Simulating Quantum Drude Oscillators on a photonic quantum computer

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(Dated: December 12, 2022)

I. INTRODUCTION

II. DEFINITION OF THE MODEL

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

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

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

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

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.

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

We define

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

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

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

with

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

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

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

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

even though we will probably focus on the dipolar approximation.

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

$$|\psi(\theta)\rangle = U(\theta)|0\rangle . \qquad (8)$$

Since we are working in the dipolar approximation, we expect that using a Gaussian state would be enough. The

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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:

$$\mathcal{C}(\theta) := \langle\psi(\theta)|H|\psi(\theta)\rangle \tag{9}$$

with the Hamiltonian defined in eq. (4). 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. (4);
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 $\alpha_i$;
Compute the energy $E$ with eq. (4);
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. (4);
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 $\theta$.
```

aged by the tensorflow backend. Is it actually implementing the shift rule? Double check that.

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

$$E = \sum_{i=1}^{N} \left(|\alpha_i|^2 + \frac{1}{2} \right) + 2 \sum_{i<j} \gamma_{ij} \mathrm{Re}(\alpha_i) \mathrm{Re}(\alpha_j) \qquad (10)$$

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

$$\langle \psi | H | \psi \rangle = \frac{1}{M} \sum_{j=1}^{M} E_j + \mathcal{O}\left(\frac{1}{\sqrt{M}} \right) \qquad (11)$$

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

V. CONCLUSION

ACKNOWLEDGMENTS

DATA AVAILABILITY

CODE AVAILABILITY

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

[1] O. Kiss, F. Tacchino, S. Vallecorsa, and I. Tavernelli, "Quantum neural networks force fields generation," *Machine Learning: Science and Technology*, vol. 3, no. 3, p. 035004, jul 2022. [Online]. Available: https://doi.org/10.1088/2632-2153/ac7d3c