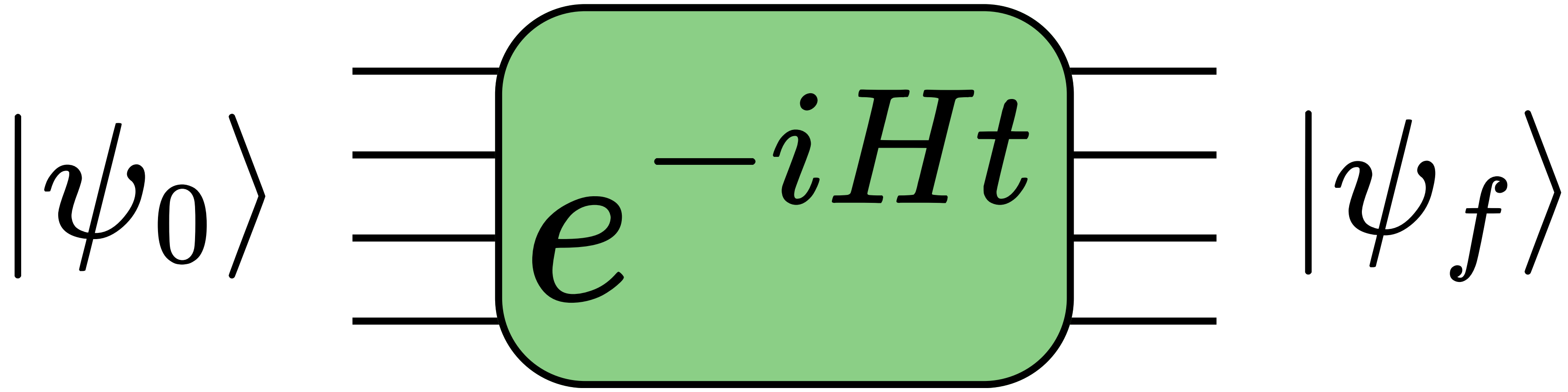
TIFPA

MOdeling Nuclear STructure and REaction

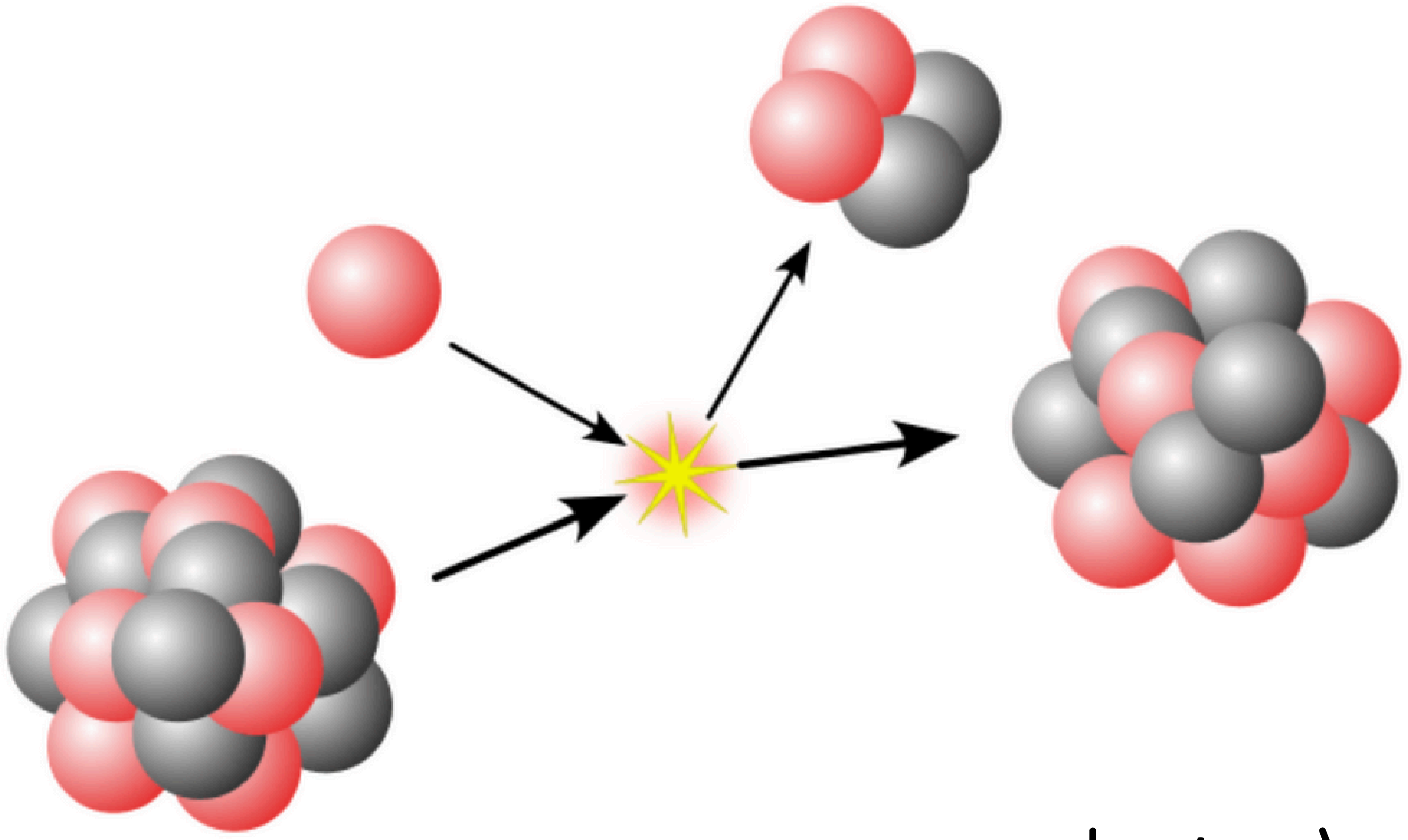
NUCLEAR PHYSICS



We want to simulate scattering processes



NUCLEAR PHYSICS



We want to simulate scattering processes

$$|\psi_0\rangle \quad \boxed{e^{-iHt}} \quad |\psi_f\rangle$$

Encoding

Evolution

IN THIS PRESENTATION

First quantization has an advantage over second quantization

IN THIS PRESENTATION

First quantization has an advantage over second quantization

First quantisation

- Hilbert space: total number of particles conserved
- Operators: position, momentum

$$H = \underbrace{\sum_i \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i<j} V(x_i - x_j)}_{V}$$

IN THIS PRESENTATION

First quantisation

- Hilbert space: total number of particles conserved
- Operators: position, momentum

First quantization has an advantage over second quantization

Second quantization

- Fock space: total number of particles not conserved
- Operators: creation and anihilation operators

$$H = \underbrace{\sum_i \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i<j} V(x_i - x_j)}_{V}$$

$$H = m \sum_i a_i^\dagger a_i + \sum_{i,j} \left(a_i^\dagger a_j + a_j^\dagger a_i \right)$$

THE ENCODING

Qubits have a finite number of states

THE ENCODING

Qubits have a finite number of states $\longrightarrow$ We need a finite single particle basis

THE ENCODING

Qubits have a finite number of states $\longrightarrow$ We need a finite single particle basis $\longrightarrow$ number of single particle orbital: Ω

THE ENCODING

Qubits have a finite number of states $\longrightarrow$ We need a finite single particle basis $\longrightarrow$ number of single particle orbital: Ω

