



# Digital quantum computation of fermion-boson interacting systems

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# Motivation

- The fermion-boson interactions are fundamental in nature
  - The Standard Model is a fermion-boson interacting system
  - Examples of fermion-boson interaction:
    - quark-gluon, fermion-Higgs, electron-photon, electron-phonon, atoms-photons
- Quantum simulations of **many-fermion** systems look very promising for **near-future devices**
  - Well developed algorithms are addressing interacting electron models in quantum chemistry and condensed matter
- What about **bosons**?
  - Bosons on qubits?
  - Can the existing fermion algorithms be extended to include bosons?

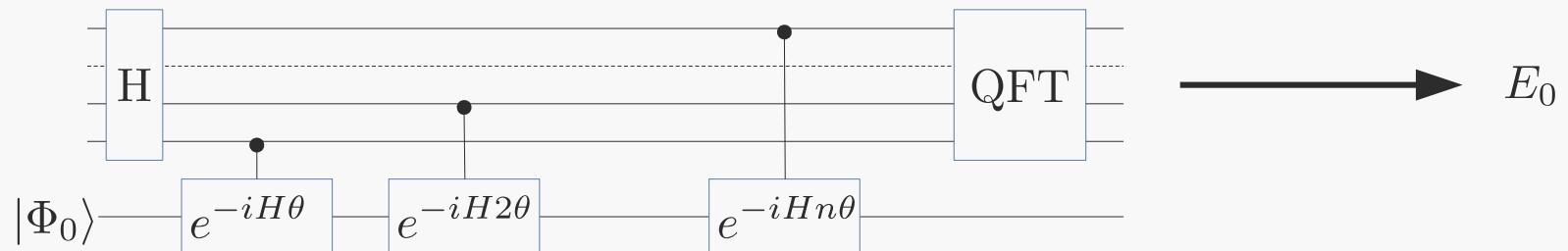
# Quantum simulation

- Represent the system Hilbert space on the qubit space
- Implement a circuit to simulate the time evolution

$$|\Phi(t)\rangle = e^{-iHt}|\Phi_0\rangle$$

- Input state preparation
- Measurements

## Example: Quantum phase estimation



$|\Phi_0\rangle$  ground state

$$|\Phi_0(t)\rangle = e^{-iE_0 t}|\Phi_0\rangle$$

# Fermion on qubits

$|\uparrow\rangle \equiv |0\rangle$  unoccupied orbital

$|\downarrow\rangle \equiv |1\rangle$  occupied orbital

$$\{c_i, c_j^\dagger\} = \delta_{ij}$$

$$c_i \longrightarrow \sigma_1^z \dots \sigma_{i-1}^z \sigma_i^+$$

$$c_i^\dagger \longrightarrow \sigma_1^z \dots \sigma_{i-1}^z \sigma_i^-$$

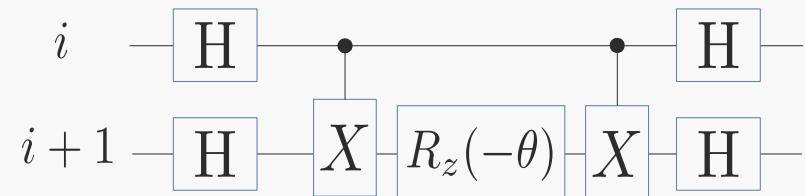
$\sigma$  – Pauli matrices

## Example (circuit for nearest-neighbor hopping):

$$H = c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \longrightarrow \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y$$

$$e^{-i\theta(\sigma_i^x \sigma_{i+1}^x)} = H_i H_{i+1} e^{-i\theta(\sigma_i^z \sigma_{i+1}^z)} H_{i+1} H_i \quad \rightarrow$$

$$H \sigma_x H = \sigma_z$$



$$X \sigma_z X = -\sigma_z$$



# Quantum simulation of bosons

## Bosons from parafermions

L.-A. Wu, D.A. Lidar, J. Math. Phys 43, 4506 (2002)

$$[\sigma_i^\pm, \sigma_j^\pm]_{i \neq j} = 0$$

$$\{\sigma_i^-, \sigma_i^+\} = 1$$

$$B^\dagger = \frac{1}{\sqrt{N}} \sum_{i=1}^N \sigma_i^+ \quad N \text{ qubits for one boson state}$$

$$[B, B^\dagger] = 1 - \frac{n}{N} \quad n \text{ - number of bosons occupying the state}$$

## $\phi^4$ - quantum field theory

S. Jordan, et al., Science, 336, 1130 (2012)

- field on a lattice
- the field amplitude is discretized at every lattice site

## Fermion-boson interaction in trapped ions devices

J. Casanova, et al, PRL 108, 190502, (2012)



qubits + ions vibrations



# Fermion-boson interaction

$$H_{fb} = \sum_{ijn} g_{ijn} (c_i^\dagger c_j + c_i^\dagger c_j)(b_n^\dagger + b_n) \equiv \sum_{ijn} F_{ij} (b_n^\dagger + b_n)$$

$$|\Psi\rangle = \sum c_{ij} |\tilde{i}, \tilde{j}\rangle \otimes |\phi\rangle \quad \text{arbitrary state}$$

