

**ALESSANDRO  
ROGGERO**



# QUANTUM SIMULATION ALGORITHMS FOR MANY FERMION SYSTEMS IN FIRST QUANTIZATION

**LUCA SPAGNOLI**



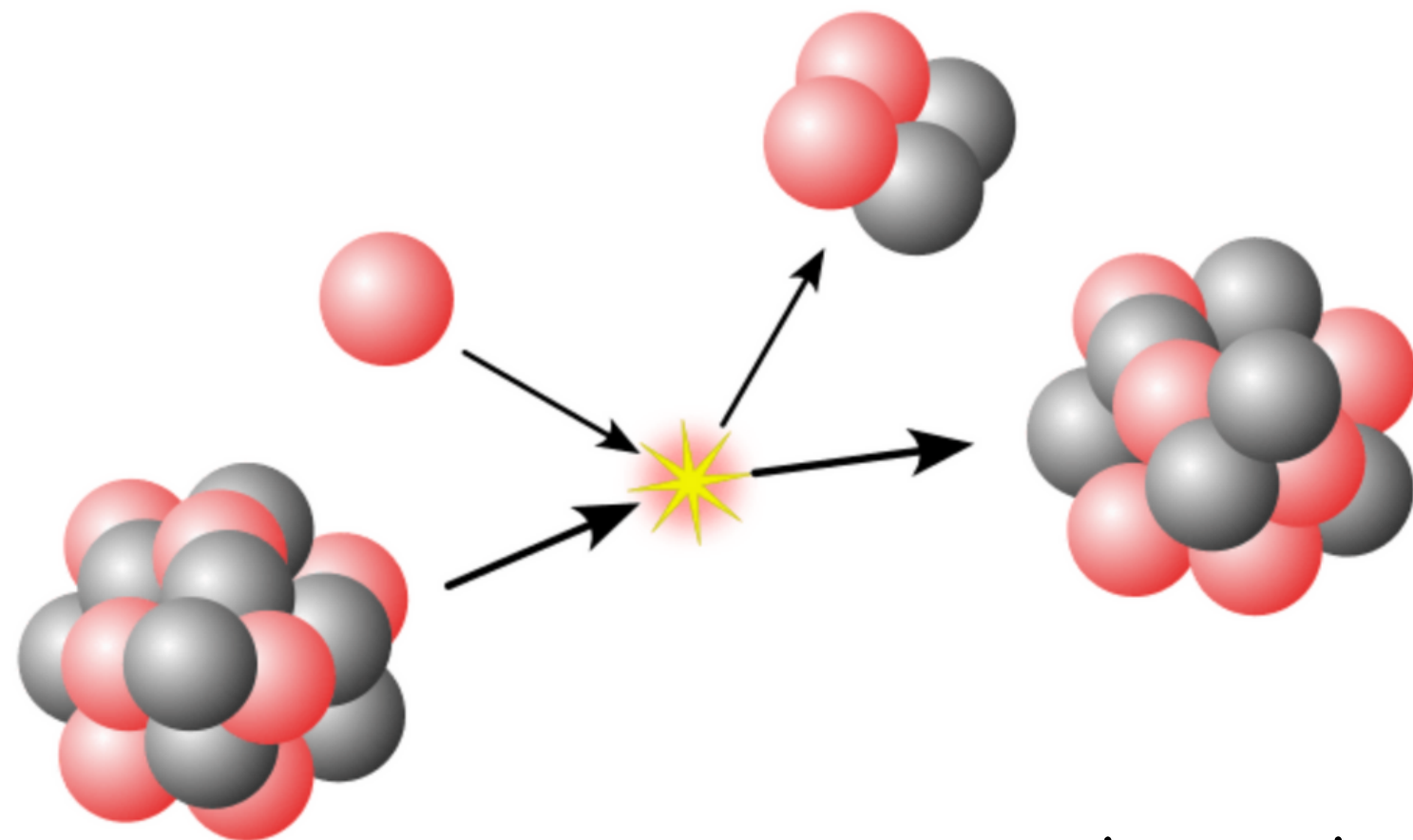
**UNIVERSITY OF TRENTO**



**TIFPA**



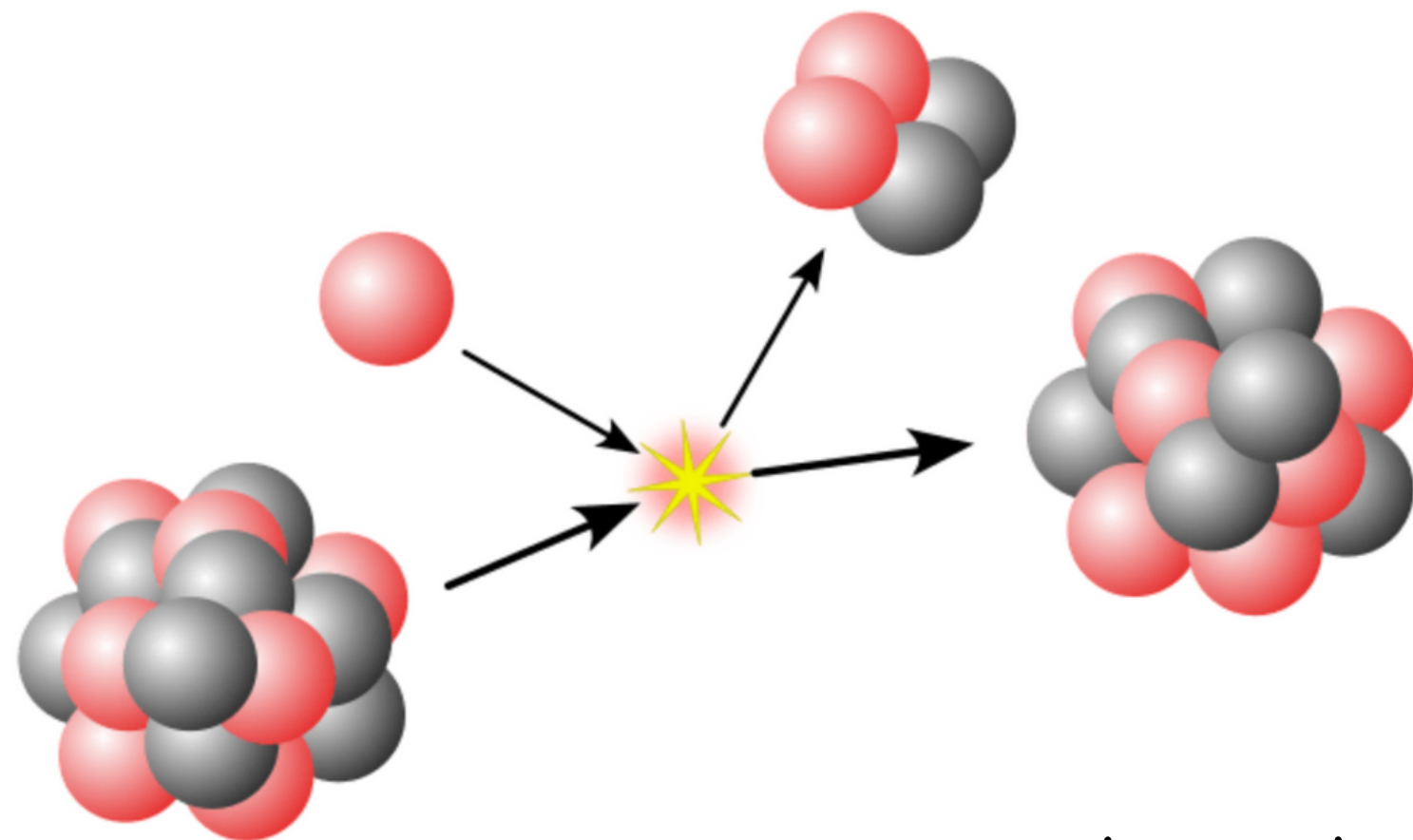
# NUCLEAR PHYSICS



We want to simulate  
scattering processes

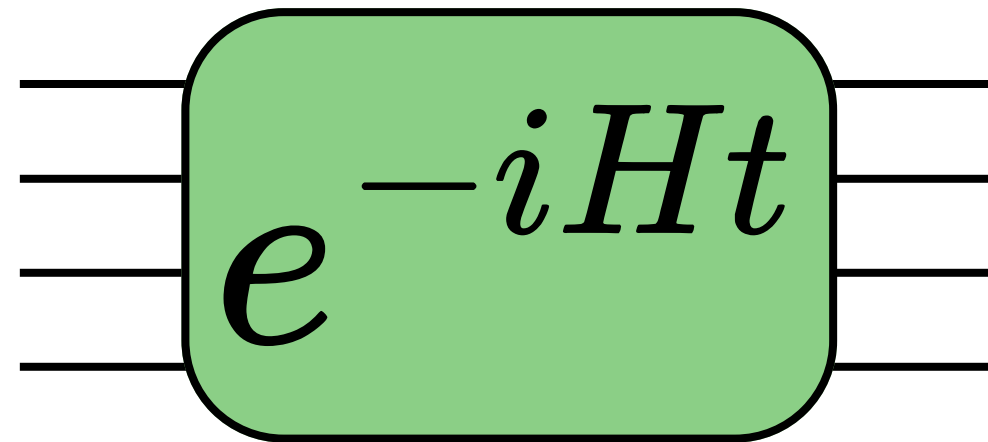
$$|\psi_0\rangle \quad \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \boxed{e^{-iHt}} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} |\psi_f\rangle$$

# NUCLEAR PHYSICS



We want to simulate scattering processes

$|\psi_0\rangle$



$|\psi_f\rangle$

Encoding

Evolution

# IN THIS PRESENTATION

First quantization  
has an advantage  
over second  
quantization

# IN THIS PRESENTATION

## First quantisation

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

First quantization  
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quantization

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

# 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 annihilation 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

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We need a finite  
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number of single  
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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

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

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

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**Trotterization:**

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

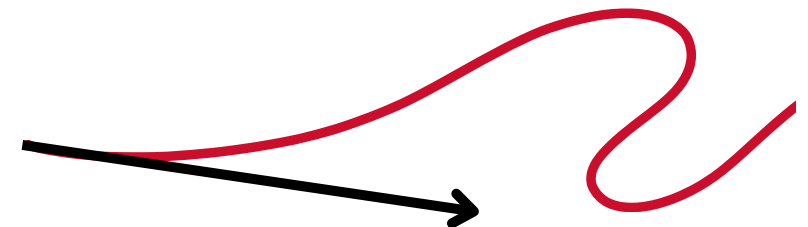
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$$e^{-itH} \approx e^{-i\frac{t}{2}T} e^{-i\frac{t}{2}V} \cdot e^{-i\frac{t}{2}T} e^{-i\frac{t}{2}V} + O\left(\frac{t^2}{2}\right)$$