First quantization

$$|\psi_3\rangle = \hat{A}|\phi_1\rangle \otimes |\phi_2\rangle \otimes |\phi_3\rangle, \quad |\phi_j\rangle = \sum_{k=0}^{\Omega-1} c_k |k\rangle$$

We need one wavefunction for every particle

$$\dim(\mathcal{H}_\eta) = \Omega^\eta$$

THE ENCODING

Qubits have a finite number of states $\longrightarrow$ We need a finite single particle basis $\longrightarrow$ number of single particle orbital: Ω

First quantization

$$|\psi_3\rangle = \hat{A}|\phi_1\rangle \otimes |\phi_2\rangle \otimes |\phi_3\rangle, \quad |\phi_j\rangle = \sum_{k=0}^{\Omega-1} c_k |k\rangle$$

We need one wavefunction for every particle

$$\dim(\mathcal{H}_\eta) = \Omega^\eta$$

We need a number of qubits equal to:

$$\eta \log_2(\Omega)$$

THE ENCODING

Qubits have a finite number of states $\longrightarrow$ We need a finite single particle basis $\longrightarrow$ number of single particle orbital: Ω

First quantization

$$|\psi_3\rangle = \hat{A}|\phi_1\rangle \otimes |\phi_2\rangle \otimes |\phi_3\rangle, \quad |\phi_j\rangle = \sum_{k=0}^{\Omega-1} c_k|k\rangle$$

We need one wavefunction for every particle

$$\dim(\mathcal{H}_\eta) = \Omega^\eta$$

We need a number of qubits equal to:

$$\eta \log_2(\Omega)$$

Second quantization

$$|\psi_3\rangle = a_1^\dagger a_2^\dagger a_3^\dagger |0\rangle$$

We need a creation operator for every single particle orbital

$$\dim(\mathcal{F}) = 2^\Omega$$

THE ENCODING

Qubits have a finite number of states $\longrightarrow$ We need a finite single particle basis $\longrightarrow$ number of single particle orbital: Ω

