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):

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

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

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

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

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

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:

$$V_0(\boldsymbol{x}_i, \boldsymbol{x}_j) = q_i q_j \frac{x_i x_j + y_i y_j - z_i z_j}{r_{ij}^3} \tag{5}$$

$$V_1(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{q_i q_j}{2r_{ij}^4} \big(-3x_i^2 z_j - 6x_i x_j z_i + 6x_i x_j z_j + 3x_j^2 z_i$$
$$- 3y_i^2 z_j - 6y_i y_j z_i + 6y_i y_j z_j + 3y_j^2 z_i$$
$$+ 6z_i^2 z_j - 6z_i z_j^2 \big) \tag{6}$$

$$V_2(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{q_i q_j}{2r_{ij}^4} \big(-6x_i^3 x_j + 9x_i^2 x_j^2 - 6x_i^2 y_i y_j + 3x_i^2 y_j^2$$
$$+ 24x_i^2 z_i z_j - 12x_i^2 z_j^2 - 6x_i x_j^3 - 6x_i x_j y_i^2$$
$$+ 12x_i x_j y_i y_j - 6x_i x_j y_j^2 + 24x_i x_j z_i^2$$
$$- 48x_i x_j z_i z_j + 24x_i x_j z_j^2 + 3x_j^2 y_i^2 - 6x_j^2 y_i y_j$$
$$- 12x_j^2 z_i^2 + 24x_j^2 z_i z_j - 6y_i^3 y_j + 9y_i^2 y_j^2$$
$$+ 24y_i^2 z_i z_j - 12y_i^2 z_j^2 - 6y_i y_j^3 + 24y_i y_j z_i^2$$
$$- 48y_i y_j z_i z_j + 24y_i y_j z_j^2 - 12y_j^2 z_i^2 + 24y_j^2 z_i z_j$$
$$- 16z_i^3 z_j + 24z_i^2 z_j^2 - 16z_i z_j^3 \big) \tag{7}$$

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 ($\alpha = 1, 2, 3$)

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

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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

Let us define one-dimensional instances of the QDO model as follows: we restrict the movement of the two electrons to be along a common axis (directed by a unit vector $\hat{\boldsymbol{e}}_\theta$) which form an angle θ with respect to the vector $\boldsymbol{r}_{ij}$ connecting the two nuclei. As particular cases, we obtain models in which the electrons are constrained to move either in the direction parallel to the axis separating the two nuclei ($\theta = 0$), or perpendicular to the latter ($\theta = \pi/2$). We therefore have a family of one-dimensional models which can be obtained from the full-fledged 3d model simply by setting to zero the contribution from the oscillator modes belonging to the plane perpendicular to $\hat{\boldsymbol{e}}_\theta$. Let us denote by x the remaining degree of freedom. As will be explained in the results section, one particular model will prove relevant, the so-called *space regularized model*, in which the angle θ is chosen to be infinitesimally small $\theta = \epsilon \ll 1$.

$$V_0(x_i, x_j) = q_i q_j \frac{x_i x_j}{r_{ij}^3} \times$$
$$\times \begin{cases} 1 - 3\cos^2\theta, & \text{generic case} \\ -2, & \text{parallel case} \\ 1, & \text{perpendicular case} \\ -\frac{1}{2}, & \text{oblique case} \\ -2 - 6\epsilon, & \text{regularized case} \end{cases} \tag{12}$$

The next terms in the multipolar expansion are:

$$V_1(x_i, x_j) = q_i q_j \frac{x_i x_j (x_i - x_j)}{r_{ij}^4} \times$$
$$\times \begin{cases} \frac{3\cos\theta(-3+5\cos^2\theta)}{2}, & \text{generic case} \\ 3, & \text{parallel case} \\ 0, & \text{perpendicular case} \\ -\frac{3}{4\sqrt{2}}, & \text{oblique case} \\ 3 + 18\epsilon, & \text{regularized case} \end{cases} \tag{13}$$

$$V_2(x_i, x_j) = q_i q_j \frac{x_i x_j (2x_i^2 - 3x_i x_j + 2x_j^2)}{r_{ij}^5} \times$$
$$\times \begin{cases} -\frac{3-30\cos^2\theta+35\cos^4\theta}{4}, & \text{generic case} \\ -2, & \text{parallel case} \\ -\frac{3}{4}, & \text{perpendicular case} \\ \frac{13}{16}, & \text{oblique case} \\ -2 - 20\epsilon, & \text{regularized case} \end{cases} \tag{14}$$