# TIME EVOLUTION

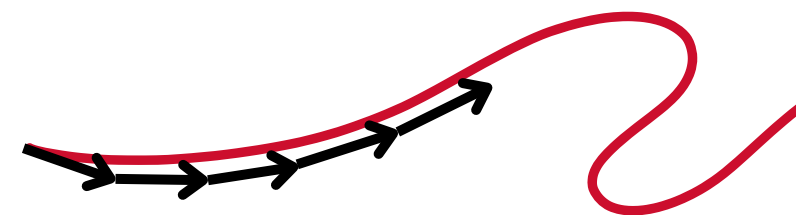
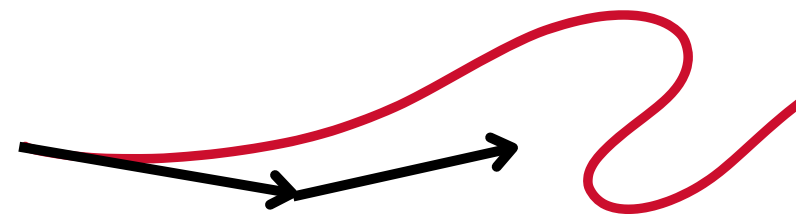
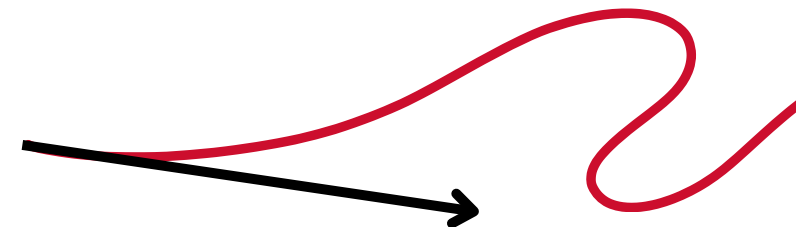
$$H = \underbrace{\sum_{i=0}^{\eta-1} \frac{p_i^2}{2m}}_T + \underbrace{\sum_{i=0}^{\eta-1} \sum_{j \neq i}^{\eta-1} C \delta(\vec{r}_i - \vec{r}_j) + \sum_{i=0}^{\eta-1} \sum_{j \neq i}^{\eta-1} \sum_{k \neq j \neq i}^{\eta-1} G \delta(\vec{r}_i - \vec{r}_j) \delta(\vec{r}_j - \vec{r}_k)}_{V=V_2+V_3}$$

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



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# NUMBER OF GATES

**Trotterization:**

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

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

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

[arXiv:2312.05344](https://arxiv.org/abs/2312.05344)

# COMPARISON

qubits

trotterization

First quantization:  
arXiv: 2507.22814

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

$$\tilde{O}\left(\frac{t^2 \eta^4}{\epsilon} \log(\Omega)\right)$$

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arXiv: 2312.05344

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# COMPARISON

|                                                  | qubits                 | trotterization                                                   | QSP                                                                                     |
|--------------------------------------------------|------------------------|------------------------------------------------------------------|-----------------------------------------------------------------------------------------|
| First quantization:<br><u>arXiv: 2507.22814</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:<br><u>arXiv: 2312.05344</u> | $O(\Omega)$            | $\tilde{O}\left(\frac{t^2 \eta}{\epsilon} \Omega\right)$         |                                                                                         |

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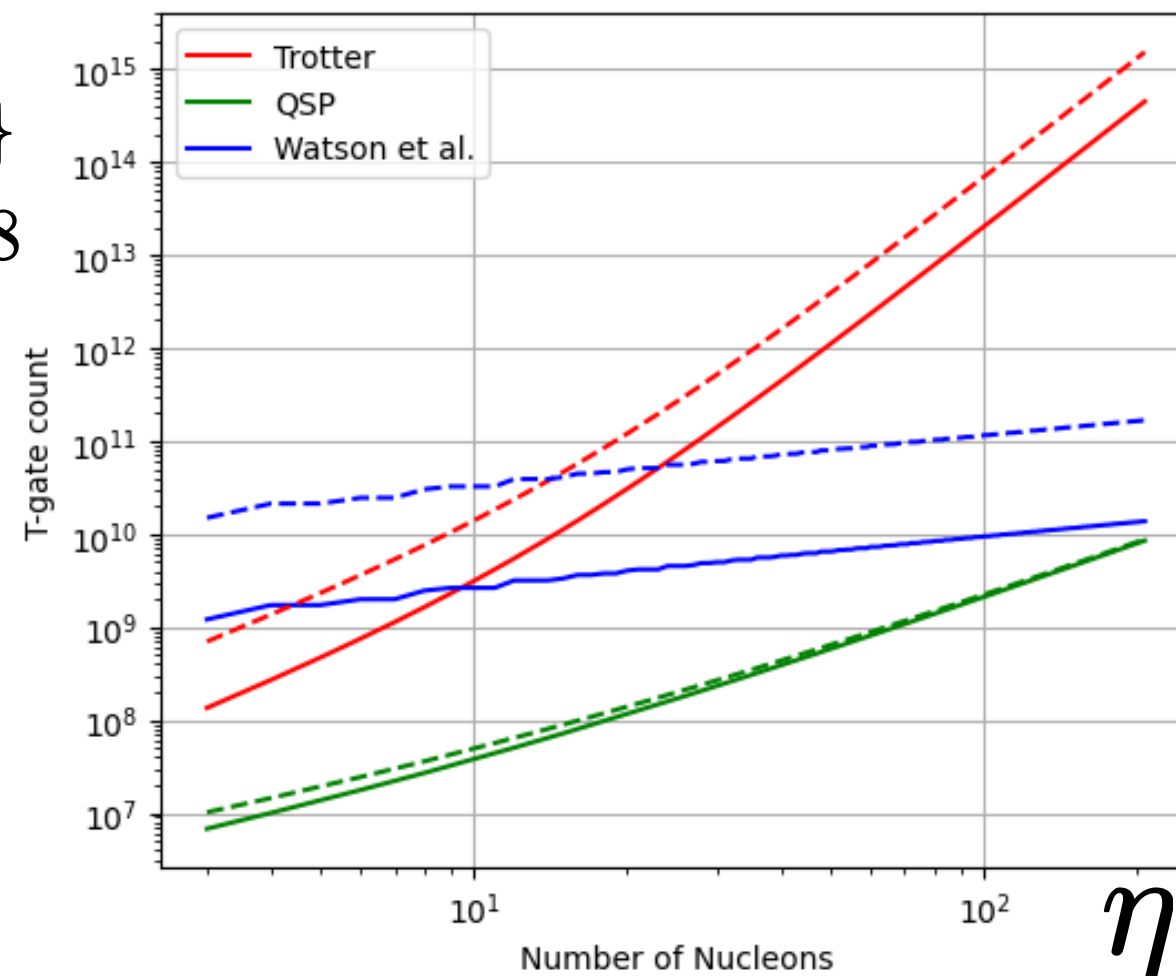
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$$\epsilon = \{10^{-1}, 10^{-3}\}$$