$|\tilde{i}, \tilde{j}\rangle$  basis of the fermion space which diagonalize  $F_{ij}$ ,  $F_{ij}|\tilde{i}, \tilde{j}\rangle = f_{ij}|\tilde{i}, \tilde{j}\rangle$   
 $|\phi\rangle$  boson state

$$e^{-i\theta H_{fb}} |\tilde{i}, \tilde{j}\rangle \otimes |\phi\rangle = |\tilde{i}, \tilde{j}\rangle \otimes e^{-i\theta f_{ij}(b_n^\dagger + b_n)} |\phi\rangle = |\tilde{i}, \tilde{j}\rangle \otimes D(-i\theta f_{ij}) |\phi\rangle$$

$$D(z) = e^{zb^\dagger - z^* b} \quad \text{displacement operator}$$

At every Trotter step a **displacement** operator acts on boson states



# Fermion-boson interaction

At every Trotter step a *displacement* operator acts on boson states

- Boson representation on qubits:

- Efficient cutoff of the boson space

- Efficient implementation of the non-interacting boson term  $H_b = \sum \omega b_n^\dagger b_n$

- Efficient implementation of the *displacement* operator

- How about the boson occupation number basis?

$$|n\rangle = 1/\sqrt{n!}(b^\dagger)^n |0\rangle$$

number of boson qubits per site  $n_b = \log(N_{cutoff})$

the boson Hamiltonian is diagonal in this basis

the *displacement*  $D(z)|n\rangle$  is difficult to implement

$$D(z)|0\rangle = e^{-|z|^2/2} \sum_n \frac{z^n}{\sqrt{n!}} |n\rangle \quad \text{Poisson distribution}$$



# Coordinate basis representation

Boson and harmonic oscillator algebra are equivalent

$$X = 1/\sqrt{2\omega}(b^\dagger + b)$$

$$P = i\sqrt{\omega/2}(b^\dagger - b)$$

$$H_b + H_{fb} = \sum_n \frac{P_n^2}{2} + \omega^2 \frac{X_n^2}{2} + \sum_{ijn} g_{ijn} (c_i^\dagger c_j + c_j^\dagger c_i) X_n$$

$\{|x\rangle\}$  coordinate basis

$$X|x\rangle = x|x\rangle$$

$$D(-i\theta f)|x\rangle = e^{-i\theta f X}|x\rangle = e^{-i\theta f x}|x\rangle$$

the **displacement** operator is diagonal in the coordinate basis

## However

$\{|x\rangle\}$  continuous set, discretization required

$N_x$  points discretization:  $\{|x_i\rangle\}, \quad x_i = i\Delta, \quad i = \overline{-N_x/2, N_x/2 - 1}$

Naive expectation  $\text{error} \propto \frac{1}{N_x}$

Actually, on the  
low-energy subspace

$\text{error} \propto e^{-N_x}$  !

# Fermion-boson model

$$H = H_f + H_b + H_{fb}$$

fermion  
*(second quantized)*

$$H_f = \sum_{ij} t_{ij} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_{ijkl} U_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

boson  
*(first quantized)*

$$H_b = \sum_{n\nu} \frac{P_{n\nu}^2}{2M_\nu} + \frac{1}{2} M_\nu \omega_{i\nu}^2 X_{n\nu}^2 + \sum_{n\nu m\mu} K_{n\nu m\mu} X_{i\nu} X_{j\mu}$$

fermion-boson

$$H_{fb} = \sum_{ijn\nu} g_{ijn\nu} (c_i^\dagger c_j + c_j^\dagger c_i) X_{n\nu}$$

Bosons are described by a set of harmonic oscillators

$$[X_{n\nu}, P_{m\mu}] = i\delta_{nm}\delta_{\nu\mu}$$

# Harmonic oscillator

$$H_h = \frac{P^2}{2} + \frac{X^2}{2}$$

$$E_n = n + 1/2$$

$$|\phi_n\rangle = \int \phi_n(x)|x\rangle dx = \int \hat{\phi}_n(p)|p\rangle dp$$

