Research Square

Preprints are preliminary reports that have not undergone peer review.
They should not be considered conclusive, used to inform clinical practice,
or referenced by the media as validated information.

Photonic Quantum Simulation of Three-Body Non-Covalent Interactions Using a Generalized Quantum Drude Oscillator Framework

Ajay Kumar
NSCBM Government College Hamirpur , Himachal Pradesh , India
Jyoti Parmar
NSCBM Government College Hamirpur , Himachal Pradesh , India
Asheesh Krishan
NSCBM Government College Hamirpur , Himachal Pradesh , India
Yavindra Kumari
Career Point University
Lavli Rana
rana.phy08@gmail.com

NSCBM Government College Hamirpur , Himachal Pradesh , India
Bhavesh Kumar Dadhich
Career Point University

Research Article

Keywords: QDO, Photonic Quantum Circuit, Coulomb Interactions, Hamiltonian, Bound States

Posted Date: October 9th, 2026

DOI: https://doi.org/10.21203/rs.3.rs-10881948/v1

License: This work is licensed under a Creative Commons Attribution 4.0 International License.
Read Full License

Additional Declarations: No competing interests reported.

Photonic Quantum Simulation of Three-Body Non-Covalent Interactions Using a Generalized Quantum Drude Oscillator Framework

Ajay Kumar[1], Jyoti Parmar[1], Asheesh Krishan[1], Yavindra Kumari[2], Lavli Rana [1,a)], Bhavesh Kumar Dadhich[2]

[1]Department of Physics, NSCBM Government College Hamirpur, Hamirpur , Himachal Pradesh, India

[2]Department of Physics, School of Basic and Applied Sciences, Career Point University, Kota, Rajasthan, India

[a)] Corresponding author: rana.phy08@gmail.com

ORCID: https://orcid.org/0009-0007-9279-5128

Abstract

Context: Non-covalent interactions, especially dispersion interactions, are crucial for defining the stability and structural characteristics of molecular systems, while accurately modeling them becomes increasingly complex for many-body arrangements. The Quantum Drude Oscillator (QDO) model offers a physically meaningful coarse-grained approach to dispersion interactions; however, previous photonic quantum simulations have primarily focused on pairwise interactions. In this work, we introduce an extended three-body Quantum Drude Oscillator (3-QDO) framework to represent geometry-sensitive non-covalent interactions in triangular molecular arrangements. This framework allows for the exploration of symmetric, asymmetric, angular-dependent, and custom-defined three-body geometries. Our simulations reveal that the interaction energy and optimal binding are highly influenced by intermolecular distances and angular arrangements. In the fully variable setup, the global minimum is found near a symmetric configuration, whereas changes in angular parameters can significantly strengthen, diminish, or even eliminate binding. These findings highlight the capability of the 3-QDO framework to advance photonic quantum simulations into the realm of more intricate many-body molecular dynamics.

Methods: The three-body QDO system was formulated as three harmonically bound quantum oscillators coupled through pairwise Coulomb interactions and mapped onto a three-mode continuous-variable photonic quantum circuit. The circuit was initialized in the three-mode Fock vacuum and implemented using Gaussian beam-splitter, rotation, squeezing, and displacement operations together with non-Gaussian Kerr gates. Numerical simulations were performed using the Strawberry Fields photonic quantum computing platform with a Fock-space cutoff of 6 and an 81-point position-quadrature grid over $X = -6$ to 6. Dimensionless

units with $\hbar = \omega_i = m_i = q_i = 1$ and an effective Coulomb constant of 0.08 were employed. Binding energies were obtained from the expectation values of the harmonic and Coulomb contributions, and the resulting energy profiles were fitted using a pairwise-summed Morse function.

Keywords: QDO, Photonic Quantum Circuit, Coulomb Interactions, Hamiltonian, Bound States

1. Introduction: Non-covalent interactions play a crucial role in determining the structural organization, stability, dynamics, and functional properties of molecular systems. [1,2] These interactions govern a wide range of physical, chemical, and biological processes, including molecular recognition, crystal packing, protein folding, supramolecular self-assembly, and the stability of nanostructured materials [2-4]. Although they are individually much weaker than covalent interactions, their collective effect often dominates the behavior of complex molecular systems and therefore an accurate theoretical description of non-covalent interactions has become a central challenge in computational chemistry, condensed matter physics, and molecular materials science [3-5]. The growing demand for reliable and computationally efficient methods to model these interactions has further motivated the development of physically meaningful quantum-mechanical frameworks capable of describing intermolecular forces with high accuracy.

Density Functional Theory (DFT), Møller–Plesset perturbation theory (MP2), and Coupled Cluster Singles and Doubles (CCSD) are among the most widely used computational methods for describing non-covalent interactions due to their high accuracy in predicting intermolecular forces [6–8]. However, these methods often become computationally expensive for larger molecular systems and may exhibit convergence limitations when treating complex many-body interactions [6–9]. To address these challenges, physically motivated models such as the Quantum Drude Oscillator (QDO) have been developed, providing an efficient and accurate framework for describing dispersion interactions through coarse-grained quantum oscillators [9–11]. In the QDO model, each atom is represented as a quantum harmonic oscillator in which the electronic cloud fluctuates about the positively charged nucleus, generating instantaneous dipoles responsible for dispersion interactions [10,11].Since these oscillators obey bosonic statistics, the QDO framework is naturally compatible with continuous-variable photonic quantum simulation [12,13].