$$\Omega = 4 \cdot 8^3 = 2048$$



# COMPARISON

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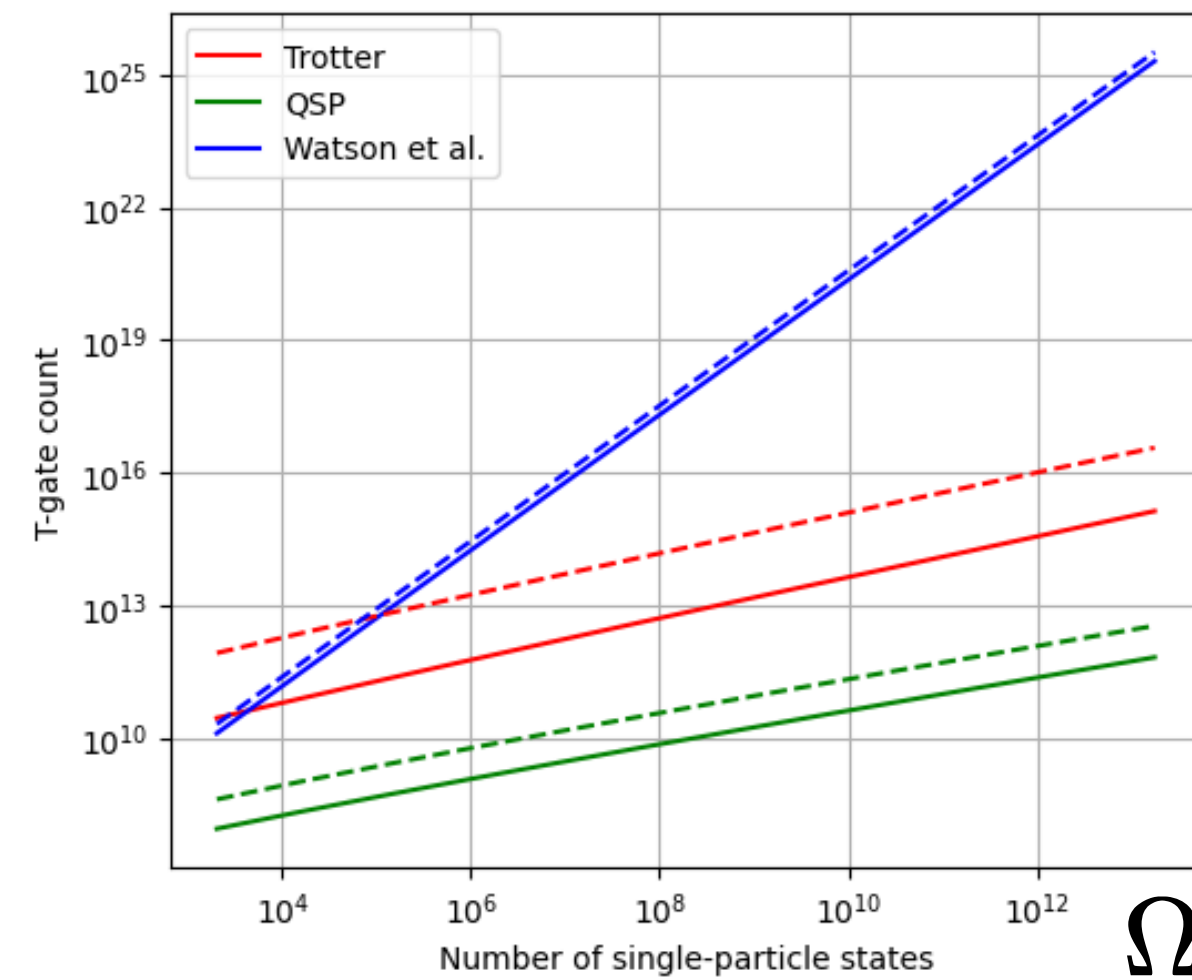
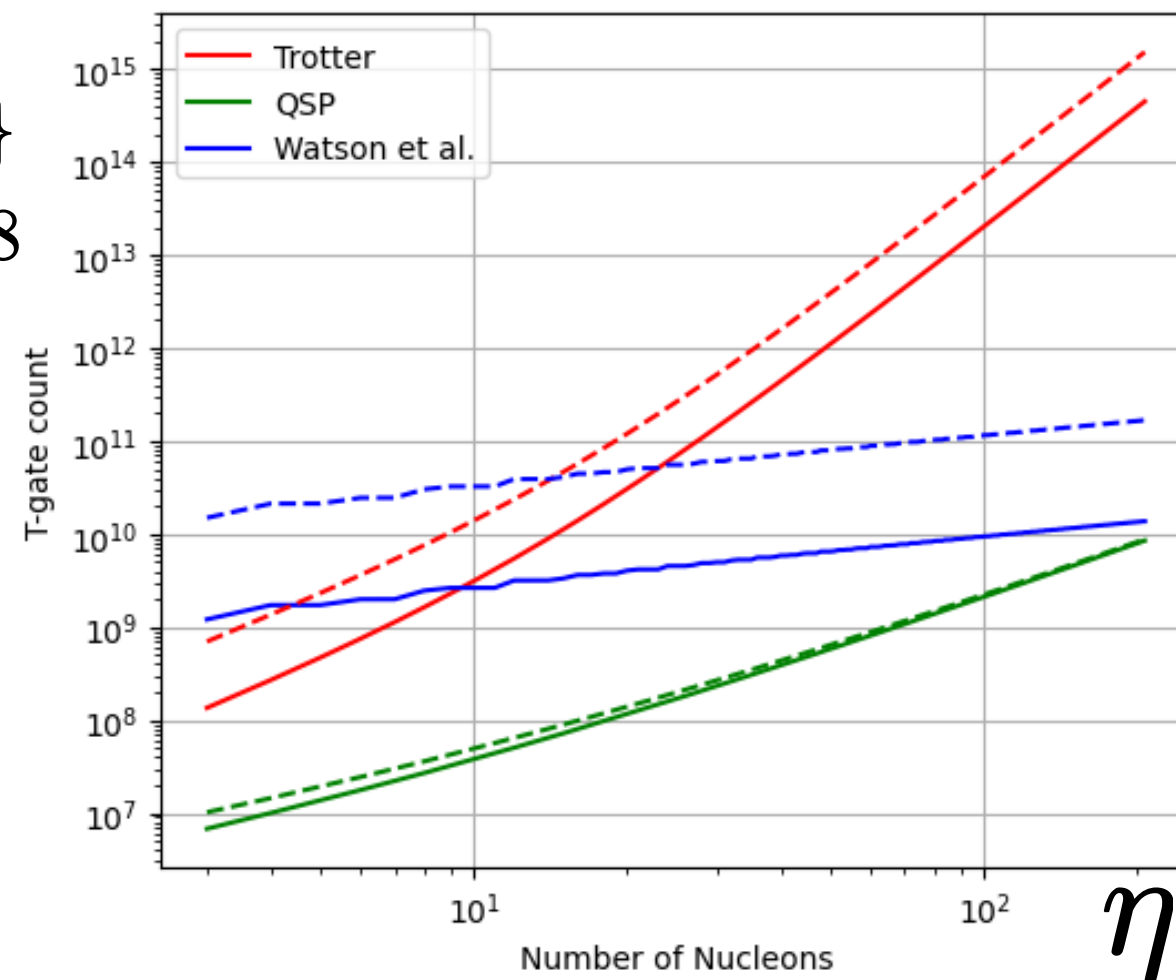
$$O(\eta \log(\Omega)) \quad \tilde{O}\left(\frac{t^2 \eta^4}{\epsilon} \log(\Omega)\right) \quad \tilde{O}\left(\eta \log(\Omega) \left(\eta t + \log \frac{1}{\epsilon}\right)\right)$$

