Simulating Quantum Drude Oscillators on a photonic quantum computer

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I. INTRODUCTION

We work in atomic units, for which $m_e = q_e = \hbar = \frac{1}{4\pi\epsilon_0} = 1$.

II. DEFINITION OF THE MODEL

A. Three-dimensional model

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

$$H_{(3,3)} = \sum_{i=1}^{N}\left[\frac{\boldsymbol{p}_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2\boldsymbol{x}_i^2\right] + \sum_{i<j}V_{\text{Coul}}\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right),\tag{1}$$

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

$$\frac{V_{\text{Coul}}\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)}{q_iq_j} = \frac{1}{r_{ij}} - \frac{1}{|\boldsymbol{r}_{ij} + \boldsymbol{x}_i|} - \frac{1}{|\boldsymbol{r}_{ij} - \boldsymbol{x}_j|} + \frac{1}{|\boldsymbol{r}_{ij} - \boldsymbol{x}_j + \boldsymbol{x}_i|}$$

The subscript $(3,3)$ in the above definition will become clear soon. In terms of components, the full Coulomb potential reads:

$$\frac{V_{\text{Coul}}(\boldsymbol{x}_i, \boldsymbol{x}_j)}{q_iq_j} = \frac{1}{r_{ij}} - \frac{1}{\sqrt{r_{ij}^2 + x_i^2 + y_i^2 + z_i^2 + 2rz_i}}$$
$$-\frac{1}{\sqrt{r_{ij}^2 + x_j^2 + y_j^2 + z_j^2 - 2r_{ij}z_j}}\tag{2}$$
$$+\frac{1}{\sqrt{r_{ij}^2 + (x_j - x_i)^2 + (y_j - y_i)^2 + (z_j - z_i)^2 - 2r_{ij}(z_j - z_i)}}$$

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

$$V_{\text{Coul}}\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right) = \sum_{n\geq 0}V_n\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right),\tag{3}$$

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

$$V_n\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right) \propto r_{ij}^{-n-3}.\tag{4}$$

The potential V_0 corresponds then to the dipole-dipole interaction, V_1 to the dipole-quadrupole interaction, and V_2 to the quadrupole-quadrupole and dipole-octupole interaction. Let us give here the expression for the multipolar potential up to quartic order:

$$V_0(\boldsymbol{x}_i, \boldsymbol{x}_j) = q_iq_j\frac{x_ix_j + y_iy_j - z_iz_j}{r_{ij}^3}\tag{5}$$

$$V_1(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{q_iq_j}{2r_{ij}^4}\big(-3x_i^2z_j - 6x_ix_jz_i + 6x_ix_jz_j + 3x_j^2z_i$$
$$- 3y_i^2z_j - 6y_iy_jz_i + 6y_iy_jz_j + 3y_j^2z_i$$
$$+ 6z_i^2z_j - 6z_iz_j^2\big)\tag{6}$$

$$V_2(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{q_iq_j}{2r_{ij}^4}\big(-6x_i^3x_j + 9x_i^2x_j^2 - 6x_i^2y_iy_j + 3x_i^2y_j^2$$
$$+ 24x_i^2z_iz_j - 12x_i^2z_j^2 - 6x_ix_j^3 - 6x_ix_jy_i^2$$
$$+ 12x_ix_jy_iy_j - 6x_ix_jy_j^2 + 24x_ix_jz_i^2$$
$$- 48x_ix_jz_iz_j + 24x_ix_jz_j^2 + 3x_j^2y_i^2 - 6x_j^2y_iy_j$$
$$- 12x_j^2z_i^2 + 24x_j^2z_iz_j - 6y_i^3y_j + 9y_i^2y_j^2$$
$$+ 24y_i^2z_iz_j - 12y_i^2z_j^2 - 6y_iy_j^3 + 24y_iy_jz_i^2$$
$$- 48y_iy_jz_iz_j + 24y_iy_jz_j^2 - 12y_j^2z_i^2 + 24y_j^2z_iz_j$$
$$- 16z_i^3z_j + 24z_i^2z_j^2 - 16z_iz_j^3\big)\tag{7}$$

We define the dimensionless position and momenta associated to QDO i:

$$\boldsymbol{X}_i := \sqrt{\frac{m_i\omega_i}{\hbar}}\,\boldsymbol{x}_i, \qquad \boldsymbol{P}_i := \frac{\boldsymbol{p}_i}{\sqrt{2\hbar m_i\omega_i}},\tag{8}$$

in terms of which the $3N$ creation and annihilation operators read ($\alpha = 1, 2, 3$)

$$\boldsymbol{a}_i = \frac{\boldsymbol{X}_i + i\boldsymbol{P}_i}{\sqrt{2}}, \qquad \boldsymbol{a}_i^\dagger = \frac{\boldsymbol{X}_i - i\boldsymbol{P}_i}{\sqrt{2}}.\tag{9}$$