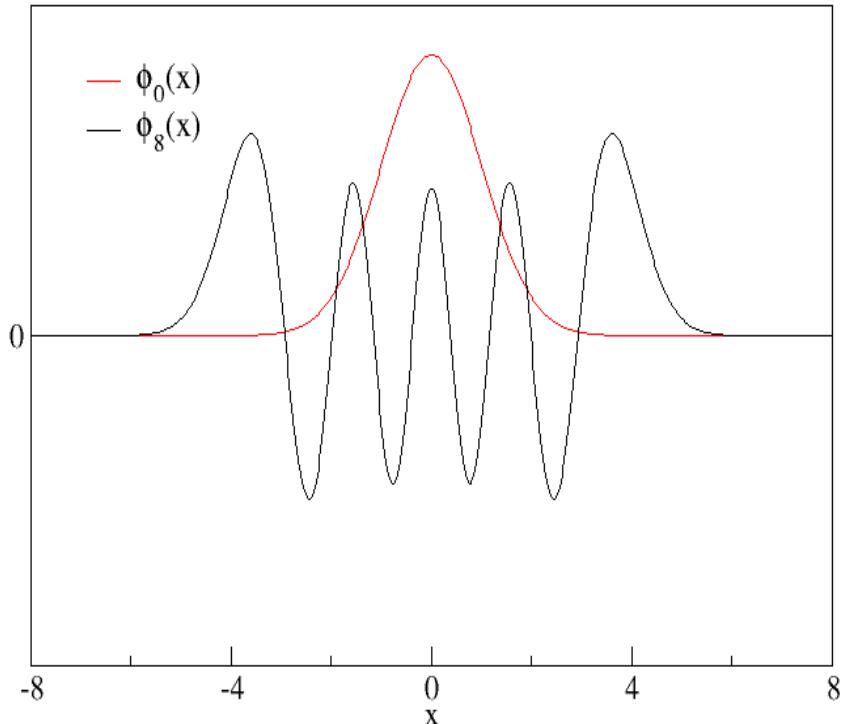
## Hermite-Gauss functions

$$\phi_n(x) = e^{-\frac{x^2}{2}} H_n(x)$$

$\hat{\phi}_n(p) = (-i)^n \phi_n(p)$  eigenfunctions of the Fourier Transform operator

$$x\phi_n(x) = \frac{1}{\sqrt{2}}[\sqrt{n+1}\phi_{n+1}(x) + \sqrt{n}\phi_{n-1}(x)]$$

$$p\hat{\phi}_n(p) = \frac{i}{\sqrt{2}}[\sqrt{n+1}\hat{\phi}_{n+1}(p) - \sqrt{n}\hat{\phi}_{n-1}(p)]$$

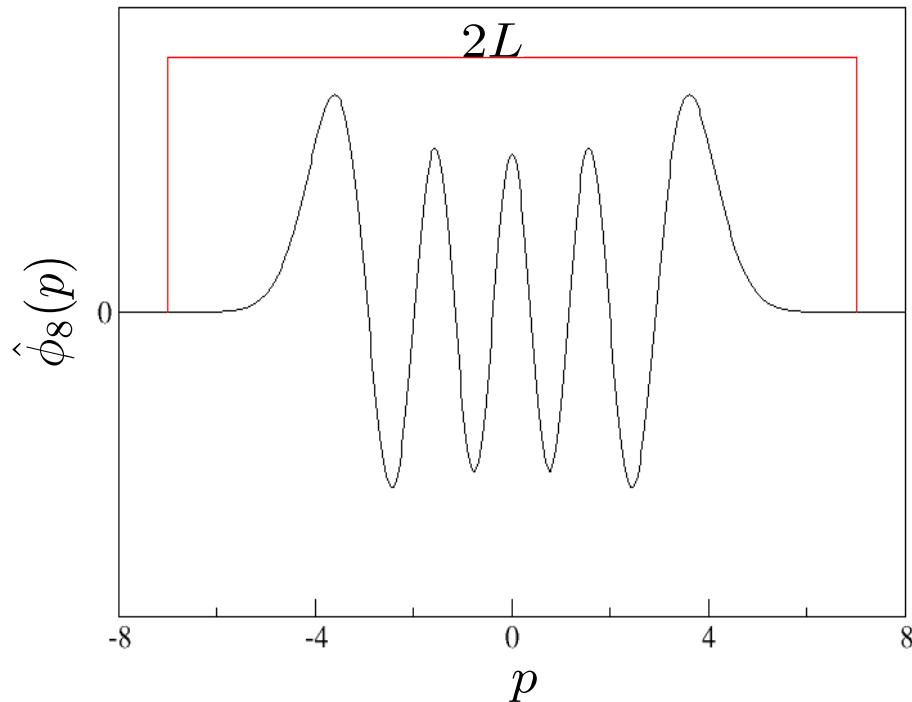


$$X = 1/\sqrt{2}(b^\dagger + b)$$

$$P = i/\sqrt{2}(b^\dagger - b)$$

$$[X, P] = i$$

# Properties of Hermite-Gaussian functions



$$\hat{\phi}(p) = \hat{\phi}_{per}(p)R(p) + \epsilon$$

$$\hat{\phi}_{per}(p) = \hat{\phi}_{per}(p + 2L)$$

$$R(p) = \begin{cases} 1, & |p| \leq L \\ 0, & |p| > L \end{cases}$$

Nyquist-Shannon sampling theorem

$$x_i = i \frac{\pi}{L} = i\Delta$$

$$\phi(x) = \sum_{i=-N_x/2}^{N_x/2-1} \phi(x_i) u(x - x_i) + \epsilon$$

The HG functions can be sampled with exponentially precision to a finite set of points