Second quantization:  
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$$O(\Omega) \quad \tilde{O}\left(\frac{t^2 \eta}{\epsilon} \Omega\right)$$

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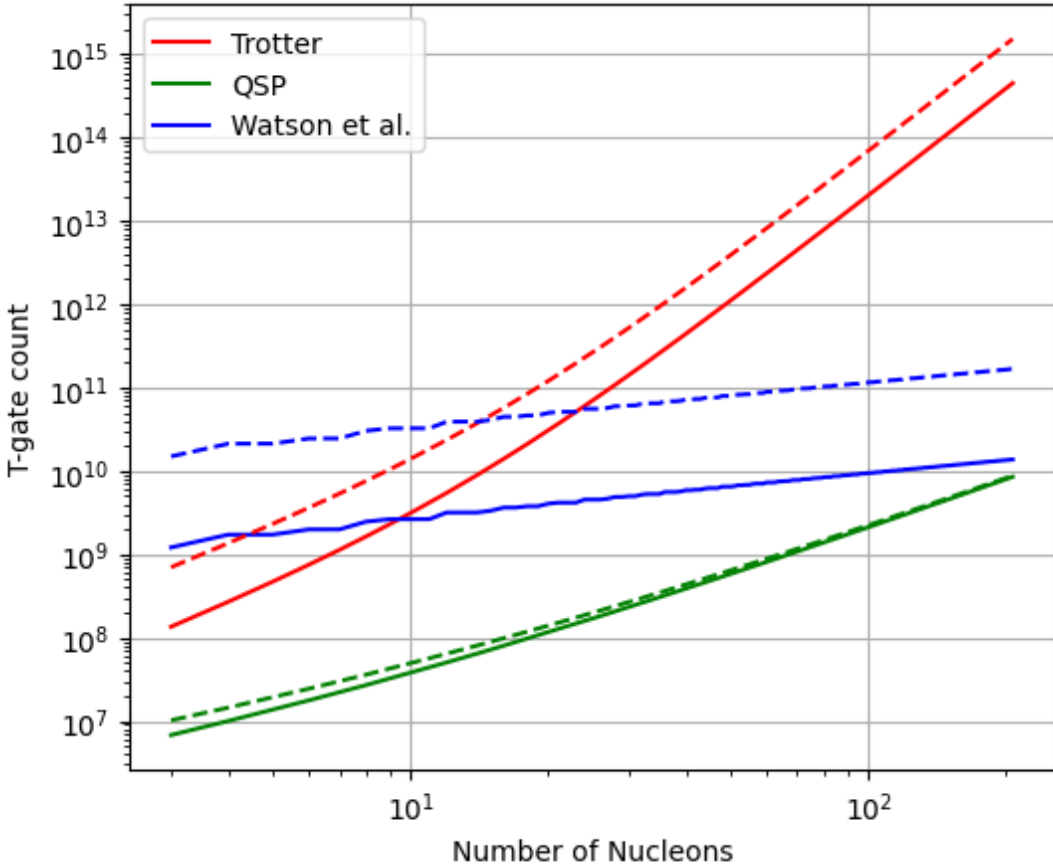