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. In the case of a generic angle θ between $\boldsymbol{r}_{ij}$ and $\boldsymbol{x}_i/\boldsymbol{x}_j$, one has

$$\frac{V_{\text{Coul}}^\theta(x_i, x_j)}{q_i q_j} = \frac{1}{r_{ij}} - \frac{1}{\sqrt{r_{ij}^2 + 2r_{ij}(\cos\theta)x_i + x_i^2}}$$
$$- \frac{1}{\sqrt{r_{ij}^2 - 2r_{ij}(\cos\theta)x_j + x_j^2}}$$
$$+ \frac{1}{\sqrt{r_{ij}^2 - 2r_{ij}(\cos\theta)(x_j - x_i) + (x_j - x_i)^2}}. \tag{16}$$

The space regularized model Coulomb potential reads

$$\frac{V_{\text{Coul}}^\epsilon(x_i, x_j)}{q_i q_j} = \frac{1}{r_{ij}} - \frac{1}{\sqrt{r_{ij}^2 + 2r_{ij}(1+\epsilon)x_i + x_i^2}}$$
$$- \frac{1}{\sqrt{r_{ij}^2 - 2r_{ij}(1+\epsilon)x_j + x_j^2}}$$
$$+ \frac{1}{\sqrt{r_{ij}^2 - 2r_{ij}(1+\epsilon)(x_j - x_i) + (x_j - x_i)^2}}. \tag{17}$$

C. 12 different models

For the simulation, we will restrict the system to two QDOs. Depending on the space dimensionality (1d oblique, 1d parallel, 1d perpendicular, 3d) and the choice of potential (quadratic, quartic, Coulomb), we therefore have 12 models to try and study, gathered in table (I).

TABLE I. The twelve models

POT \ DIM	1d oblique	1d parallel	1d perpendicular	3d
QUAD	$H_{(1,0)}$	$H_{(1,1)}$	$H_{(1,2)}$	$H_{(1,3)}$
QUART	$H_{(2,0)}$	$H_{(2,1)}$	$H_{(2,2)}$	$H_{(2,3)}$
COULOMB	$H_{(3,0)}$	$H_{(3,1)}$	$H_{(3,2)}$	$H_{(3,3)}$

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

$$|\psi(\theta)\rangle = U(\theta)|0\rangle. \tag{18}$$

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

$$\langle\psi(\theta)|H|\psi(\theta)\rangle \tag{19}$$

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

$$\langle H_{(3,3)}\rangle = \sum_{i=1}^{N} \frac{\hbar\omega_i}{2}\left(\langle n_{i,x}\rangle + \langle n_{i,y}\rangle + \langle n_{i,z}\rangle + \frac{3}{2}\right) \\ + \sum_{i<j}\left\langle V_{\mathrm{Coul}}\left(\sqrt{\frac{\hbar}{m_i\omega_i}}\boldsymbol{X}_i, \sqrt{\frac{\hbar}{m_j\omega_j}}\boldsymbol{X}_j\right)\right\rangle \tag{20}$$

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

$$\langle f(X_{i,\alpha})\rangle = \int_{\mathbb{R}^{3N}} f(x_{i,\alpha})\rho(x_{i,\alpha})\prod_{i,\alpha}\mathrm{d}x_{i,\alpha}. \tag{21}$$

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:

$$|\psi\rangle = \sum_{n_1,\ldots,n_K=0}^{\infty} \alpha_{n_1\ldots n_K}|n_1\rangle \otimes \cdots \otimes |n_K\rangle. \tag{22}$$

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

$$\rho(X_1, \ldots, X_K) = \sum_{\substack{n_1,\ldots,n_K \\ m_1,\ldots,m_K}} \alpha_{n_1\ldots n_K}\alpha^*_{m_1\ldots m_K} \\ \times \prod_{i=1}^{K}\frac{e^{-X_i^2}H_{n_i}(X_i)H_{m_i}(X_i)}{\sqrt{\pi^{1/2}2^{n_i}n_i!}\sqrt{\pi^{1/2}2^{m_i}m_i!}} \tag{23}$$

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:

$$\mathcal{C}_{(\mu,\nu)}(\theta) := \langle\psi(\theta)|H_{(\mu,\nu)}|\psi(\theta)\rangle \tag{24}$$

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 distribution 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 $|\psi$ 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. (20);
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. QUANTUM MUTUAL INFORMATION

Recall the definition here.

Since the state of the total system is pure, the von Neumann entropy of the total density matrix is zero. QDO number 2 can then be interpreted as purifying the system composed solely of QDO number 1. The two QDO therefore have identical von Neumann entropy $S(\rho_1)$, the entanglement entropy. The quantum mutual information of the system is therefore given by

$$I(1:2) = S(\rho_1) + S(\rho_2) - S(\rho_{12}) = 2S(\rho_1) = -2\mathrm{Tr}\rho_1 \log \rho_1 \,. \tag{25}$$

The profile of the quantum mutual information as a function of the interatomic distance is provided in fig. (...)

VII. CONCLUSION

ACKNOWLEDGMENTS

CODE AVAILABILITY

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

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