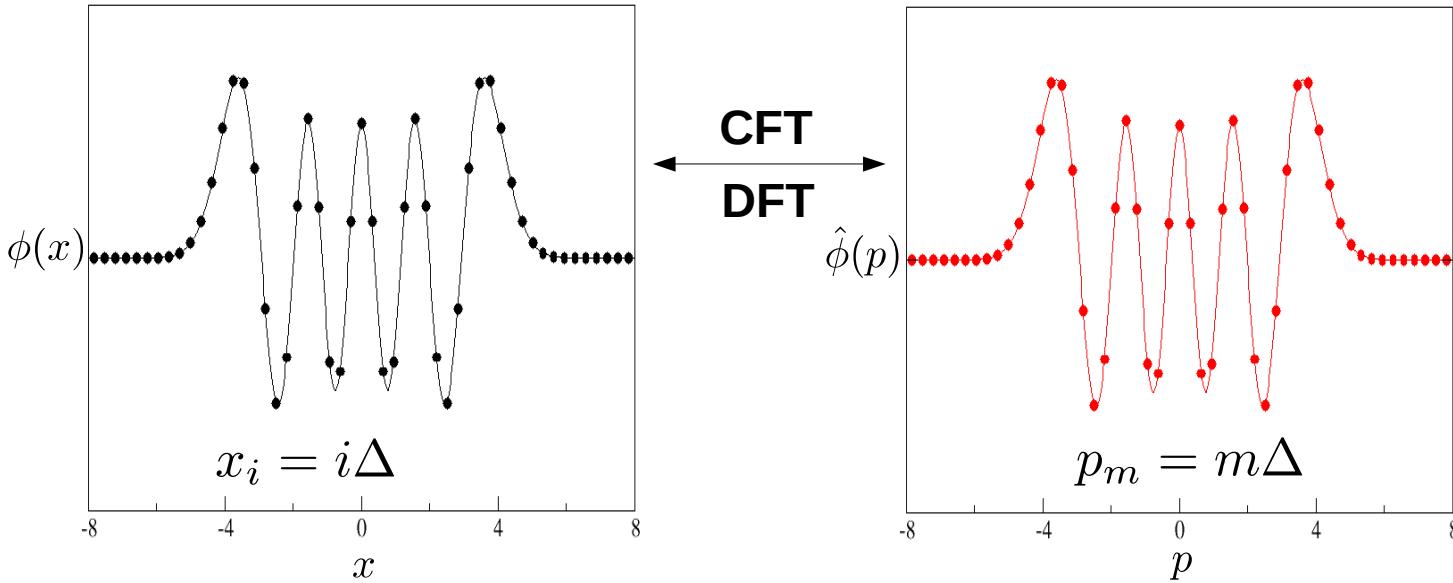
The grid of  $N_x$  points should be large enough to cover the width  $2L$

$$2L = \sqrt{2\pi N_x}$$

$$\Delta = \sqrt{2\pi/N_x}$$

# Fourier transform of the HG functions

$$\hat{\phi}(p_m) = \sum_{i=N_x/2}^{N_x/2-1} \phi(x_i) e^{-i2\pi im/N_x} \quad \text{discrete FT}$$



$$x_i \phi_n(x_i) = \frac{1}{\sqrt{2}} [\sqrt{n+1} \phi_{n+1}(x_i) + \sqrt{n} \phi_{n-1}(x_i)]$$

$$p_m \hat{\phi}_n(p_m) = \frac{i}{\sqrt{2}} [\sqrt{n+1} \hat{\phi}_{n+1}(p_m) - \sqrt{n} \hat{\phi}_{n-1}(p_m)]$$

On the grid points the **discrete Fourier transform (DFT)** replaces with exponential precision the **continuous Fourier transform (CFT)**

# Finite representation of the harmonic oscillator space

- Define a size  $N_x$  Hilbert space spanned by  $\{|x_i\rangle\}$  vectors

- Define the operators  $\tilde{X}|x_i\rangle = x_i|x_i\rangle$ ,  $x_i = i\Delta$

$$\tilde{P}|p_m\rangle = p_m|p_m\rangle, p_m = m\Delta$$

where  $|p_m\rangle = \sum_{i=-N_x/2}^{N_x/2-1} |x_i\rangle e^{i2\pi im/N_x}$

- Define the orthonormal vectors  $|\tilde{\phi}_n\rangle = \sum_i \phi_n(x_i)|x_i\rangle$

- There is a cutoff  $N_c < N_x$  such that for  $n < N_c$  one has

$$\begin{aligned}\tilde{P}|\tilde{\phi}_n\rangle &= \frac{i}{\sqrt{2}} \left( \sqrt{n+1}|\tilde{\phi}_{n+1}\rangle - \sqrt{n}|\tilde{\phi}_{n-1}\rangle \right) \\ \tilde{X}|\tilde{\phi}_n\rangle &= \frac{1}{i}\sqrt{2} \left( \sqrt{n+1}|\tilde{\phi}_{n+1}\rangle + \sqrt{n}|\tilde{\phi}_{n-1}\rangle \right)\end{aligned}\qquad\qquad\qquad \xrightarrow{\hspace{1cm}} \qquad [ \tilde{X}, \tilde{P} ] = i$$

## Harmonic Oscillator

$$H = \frac{P^2}{2} + \frac{1}{2}\omega^2 X^2$$

$$E_n = \omega \left( n + \frac{1}{2} \right)$$

$$[X, P] = i$$



$\cong$

*Isomorphism on the  
low-energy subspace*

## Discrete Harmonic Oscillator

$$\tilde{H} = \frac{\tilde{P}^2}{2} + \frac{1}{2}\omega^2 \tilde{X}^2$$

—  $N$  finite size space

—  $N_c$  low-energy cutoff

$$[\tilde{X}, \tilde{P}] \approx i$$

$$\epsilon < 10e^{-(0.51N - 0.76N_c)} \\ n_{\text{boson qubits}} = O(\log(\log \epsilon^{-1}))$$