In terms of the dimensionless canonical variables, the Hamiltonian reads

$$H_{(3,3)} = \sum_{i=1}^{N} \frac{\hbar\omega_i}{2} \left(\boldsymbol{X}_i^2 + \boldsymbol{P}_i^2 \right)$$
$$+ \sum_{i<j} V_{\text{Coul}} \left(\sqrt{\frac{\hbar}{m_i\omega_i}} \boldsymbol{X}_i, \sqrt{\frac{\hbar}{m_j\omega_j}} \boldsymbol{X}_j \right) \tag{10}$$

and can be rewritten

$$H_{(3,3)} = \sum_{i=1}^{N} \frac{\hbar\omega_i}{2} \left(\boldsymbol{a}_i^\dagger \cdot \boldsymbol{a}_i + \frac{3}{2} \right)$$
$$+ \sum_{i<j} V_{\text{Coul}} \left(\sqrt{\frac{\hbar}{m_i\omega_i}} \frac{\boldsymbol{a}_i + \boldsymbol{a}_i^\dagger}{\sqrt{2}}, \sqrt{\frac{\hbar}{m_j\omega_j}} \frac{\boldsymbol{a}_j + \boldsymbol{a}_j^\dagger}{\sqrt{2}} \right) \tag{11}$$

B. One-dimensional case

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. Those two cases can be obtained simply by setting to zero the contribution from all the terms involving the (x,y) Cartesian axes in the parallel case, and the (y,z) Cartesian axes in the perpendicular case. In both cases, we denote by x the remaining degree of freedom.

$$V_0(x_i, x_j) = q_i q_j \frac{x_i x_j}{r_{ij}^3} \times \begin{cases} -2, & \text{parallel case} \\ 1, & \text{perpendicular case} \end{cases} \tag{12}$$

The next terms in the multipolar expansion are:

$$V_1(x_i, x_j) = q_i q_j \frac{x_i x_j (x_i - x_j)}{r_{ij}^4} \times \begin{cases} 3, & \text{parallel case} \\ 0, & \text{perpendicular case} \end{cases} \tag{13}$$

$$V_2(x_i, x_j) = q_i q_j \frac{x_i x_j (2x_i^2 - 3x_i x_j + 2x_j^2)}{r_{ij}^5}$$
$$\times \begin{cases} -2, & \text{parallel case} \\ -\frac{3}{4}, & \text{perpendicular case} \end{cases} \tag{14}$$

For the full Coulomb potential, assuming that the electrons are constrained to move along an axis, we get the following expressions:

$$\frac{V_{\text{Coul}}^\perp(x_i, x_j)}{q_i q_j} = \frac{1}{r_{ij}} - \frac{1}{\sqrt{r_{ij}^2 + x_i^2}} - \frac{1}{\sqrt{r_{ij}^2 + x_j^2}}$$
$$+ \frac{1}{\sqrt{r_{ij}^2 + (x_j - x_i)^2}} \tag{15}$$

in the case where the electrons move perpendicular to the axis joining the two nuclei, and

$$\frac{V_{\text{Coul}}^{||}(x_i, x_j)}{q_i q_j} = \frac{1}{r_{ij}} - \frac{1}{|r_{ij} + x_i|} - \frac{1}{|r_{ij} - x_j|} + \frac{1}{|r_{ij} + x_i - x_j|}$$

in the case where they move parallel to the latter.

C. 9 different models

For the simulation, we will restrict the system to two QDOs. Depending on the space dimensionality (1d parallel, 1d perpendicular, 3d) and the choice of potential (quadratic, quartic, Coulomb), we therefore have 9 models to try and study, gathered in table (I).

TABLE I. The nine models

POTENTIAL \ DIMENSION	1d parallel	1d perpendicular	3d
DD	$H_{(1,1)}$	$H_{(1,2)}$	$H_{(1,3)}$
DD+DQ+QQ+DO	$H_{(2,1)}$	$H_{(2,2)}$	$H_{(2,3)}$
COULOMB	$H_{(3,1)}$	$H_{(3,2)}$	$H_{(3,3)}$

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

$$|\psi(\theta)\rangle = U(\theta)|0\rangle. \tag{16}$$

In the dipolar approximation, namely for the Hamiltonians $H_{(1,1)}$, $H_{(1,2)}$ and $H_{(1,3)}$, 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). However for the other models, non-Gaussian operation should be added in the end of each layer in the ansatz circuit.

One the ansatz state $|\psi(\theta)\rangle$ has been produced, one should extract the value of the energy in that state, namely compute the value of

$$\langle \psi(\theta)|H|\psi(\theta)\rangle \tag{17}$$

To be specific, let us take the model $H_{(3,3)}$, and let us denote by angular brackets the expectation in state $|\psi(\theta)\rangle$. One has

$$\langle H_{(3,3)} \rangle = \sum_{i=1}^{N} \frac{\hbar\omega_i}{2} \left(\langle n_{i,x} \rangle + \langle n_{i,y} \rangle + \langle n_{i,z} \rangle + \frac{3}{2} \right)$$
$$+ \sum_{i<j} \left\langle V_{\text{Coul}} \left(\sqrt{\frac{\hbar}{m_i\omega_i}} \boldsymbol{X}_i, \sqrt{\frac{\hbar}{m_j\omega_j}} \boldsymbol{X}_j \right) \right\rangle \tag{18}$$