First quantization

$$|\psi_3\rangle = \hat{A}|\phi_1\rangle \otimes |\phi_2\rangle \otimes |\phi_3\rangle, \quad |\phi_j\rangle = \sum_{k=0}^{\Omega-1} c_k|k\rangle$$

We need one wavefunction for every particle

$$\dim(\mathcal{H}_\eta) = \Omega^\eta$$

We need a number of qubits equal to:

$$\eta \log_2(\Omega)$$

Second quantization

$$|\psi_3\rangle = a_1^\dagger a_2^\dagger a_3^\dagger|0\rangle$$

We need a creation operator for every single particle orbital

$$\dim(\mathcal{F}) = 2^\Omega$$

We need a number of qubits equal to:

$$\Omega$$

TIME EVOLUTION

$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j \neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j \neq i}^{\eta-1} \sum_{k \neq j \neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V = V_2 + V_3}$$

TIME EVOLUTION

$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

Trotterization:

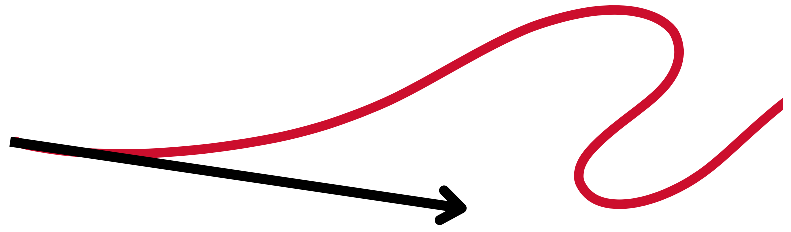
$$e^{-itH} \approx e^{-itT} e^{-itV} + O(t^2)$$

TIME EVOLUTION

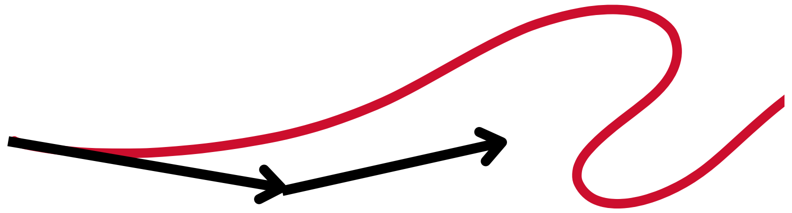
$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

Trotterization:

$$e^{-itH} \approx e^{-itT} e^{-itV} + O(t^2)$$



$$e^{-itH} \approx e^{-i\frac{t}{2}T} e^{-i\frac{t}{2}V} \cdot e^{-i\frac{t}{2}T} e^{-i\frac{t}{2}V} + O\left(\frac{t^2}{2}\right)$$

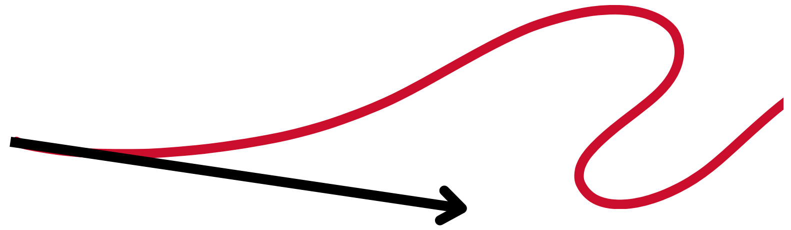


TIME EVOLUTION

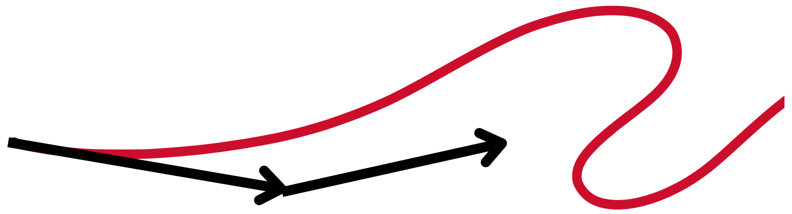
$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

Trotterization:

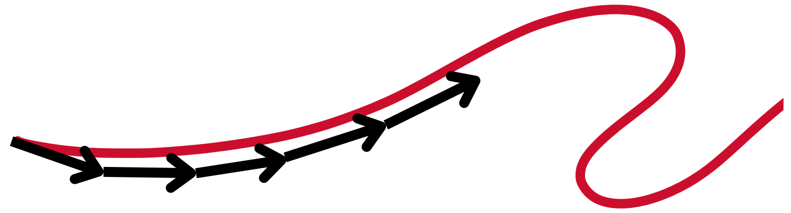
$$e^{-itH} \approx e^{-itT} e^{-itV} + O(t^2)$$



$$e^{-itH} \approx e^{-i\frac{t}{2}T} e^{-i\frac{t}{2}V} \cdot e^{-i\frac{t}{2}T} e^{-i\frac{t}{2}V} + O\left(\frac{t^2}{2}\right)$$



$$e^{-itH} \approx \underbrace{e^{-i\frac{t}{r}T} e^{-i\frac{t}{r}V} \cdots e^{-i\frac{t}{r}T} e^{-i\frac{t}{2}V}}_{r \text{ times}} + O\left(\frac{t^2}{r}\right)$$