A. Macridin, P. Spentzouris, J. Amundson, R. Harnik, Phys. Rev. Lett. 121, 110504, 2018

A. Macridin, P. Spentzouris, J. Amundson, R. Harnik, Phys. Rev. A 98, 042312, 2018



# Algorithm implementation

fermion

$$H_f = \sum_{ij} t_{ij} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_{ijkl} U_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

boson

$$H_b = \sum_{n\nu} \frac{P_{n\nu}^2}{2M_\nu} + \frac{1}{2} M_\nu \omega_{i\nu}^2 X_{n\nu}^2 + \sum_{n\nu m\mu} K_{n\nu m\mu} X_{i\nu} X_{j\mu}$$

fermion-boson

$$H_{fb} = \sum_{ijn\nu} g_{ijn\nu} (c_i^\dagger c_j + c_j^\dagger c_i) X_{n\nu}$$

I will show circuits for the evolution operators  $e^{-i\theta X^2}$ ,  $e^{-i\theta P^2}$ ,  $e^{-i\theta c_i^\dagger c_i X_n}$

## Bosons on qubits

On a quantum computer each harmonic oscillator state is a superposition of  $\{|x\rangle\}$  states stored on  $n_x$  qubits.

$$n_x = \log N_x = \mathcal{O}(\log(\log \epsilon^{-1}))$$

$$|\phi\rangle = \sum_{x=0}^{2^n - 1} a_x |x\rangle$$

$$[0, N_x - 1] \ni x \longrightarrow x - \frac{N_x}{2} \in \left[ -\frac{N_x}{2}, \frac{N_x}{2} - 1 \right] \quad \text{subtract} \quad \frac{N_x}{2} = 2^{n_x - 1}$$

$$\tilde{X}|x\rangle = (x - N_x/2)|x\rangle$$

$$\tilde{P}|p\rangle = [(p + N_x/2) \bmod N_x - N_x/2]|p\rangle$$

# Evolution of the boson term $X^2$

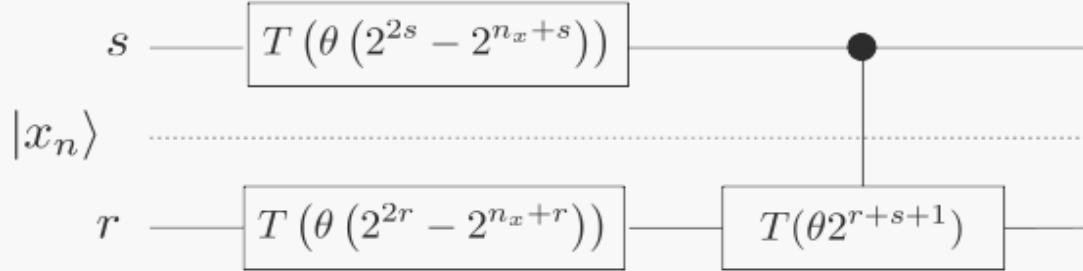
$$e^{-i\theta \tilde{X}_n^2} |x_n\rangle = e^{-i\theta(x_n - N_x/2)^2} |x_n\rangle \quad n\text{- site index here}$$

Write the phase term in the binary form

$$(x_n - N_x/2)^2 = \sum_{r=0}^{n_x-1} x_n^r (2^{2r} - 2^{n_x+r}) + \sum_{r < s} x_n^r x_n^s 2^{r+s+1} + 2^{2n_x-2}$$

$$x_n = \sum_{r=0}^{n_x-1} x_n^r 2^r \quad \{x_n^r\}_{r=\overline{0,n_x-1}} \in \{0, 1\}$$

Circuit for  $|x_n\rangle \rightarrow \exp(i2^{n_x-2}\theta) \exp[-i(x_n - N_x/2)^2\theta] |x_n\rangle$



$$T(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\theta} \end{pmatrix}$$

# Evolution of the boson term $\tilde{P}^2$

Simulation of  $e^{-i\theta \tilde{P}^2} |x\rangle$

$$|x\rangle \xrightarrow{QFT} |p\rangle \quad \text{Quantum Fourier transform circuit}$$

$$e^{-i\theta \tilde{P}^2} |p\rangle = e^{-i\theta p^2} |p\rangle \quad \text{Circuit as for } e^{-i\theta \tilde{X}^2}$$

$$|p\rangle \xrightarrow{QFT}^{-1} |x\rangle \quad \text{Inverse Quantum Fourier transform circuit}$$

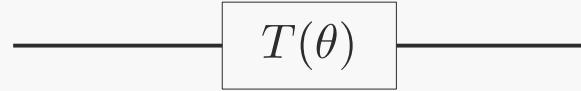
**One can consider**  $\tilde{P}^2 = QFT^{-1} \tilde{X}^2 QFT$

