Simulating Quantum Drude Oscillators on a photonic quantum computer

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I. INTRODUCTION

II. DEFINITION OF THE MODEL

The Hamiltonian describing a system of N QDOs in 3d is given by:

$$H = \sum_{i=1}^{N}\left[\frac{\vec{p}_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2\vec{x}_i^2\right] + \sum_{i<j}V_{\text{Coul}}\left(\vec{x}_i,\vec{x}_j\right), \quad (1)$$

with the Coulomb interaction receiving contributions from every pair of constituents (centers and point particles):

$$\frac{V_{\text{Coul}}\left(\vec{x}_i,\vec{x}_j\right)}{q_iq_j(4\pi\epsilon_0)^{-1}} = \frac{1}{r} - \frac{1}{|\vec{r}+\vec{x}_i|} - \frac{1}{|\vec{r}-\vec{x}_j|} + \frac{1}{|\vec{r}-\vec{x}_j+\vec{x}_i|}$$

In the multipolar expansion, this can be expressed as a power series in the inverse distance separating the two centers:

$$V_{\text{Coul}}\left(\vec{x}_i,\vec{x}_j\right) = \sum_{n\geq 0}V_n\left(\vec{x}_i,\vec{x}_j\right),$$

with the following scaling behavior in terms of the distance between the centers:

$$V_n\left(\vec{x}_i,\vec{x}_j\right) \propto r_{ij}^{-n-3}.$$

We consider the one dimensional system in which the electrons are constrained to move either in the direction parallel to the axis separating the two nuclei, or perpendicular to the latter.

$$V_0(x_i,x_j) = \frac{q_iq_j}{4\pi\epsilon_0}\frac{x_ix_j}{r_{ij}^3} \times \begin{cases} -2, & \text{parallel case} \\ 1, & \text{perpendicular case} \end{cases} \quad (2)$$

We define

$$\gamma_{ij} := \frac{q_iq_j}{4\pi\epsilon_0 r_{ij}^3} \times \begin{cases} -2, & \text{parallel case} \\ 1, & \text{perpendicular case} \end{cases} \quad (3)$$

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We therefore reach the following one dimensional model for N QDOs in the dipolar approximation:

$$\begin{aligned}H &= \sum_{i=1}^{N}\left(\frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2x_i^2\right) + \sum_{i<j}\gamma_{ij}x_ix_j \\ &= \sum_{i=1}^{N}\hbar\omega_i\left(a_i^\dagger a_i + \frac{1}{2}\right) + \sum_{i<j}\gamma_{ij}x_ix_j \\ &= \sum_{i=1}^{N}\hbar\omega_i\left(a_i^\dagger a_i + \frac{1}{2}\right) + \frac{\hbar}{2}\sum_{i<j}\frac{\gamma_{ij}}{\sqrt{m_im_j\omega_i\omega_j}}\left(a_i + a_i^\dagger\right)\left(a_j + a_j^\dagger\right)\end{aligned} \quad (4)$$

with the annihilation and creation operators:

$$\begin{aligned}a_i &= \sqrt{\frac{m_i\omega_i}{2\hbar}}\,x_i + \frac{i}{\sqrt{2\hbar m_i\omega_i}}\,p_i, \\ a_i^\dagger &= \sqrt{\frac{m_i\omega_i}{2\hbar}}\,x_i - \frac{i}{\sqrt{2\hbar m_i\omega_i}}\,p_i.\end{aligned} \quad (5)$$

Just in case, let me write down the next terms in the multipolar expansion:

$$V_1(x_i,x_j) = \frac{q_iq_j}{4\pi\epsilon_0}\frac{x_ix_j(x_i-x_j)}{r_{ij}^4} \times \begin{cases} 3, & \text{parallel case} \\ 0, & \text{perpendicular case} \end{cases} \quad (6)$$

$$V_2(x_i,x_j) = \frac{q_iq_j}{4\pi\epsilon_0}\frac{x_ix_j(2x_i^2-3x_ix_j+2x_j^2)}{r_{ij}^5} \times \begin{cases} -2, & \text{parallel case} \\ -\frac{3}{4}, & \text{perpendicular case} \end{cases} \quad (7)$$

even though we will probably focus on the dipolar approximation.

For simplicity in the following, we will perform the following simplifications:

- All the masses are equal to a common value m, that we set equal to 1.

- All the frequences are equal to a common value ω, that we set equal to 1.

- All the charges are equal to a common value q, that we set equal to 1.

- We also set $\hbar = 1$ and $\frac{1}{4\pi\epsilon_0} = 1$.

The model therefore reads:

$$H = \sum_{i=1}^{N} \left(a_i^\dagger a_i + \frac{1}{2} \right) + \frac{1}{2} \sum_{i<j} \gamma_{ij} \left(a_i + a_i^\dagger \right) \left(a_j + a_j^\dagger \right).$$

(8)

In the case of two QDOs we have:

$$H = a_1^\dagger a_1 + a_2^\dagger a_2 + \frac{\gamma}{2} \left(a_1 + a_1^\dagger \right) \left(a_2 + a_2^\dagger \right) + 1, \quad (9)$$

with

$$\gamma := \frac{1}{r^3} \times \begin{cases} -2, & \text{parallel case} \\ 1, & \text{perpendicular case} \end{cases} \quad (10)$$

where r is the distance between the two nuclei.