TIME EVOLUTION

$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

Kinetic term:

$$e^{itT} = \prod_{j=0}^{\eta-1} e^{i\frac{t}{2m}p_i^2}$$

TIME EVOLUTION

$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

Kinetic term:

$$e^{itT} = \prod_{j=0}^{\eta-1} e^{i\frac{t}{2m}p_i^2}$$

$$\boxed{C\left(e^{itT}\right) = O(\eta \log(\Omega))}$$

TIME EVOLUTION

$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

Kinetic term:

$$e^{itT} = \prod_{j=0}^{\eta-1} e^{i\frac{t}{2m}p_i^2}$$

$$\boxed{C\left(e^{itT}\right) = O(\eta \log(\Omega))}$$

Potential term:

$$e^{itV} = \prod_{j=0}^{\eta-1} \prod_{j=i+1}^{\eta-1} e^{itC\delta(x_i - x_j)}$$

TIME EVOLUTION

$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

Kinetic term:

$$e^{itT} = \prod_{j=0}^{\eta-1} e^{i\frac{t}{2m}p_i^2}$$

$$\boxed{C\left(e^{itT}\right) = O(\eta \log(\Omega))}$$

Potential term:

$$e^{itV} = \prod_{j=0}^{\eta-1} \prod_{j=i+1}^{\eta-1} e^{itC\delta(x_i - x_j)}$$

$$\boxed{C\left(e^{itV}\right) = O(\eta^2 \log(\Omega) + \eta^3 \log(\Omega))}$$

TIME EVOLUTION

$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

Kinetic term:

$$e^{itT} = \prod_{j=0}^{\eta-1} e^{i\frac{t}{2m}p_i^2}$$

$$\boxed{C\left(e^{itT}\right) = O(\eta \log(\Omega))}$$

$$O(\eta^3 \log(\Omega))$$

Potential term:

$$e^{itV} = \prod_{j=0}^{\eta-1} \prod_{j=i+1}^{\eta-1} e^{itC\delta(x_i - x_j)}$$

$$\boxed{C\left(e^{itV}\right) = O(\eta^2 \log(\Omega) + \eta^3 \log(\Omega))}$$

NUMBER OF GATES

Trotterization:

$$||e^{-itH} - \left(e^{-i\frac{t}{r}T}e^{-i\frac{t}{r}V}\right)^r|| \leq \epsilon \quad \Rightarrow \quad r = O\left(\frac{t^2\eta}{\epsilon}\right)$$

NUMBER OF GATES

Trotterization:

$$||e^{-itH} - \left(e^{-i\frac{t}{r}T}e^{-i\frac{t}{r}V}\right)^r|| \leq \epsilon \quad \Rightarrow \quad r = O\left(\frac{t^2\eta}{\epsilon}\right)$$

The total cost will be: $$r\left(C\left(e^{i\frac{t}{r}T}\right) + C\left(e^{i\frac{t}{r}V}\right)\right)$$

NUMBER OF GATES

Trotterization:

$$||e^{-itH} - \left(e^{-i\frac{t}{r}T}e^{-i\frac{t}{r}V}\right)^r|| \leq \epsilon \quad \Rightarrow \quad r = O\left(\frac{t^2\eta}{\epsilon}\right)$$

The total cost will be:

$$r\left(C\left(e^{i\frac{t}{r}T}\right) + C\left(e^{i\frac{t}{r}V}\right)\right) = O\left(\frac{t^2\eta^4}{\epsilon}\log(\Omega)\right)$$

NUMBER OF GATES

Trotterization:

$$||e^{-itH} - \left(e^{-i\frac{t}{r}T}e^{-i\frac{t}{r}V}\right)^r|| \leq \epsilon \quad \Rightarrow \quad r = O\left(\frac{t^2\eta}{\epsilon}\right)$$

The total cost will be: $$r\left(C\left(e^{i\frac{t}{r}T}\right) + C\left(e^{i\frac{t}{r}V}\right)\right) = O\left(\frac{t^2\eta^4}{\epsilon}\log(\Omega)\right)$$

In second quantization: $$\widetilde{O}\left(\frac{t^2\eta}{\epsilon}\Omega\right)$$

COMPARISON

	qubits	trotterization
First quantization: <u>work in progress</u>	$O(\eta \log(\Omega))$	$\widetilde{O}\left(\frac{t^2\eta^4}{\epsilon}\log(\Omega)\right)$
Second quantization: <u>arXiv:2312.05344</u>	$O(\Omega)$	$\widetilde{O}\left(\frac{t^2\eta}{\epsilon}\Omega\right)$