# Evolution of the local fermion-boson interacting term

Consider the fermion term  $H = \sum_i E_i c_i^\dagger c_i$

Jordan Wigner representation  $c_i^\dagger c_i \longrightarrow \frac{1 - \sigma_i^z}{2}$

$$e^{-i\frac{\theta}{2}(1-\sigma_i^z)}|i\rangle = T(\theta)|i\rangle$$

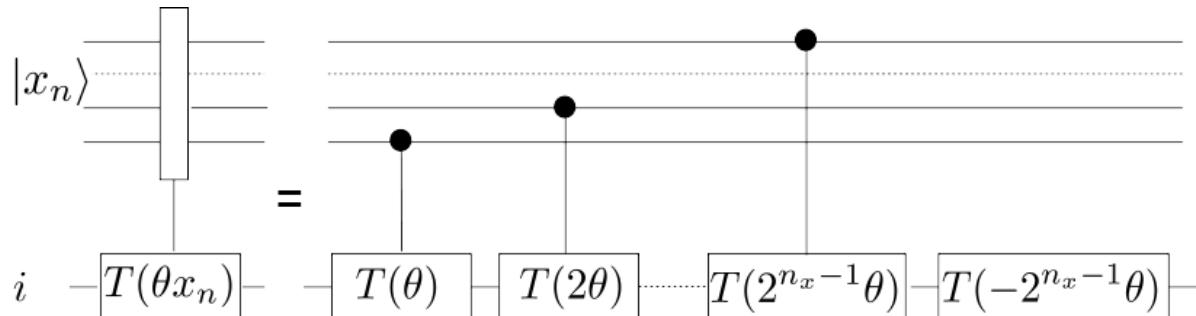


$$T(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\theta} \end{pmatrix}$$

The local fermion-boson interaction term is similar

$$H = \sum_{i,n} g c_i^\dagger c_i X_n$$

$$e^{-i\frac{\theta}{2}(1-\sigma_i^z)X_n} (|i\rangle \otimes |x_n\rangle) = T(\theta x_n)|i\rangle \otimes |x_n\rangle \quad \text{but the phase is proportional to } x_n$$

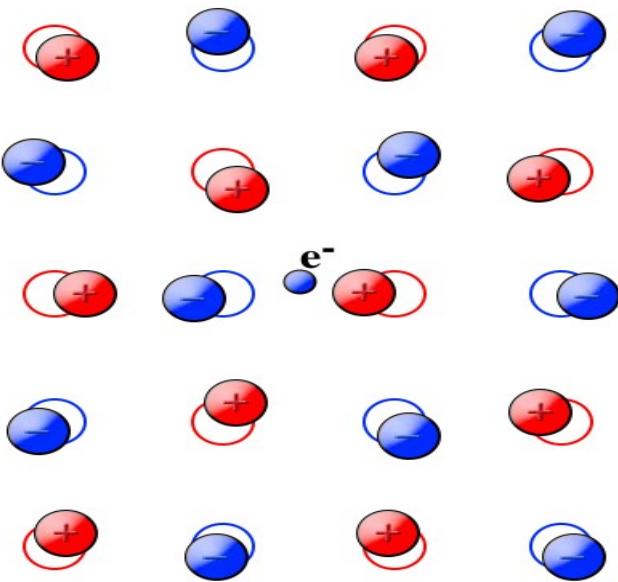


$$x_n = \sum_{r=0}^{n_x-1} x_n^r 2^r$$

$$\{x_n^r\}_{r=\overline{0,n_x-1}} \in \{0, 1\}$$



# Benchmark. Holstein polaron



- **Polaron**

- One electron interacting with the vibration of the crystalline lattice
- Can be seen as an electron dressed by phonons

Figure from Wikipedia

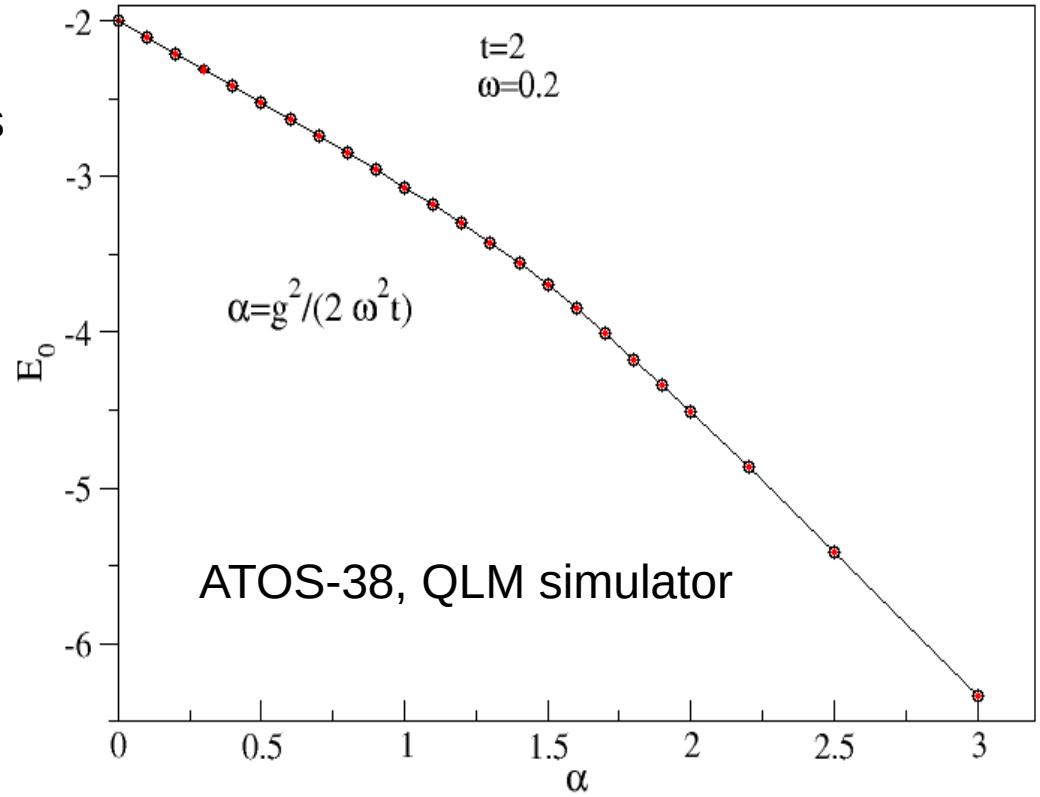
$$H = -t \sum_{ij} (c_i^\dagger c_j + c_j^\dagger c_i) + g \sum_i c_i^\dagger c_i X_i + \sum_i \frac{P_i^2}{2} + \frac{1}{2} \omega^2 X_i^2$$