$$\epsilon = \{10^{-1}, 10^{-3}\}$$

$$\eta = 40$$

# CONCLUSIONS

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



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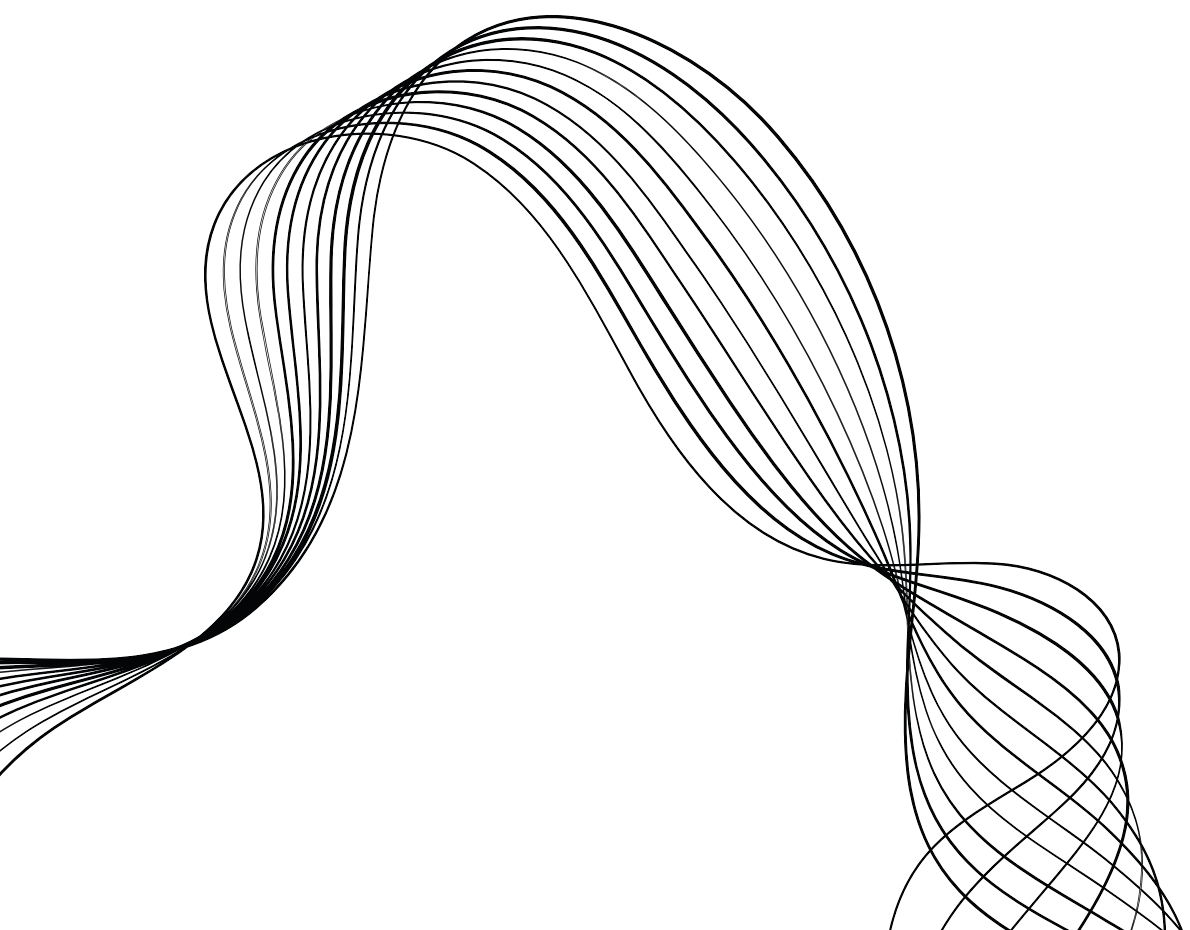
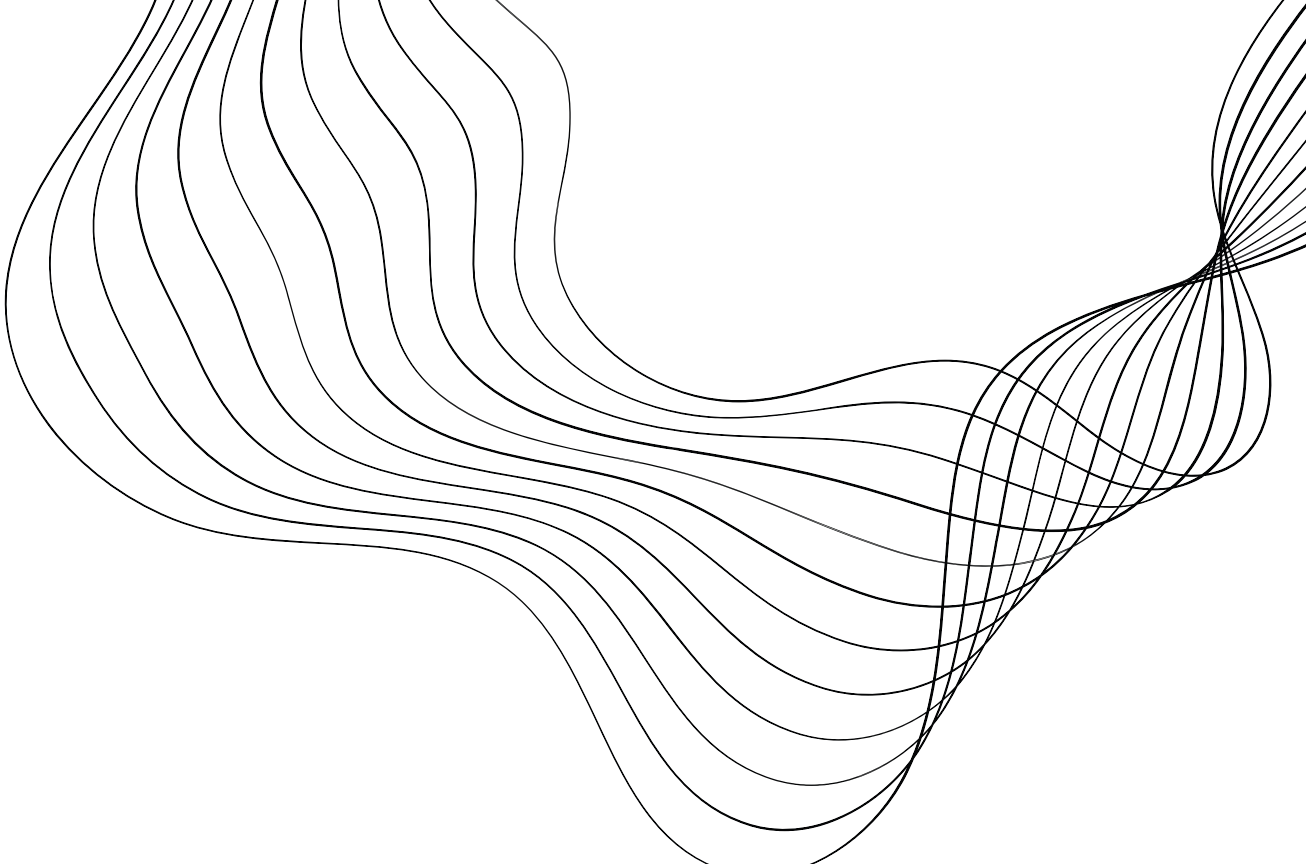
$$\tilde{O}\left(\eta \log(\Omega) \left(\eta t + \log \frac{1}{\epsilon}\right)\right)$$