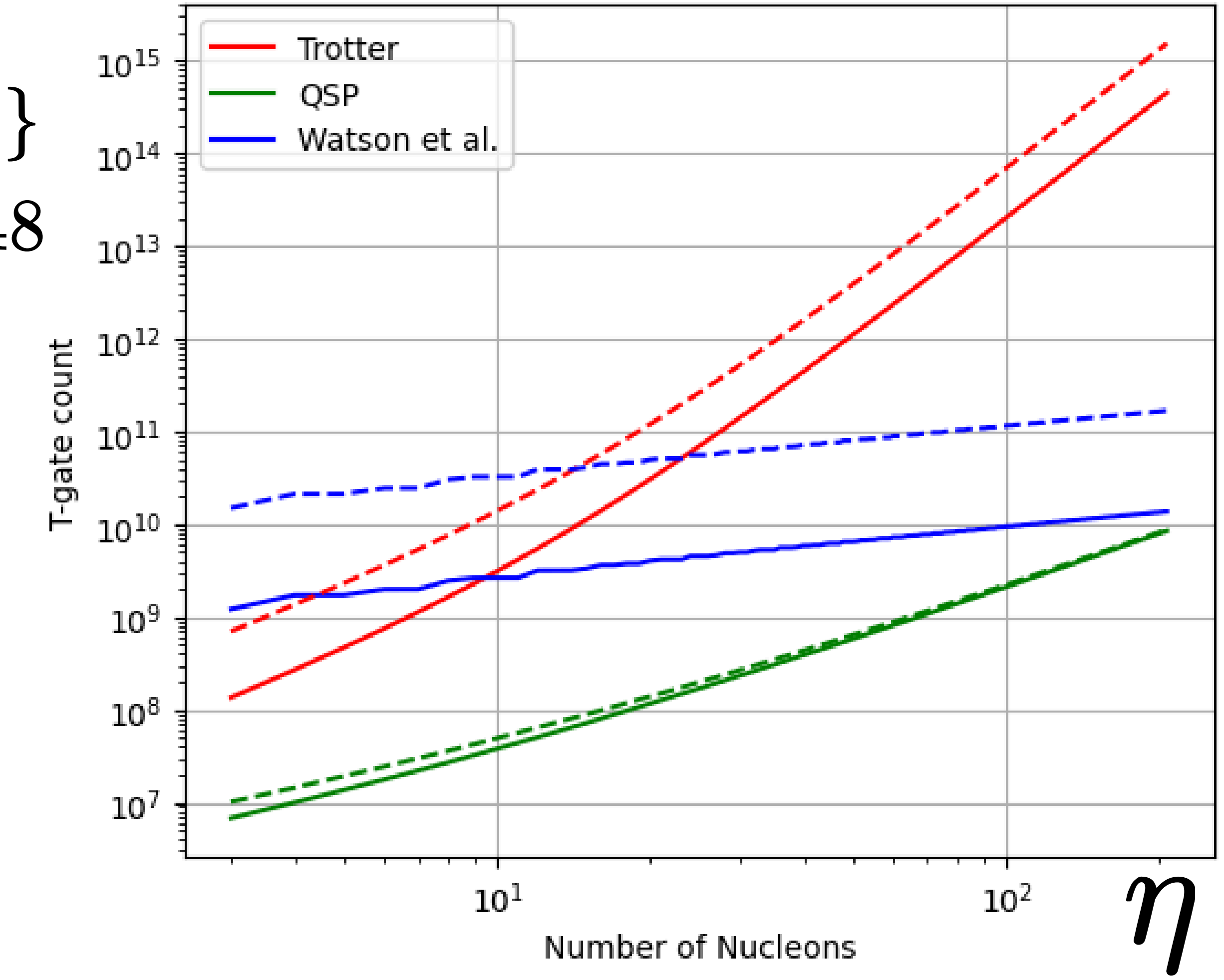
COMPARISON

	qubits	trotterization	QSP
First quantization: work in progress	$O(\eta \log(\Omega))$	$\widetilde{O}\left(\frac{t^2\eta^4}{\epsilon}\log(\Omega)\right)$	$\widetilde{O}\left(\eta\log(\Omega)\left(\eta t + \log\frac{1}{\epsilon}\right)\right)$
Second quantization: arXiv:2312.05344	$O(\Omega)$	$\widetilde{O}\left(\frac{t^2\eta}{\epsilon}\Omega\right)$	