## 2 site Holstein polaron. Quantum Phase Estimation

$$H = -t \sum_{ij} (c_i^\dagger c_j + c_j^\dagger c_i) + g \sum_i c_i^\dagger c_i X_i + \sum_i \frac{P_i^2}{2} + \frac{1}{2} \omega^2 X_i^2$$

1 electron, 2 harmonic oscillators

2 sites  $N = 2$   
 $n_x = 6$



total number of qubits

$$Nn_x + N + n_{qpe} = 12 + 2 + 6 = 20$$

## 2 site Holstein polaron. Phonon distribution measurement

$$|\Phi\rangle = \sum_{n=0,r} a_{nr}|n, r\rangle \quad \text{ground state}$$

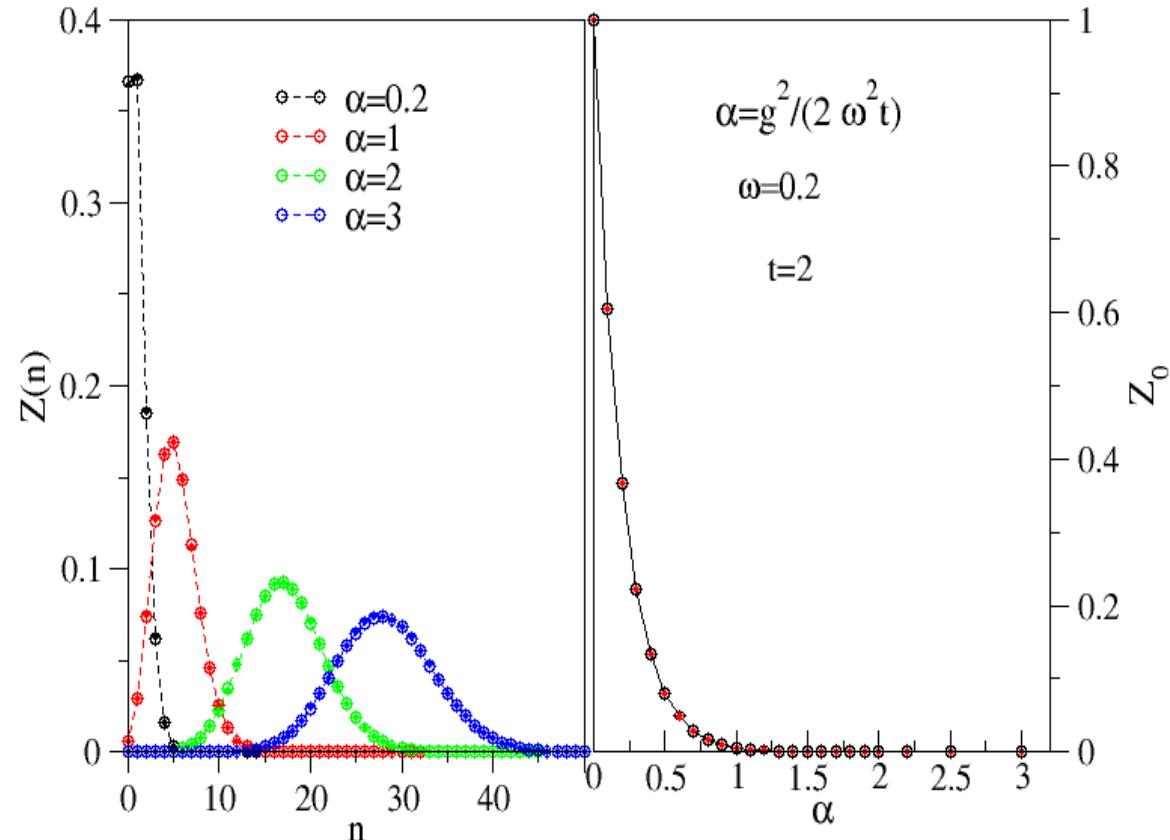
$$Z(n) = \sum_r |a_{nr}|^2 \quad \text{phonon distribution}$$