III. PHOTONIC CIRCUIT

The circuit implements a unitary $U(\theta)$ acting on an input reference state (the Fock vacuum for instance) that we simply take to be the vacuum state $|0\rangle$. The state prepared by the circuit is therefore given by

$$|\psi(\theta)\rangle = U(\theta)|0\rangle. \quad (11)$$

Since we are working in the dipolar approximation, we expect that using a Gaussian state would be enough. The circuit is therefore composed of at most quadratic optical components (squeezing operations for our ansatz). A non-Gaussian operation can optionally be added in the end of each layer in the ansatz circuit.

IV. VARIATIONAL ALGORITHM

We define the following loss function:

$$\mathcal{C}(\theta) := \langle \psi(\theta) | H | \psi(\theta) \rangle \quad (12)$$

with the Hamiltonian defined in eq. (8). In order to compute this loss, one therefore has to measure both the photon number operator on each channel, as well as the position quadrature operator on each channel.

Algorithm 1: Computation of the energy using photon numbers and quadratures

Parameters: reference statevector $|0\rangle$, circuit U
Result: Value of the energy E

Prepare statevector $|\psi\rangle = U|0\rangle$;
Measure the position quadratures x_i;
Prepare statevector $|\psi\rangle = U|0\rangle$;
Measure the photon numbers n_i;
Compute the energy E with eq. (8);
return E.

Algorithm 2: Computation of the energy using coherent state basis

Parameters: reference statevector $|0\rangle$, circuit U
Result: Value of the energy E

Prepare statevector $|\psi\rangle = U|0\rangle$;
Perform heterodyne measurement on each channel to get α_i;
Compute the energy E with eq. (8);
return E.

Algorithm 3: Computation of the energy using quadratures

Parameters: reference statevector $|0\rangle$, circuit U
Result: Value of the energy E

Prepare statevector $|\psi\rangle = U|0\rangle$;
Perform homodyne measurement on each channel to get the position quadratures x_i;
Prepare statevector $|\psi\rangle = U|0\rangle$;
Perform homodyne measurement on each channel to get the momentum quadratures p_i;
Compute the energy E with eq. (8);
return E.

Questions that should be addressed:

- Are alg. (1) or (3) the best since one needs to prepare the state twice to measure both the position quadratures and the photon numbers. Maybe a single measure in the coherent states basis would be possible? This can be achieved by a heterodyne measurement. With strawbery fields it can only be performed in the Gaussian or Bosonic backends, but not the tensorflow backend...

- What is the role of the parameter M in alg. (4)? Could one safely set $M = 1$ and still hope for convergence, a bit like in reinforcement learning? Setting $M = 1$ is of course a very rough estimate of the expected value, but since it is embedded in the training loop, maybe this estimate is actually enough?

- In strawberryfields the training procedure is man-

Algorithm 4: Computation of the loss

Parameters: $M \in \mathbb{N}$
Result: Value of the loss $\mathcal{C}$

Initialize $\mathcal{C} \leftarrow 0$;
for $j = 1$ *to* M **do**
    Compute the energy E with alg. (1), (2) or (3);
    Update the loss $\mathcal{C} \leftarrow \mathcal{C} + E$;
end for
$\mathcal{C} \leftarrow \mathcal{C}/M$;
return $\mathcal{C}$.

Algorithm 5: Training of the parameterized photonic circuit

Parameters: $N_{\text{steps}} \in \mathbb{N}$, initial parameters $\theta_0 \in \mathbb{R}^K$, learning rate $\eta \in \mathbb{R}_+$
Result: Optimized hyperparameters $\theta \in \mathbb{R}^K$

Initialize hyperparameters $\theta \leftarrow \theta_0$;
for $i = 1$ *to* N_{steps} **do**
    Compute the loss $\mathcal{C}$ with alg. (4);
    Compute the gradient $\nabla_\theta \mathcal{C}$ with shift rule and alg. (4);
    Update the parameters $\theta \leftarrow \theta - \eta \nabla_\theta \mathcal{C}$;
end for
return θ.

After measuring the amplitude α_i on each channel with heterodyne detections, the measured energy reads

$$E = \sum_{i=1}^{N} \left(|\alpha_i|^2 + \frac{1}{2} \right) + 2 \sum_{i<j} \gamma_{ij} \text{Re}(\alpha_i) \text{Re}(\alpha_j) \quad (13)$$

The expected value of the energy in state $|\psi\rangle$ is obtained by averaging the result of $M \in \mathbb{N}$ such measurements:

$$\langle\psi|H|\psi\rangle = \frac{1}{M} \sum_{j=1}^{M} E_j + \mathcal{O}\left(\frac{1}{\sqrt{M}}\right) \quad (14)$$

A very rough estimate would consist in setting $M = 1$.

V. CONCLUSION

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DATA AVAILABILITY

CODE AVAILABILITY

The reader will find an open source python code accompanying this paper following this github repository.

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[2] J. M. Arrazola, T. R. Bromley, J. Izaac, C. R. Myers, K. Brádler, and N. Killoran, "Machine learning method for state preparation and gate synthesis on photonic quantum computers," *Quantum Science and Technology*, vol. 4, no. 2, p. 024004, 2019.