COMPARISON

	qubits	trotterization	QSP
First quantization: <u>work in progress</u>	$O(\eta \log(\Omega))$	$\tilde{O}\left(\frac{t^2\eta^4}{\epsilon}\log(\Omega)\right)$	$\tilde{O}\left(\eta \log(\Omega)\left(\eta t + \log\frac{1}{\epsilon}\right)\right)$
Second quantization: <u>arXiv:2312.05344</u>	$O(\Omega)$	$\tilde{O}\left(\frac{t^2\eta}{\epsilon}\Omega\right)$	

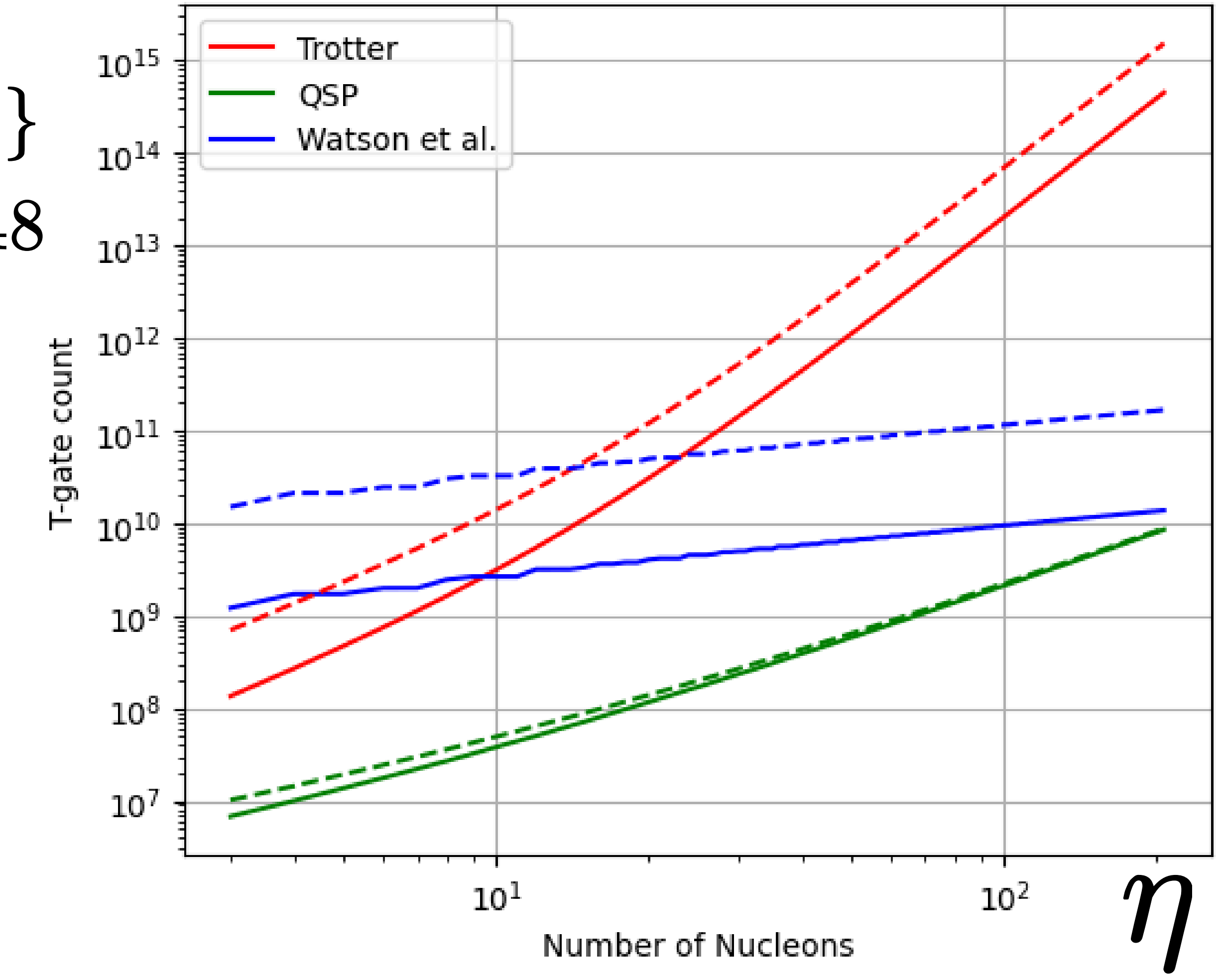
$$\epsilon = \{10^{-1}, 10^{-3}\}$$
$$\Omega = 4 \cdot 8^3 = 2048$$