**QPE for the noninteracting phonon part of the Hamiltonian**

$$H_p = \sum_i \frac{P_i^2}{2} + \frac{1}{2}\omega^2 X_i^2$$

$$H_p|n, r\rangle = E_n|n, r\rangle$$

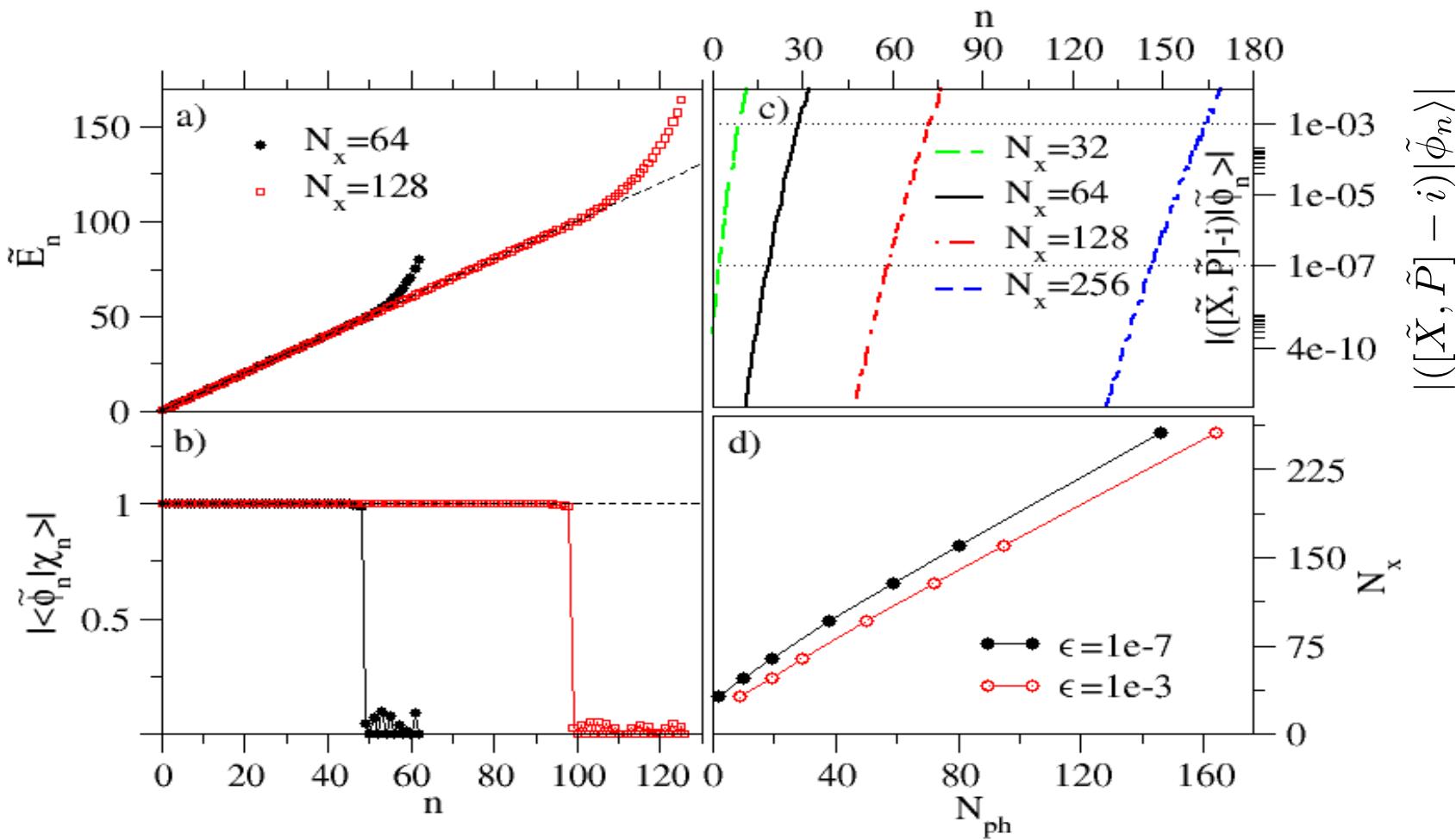
$$e^{-iH_p t}|\Phi\rangle \quad \text{measure} \quad E_n = \omega \left( n + \frac{1}{2} \right) \quad \text{with probability} \quad Z(n)$$



# Summary

- We present a quantum algorithm addressing fermion-boson and boson-boson interacting systems.
- The low-energy space of the boson space can be digitized with exponential precision and mapped on qubit space.
- This representation allows efficient implementation of the Hamiltonian evolution operators.
- We benchmarked the algorithm by implementing it for Holstein polaron on an ATOS quantum simulator. The agreement between the simulation and the exact diagonalization is excellent.

# Numerical results



- (d) The truncated Hilbert space size is proportional to the boson cutoff number

$$N_x \propto N_{ph}$$

# Errors, scaling

$$\epsilon < 10e^{-(0.51N - 0.76N_c)}$$

$$n_{boson \ qubits} = O(\log(\log \epsilon^{-1}))$$

$$n_{boson \ qubits} = O(\log g_{eff})$$

$$n_{boson \ qubits} = O(\log N_E)$$