by linearity of the expectation. On the second line one has to compute something of the form $\langle f(X_{i,\alpha})\rangle$, where $(X_{i,\alpha})$ denotes collectively the position quadrature of all the photon channels (including QDO and spatial index). One therefore needs to extract the statistics of quadratures by preparing and measuring the state $|\psi(\theta)\rangle$ in the quadrature basis. Once the joint density ρ of $(X_{i,\alpha})$ in the state $|\psi(\theta)\rangle$ is known, one can compute

$$\langle f(X_{i,\alpha})\rangle = \int_{\mathbb{R}^{3N}} f(x_{i,\alpha})\rho(x_{i,\alpha}) \prod_{i,\alpha} \mathrm{d}x_{i,\alpha}. \tag{19}$$

There is a complication related to the fact that strawberryfields does not allow to access the joint law of the position quadratures. We therefore have to extract it by ourselves. Let us first suppose that there are K photon modes. The statevector is represented in the Fock basis as follows:

$$|\psi\rangle = \sum_{n_1,\ldots,n_K=0}^{\infty} \alpha_{n_1\ldots n_K}|n_1\rangle \otimes \cdots \otimes |n_K\rangle. \tag{20}$$

The amplitude of a specific tuple of the quadratures $(X_1,\ldots,X_K)$ is therefore given by:

$$\langle X_1,\ldots,X_K|\psi\rangle = \sum_{n_1,\ldots,n_K=0}^{\infty} \alpha_{n_1\ldots n_K} \prod_{i=1}^{K} \frac{e^{-\sum_{i=1}^{K}\frac{X_i^2}{2}}H_{n_i}(X_i)}{\sqrt{\pi^{1/2}2^{n_i}n_i!}},$$

in terms of the Hermite polynomials. The joint law of the quadratures in the state $|\psi\rangle$ is therefore given by

$$\rho(X_1,\ldots,X_K) = \sum_{\substack{n_1,\ldots,n_K \\ m_1,\ldots,m_K}} \alpha_{n_1\ldots n_K}\alpha^*_{m_1\ldots m_K}$$
$$\times \prod_{i=1}^{K} \frac{e^{-X_i^2}H_{n_i}(X_i)H_{m_i}(X_i)}{\sqrt{\pi^{1/2}2^{n_i}n_i!}\sqrt{\pi^{1/2}2^{m_i}m_i!}} \tag{21}$$

Notice that the tensor $\alpha_{n_1,\ldots,n_K}$ is precisely the output of 'state.ket()' in strawberryfields. Also the Hermite polynomials are implemented in 'scipy.special.hermite':

```
from scipy import special
p = special.hermite(3, monic=False)
```

After extracting as well the mean photon numbers $\langle n_{i,\alpha}\rangle$, one obtains $\langle H_{(3,3)}\rangle$.

IV. VARIATIONAL ALGORITHM

Depending on the model $H_{(\mu,\nu)}$ of interest, we define the following loss function:

$$\mathcal{C}_{(\mu,\nu)}(\theta) := \langle\psi(\theta)|H_{(\mu,\nu)}|\psi(\theta)\rangle \tag{22}$$

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, as described in the previous section.

Algorithm 1: Extract sdistribution of observable

Parameters: statevector $|\psi\rangle$, observable $\mathcal{O}$, shots $M \in \mathbb{N}$
Result: Probability distribution of $\mathcal{O}$ in state $|\psi\rangle$

for $m = 1$ *to* $\dim(spec(\mathcal{O}))$ **do**
   Initialize $N_m \leftarrow 0$;
for $j = 1$ *to* M **do**
   Measure the state $|\psi\rangle$ in the basis $\mathcal{O}$, obtain the eigenvalue o_m, set $N_m \leftarrow N_m + 1$;
for $m = 1$ *to* $\dim(spec(\mathcal{O}))$ **do**
   Normalize $N_m \leftarrow N_m/M$;
return $(N_m)_m$.

Algorithm 2: Computation of the loss

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

Initialize $\mathcal{C} \leftarrow 0$;
Get the position quadratures distribution with alg. (1);
Get the photon numbers distribution with alg. (1);
Compute the loss $\mathcal{C}$ using eq. (18);
return $\mathcal{C}$.

Algorithm 3: 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. (2);
   Compute the gradient $\nabla_\theta\mathcal{C}$ with shift rule and alg. (2);
   Update the parameters $\theta \leftarrow \theta - \eta\nabla_\theta\mathcal{C}$;
   end for
return θ.

V. RESULTS

We gather here the results of the simulations. We focus on the case of 2 QDOs. In particular we plot the profile of the binding energy as a function of the distance between the two nuclei. The binding energy is simply defined as the ground state energy of the interacting system to which one substract the ground state energy of the uninteracting system, namely that of a pair of free harmonic oscillators in this Drude model.

VI.   CONCLUSION

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CODE AVAILABILITY

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

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