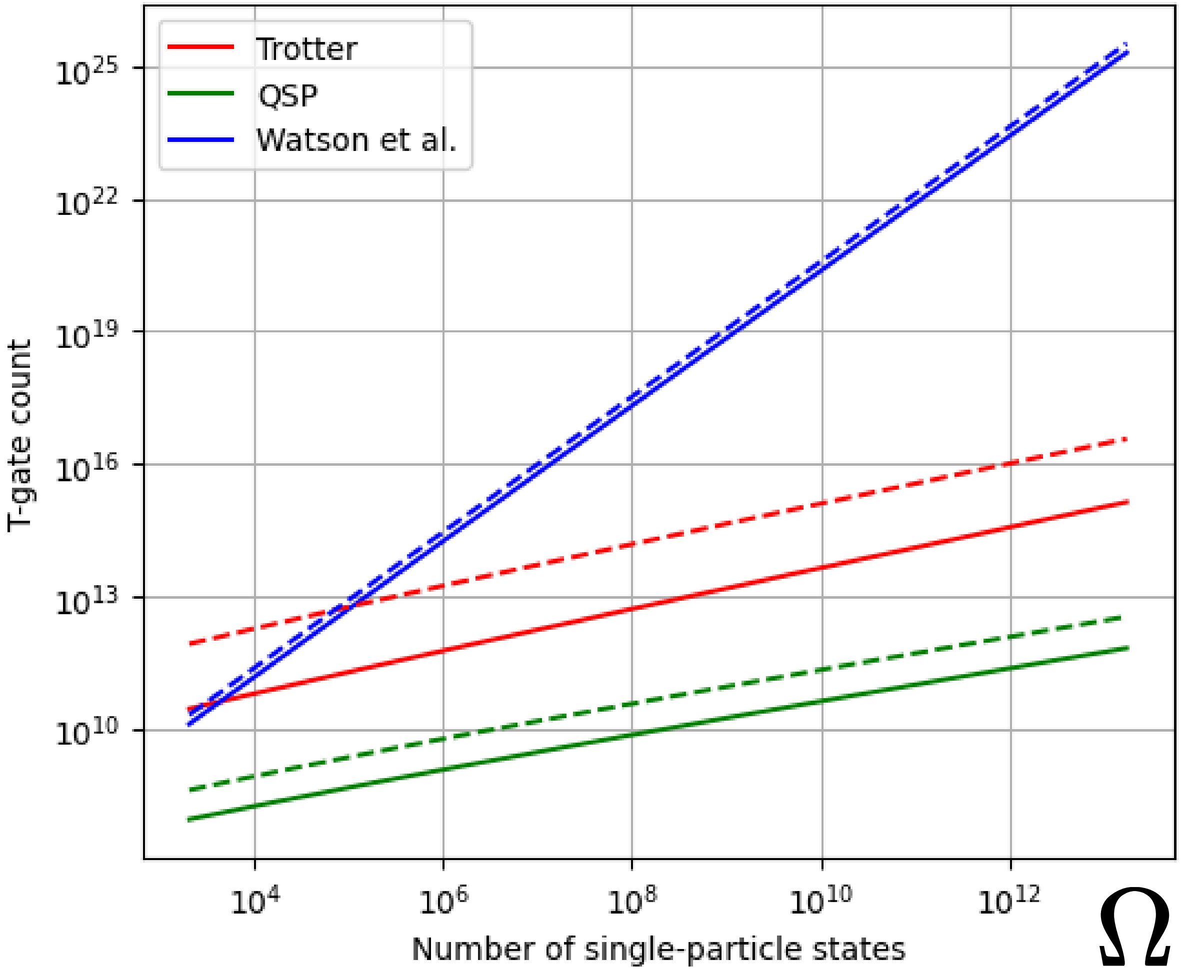


COMPARISON

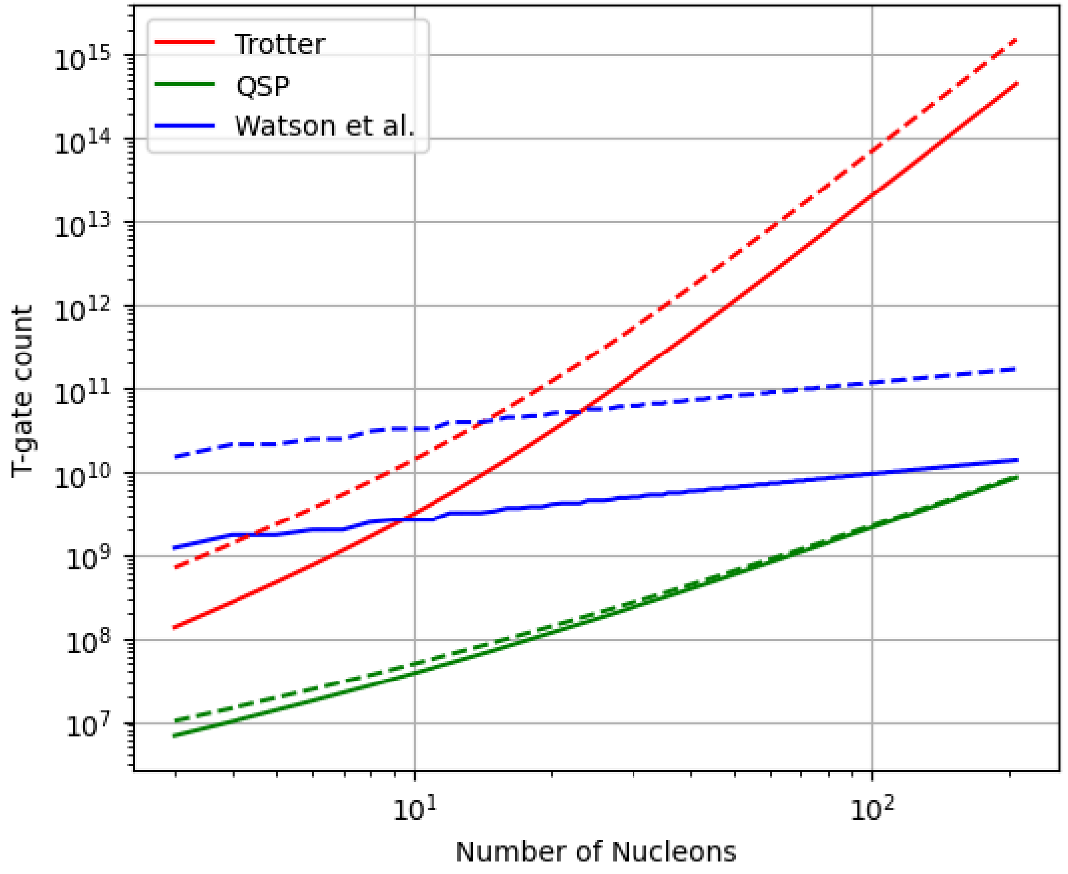
	qubits	trotterization	QSP
First quantization: <u>work in progress</u>	$O(\eta\log(\Omega))$	$\tilde{O}\left(\frac{t^2\eta^4}{\epsilon}\log(\Omega)\right)$	$\tilde{O}\left(\eta\log(\Omega)\left(\eta t+\log\frac{1}{\epsilon}\right)\right)$
Second quantization: <u>arXiv:2312.05344</u>	$O(\Omega)$	$\tilde{O}\left(\frac{t^2\eta}{\epsilon}\Omega\right)$	

$$\epsilon=\{10^{-1},10^{-3}\}$$
$$\Omega=4\cdot 8^3=2048$$





$$\epsilon=\{10^{-1},10^{-3}\}$$
$$\eta=40$$



CONCLUSIONS

$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

	qubits	trotterization	QSP
First quantization: work in progress	$O(\eta \log(\Omega))$	$\tilde{O}\left(\frac{t^2\eta^4}{\epsilon}\log(\Omega)\right)$	$\tilde{O}\left(\eta \log(\Omega)\left(\eta t + \log\frac{1}{\epsilon}\right)\right)$
Second quantization: arXiv:2312.05344	$O(\Omega)$	$\tilde{O}\left(\frac{t^2\eta}{\epsilon}\Omega\right)$	

First quantization is exponentially better in termos of the lattice size, while it is polynomially worst in terms of the number of particles

THANK YOU

NUMBER OF GATES