Second quantization:  
[arXiv: 2312.05344](#)

$$O(\Omega)$$

$$\tilde{O}\left(\frac{t^2 \eta}{\epsilon} \Omega\right)$$

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



**THANK YOU**

# NUMBER OF GATES

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**Trotterization:**

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

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

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

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

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

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

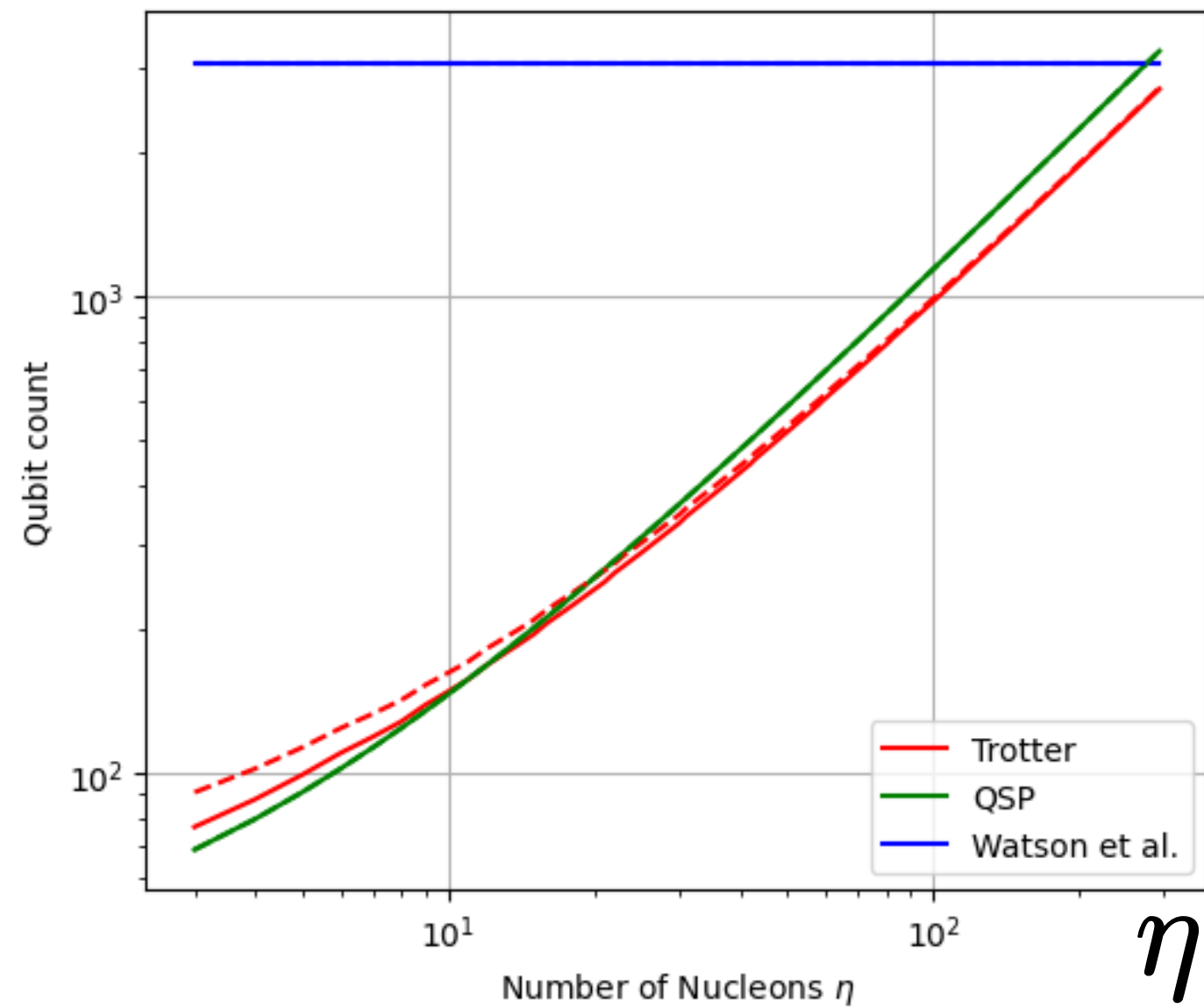
Which means that we can bound the  
error by choosing  $r$  as follows:

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

**The total cost will be:**

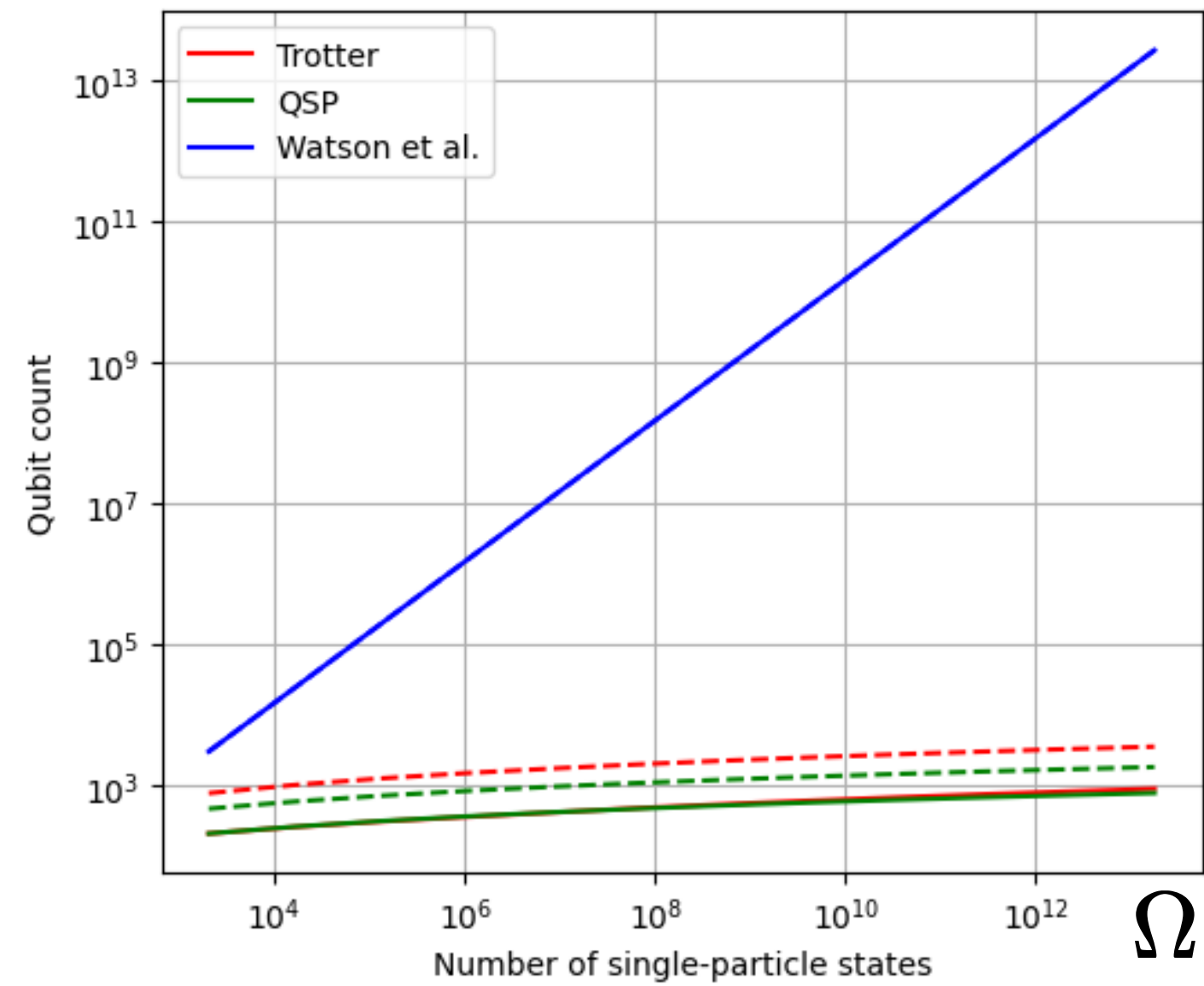
$$r \left( C(e^{itT}) + C(e^{itV}) \right) = \tilde{O}\left(\frac{t^2 \eta^4}{\epsilon} \log(V)\right)$$

# NUMBER OF QUBITS



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