$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_{T} + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} C\delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j\neq i}^{\eta-1} \sum_{k\neq j\neq i}^{\eta-1} G\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

Trotterization:

$$e^{itH} \approx e^{itT} e^{itV} \quad \rightarrow \quad ||e^{itH} - e^{itT}e^{itV}|| \leq \frac{t^2}{2} ||[T,V]||$$

$$\rightarrow \quad ||e^{i\frac{t}{r}H} - e^{i\frac{t}{r}T}e^{i\frac{t}{r}V}|| \leq \frac{t^2}{2r^2} ||[T,V]||$$

$$\rightarrow \quad ||e^{itH} - \left(e^{i\frac{t}{r}T}e^{i\frac{t}{r}V}\right)^r|| \leq \frac{t^2}{2r} ||[T,V]||$$

NUMBER OF GATES

Trotterization:

$$||e^{itH} - \left(e^{i\frac{t}{r}T} e^{i\frac{t}{r}V}\right)^r|| \leq \frac{t^2}{2r} ||[T, V]||$$

The norm of the commutator scales as the number of particles:

$$||[T, V]|| = O(\eta)$$

Which means that we can bound the error by choosing r as follows:

$$\frac{t^2}{r}\eta \leq \epsilon \;\; \Rightarrow \;\; r = O\left(\frac{t^2\eta}{\epsilon}\right)$$

The total cost will be:

$$r\left(C\left(e^{itT}\right) + C\left(e^{itV}\right)\right) = \widetilde{O}\left(\frac{t^2\eta^4}{\epsilon}\log(V)\right)$$