Recent studies have successfully demonstrated the feasibility of photonic quantum simulation for modeling non-covalent interactions using the two-body Quantum Drude Oscillator (2-

QDO) framework [14]. However, the existing framework is primarily demonstrated for pairwise interactions and does not explicitly address generalized three-body systems, where non-additive many-body effects become increasingly significant [11,14]. Since three interacting particles constitute the simplest many-body system, extending the QDO framework beyond pairwise interactions provides a natural pathway toward more realistic molecular modeling [11]. In the present work, we develop a generalized three-body Quantum Drude Oscillator (3-QDO) framework for the photonic quantum simulation of non-covalent interactions using the Strawberry Fields photonic quantum computing platform [12,14]. The proposed framework extends the existing two-body formulation by enabling the investigation of three-body molecular configurations and provides a foundation for exploring geometry-dependent non-covalent interactions in more complex molecular systems.

2. Theoretical Framework

The theoretical framework developed in this work is based on the Quantum Drude Oscillator (QDO) model and its implementation using photonic quantum simulation in Strawberry Fields. [10,12,14]. The three-body Quantum Drude Oscillator (3-QDO) framework extends the conventional two-body Quantum Drude Oscillator (2-QDO) model to describe non-covalent interactions by incorporating non-additive dispersion effects. In this framework, three interacting Quantum Drude Oscillators are considered simultaneously to model many-body interactions. Each oscillator follows the same physical description introduced in the conventional QDO model, while the generalized framework accounts for the pairwise and collective interactions among all three oscillators. This extension enables the investigation of geometry-dependent non-covalent interactions beyond the pairwise approximation.

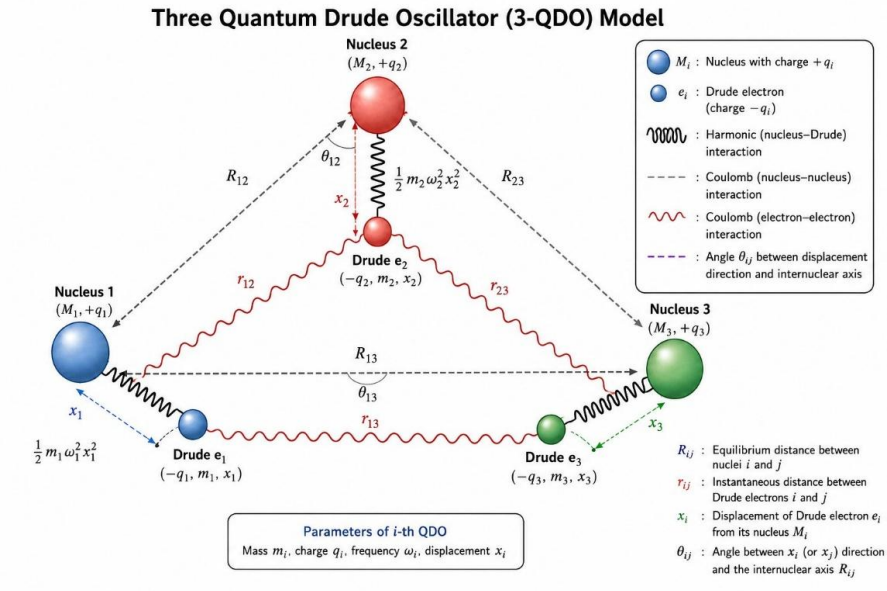


Fig.1 Schematic representation of the three Quantum Drude Oscillator (3-QDO) model arranged in a triangular geometry. Each atom consists of a positively charged nucleus and a harmonically bound Drude particle, with pairwise Coulomb interactions between all oscillator pairs.

The three QDOs are arranged in an all-to-all triangular configuration, allowing each oscillator to interact with the other two through Coulomb interactions. The equilibrium positions of the nuclei are separated by the inter-nuclear distancesR_{12}, R_{13}, and R_{23}. The instantaneous positions of the drudons relative to their parent nuclei are represented by the displacement coordinates x_1, x_2, and x_3. Consequently, the instantaneous separations between interacting particles become functions of both the equilibrium nuclear geometry and the drudon displacements. This triangular arrangement provides the geometric framework for constructing the total Hamiltonian and evaluating the pairwise Coulomb interactions among the three oscillators. The complete Hamiltonian of the 3-QDO system is:

$$H = \sum_{i=1}^{3} \left[\frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2 x_i^2\right] + \sum_{i<j}^{3} V_{Coul}(i,j) \qquad (1)$$

For a simplified symmetric 3-QDO system, all three oscillators may be taken as identical. In this approximation,

$$m_1 = m_2 = m_3 = m$$
$$q_1 = q_2 = q_3 = q$$
$$\omega_1 = \omega_2 = \omega_3 = \omega$$

With these assumptions, the Hamiltonian becomes:

$$H = \sum_{i=1}^{3} \left[\frac{p_i^2}{2m} + \frac{1}{2}m\omega^2 x_i^2\right] + \sum_{i<j}^{3} V_{Coul}(i,j) \qquad (2)$$

This Hamiltonian forms the basis for the dimensionless formulation employed in the photonic quantum simulation. To express the Hamiltonian of the three Quantum Drude Oscillator system in a form suitable for photonic quantum computation, we have to evaluate the equations in dimensionless form. The dimensionless position and momentum coordinate in 3QDO framework is defined as:

$$X_i = \sqrt{\frac{m_i\omega_i}{\hbar}}x_i \qquad P_i = \frac{p_i}{\sqrt{\hbar m_i \omega_I}} \qquad \text{where } i = 1,2,3$$

Using these dimensionless variables, the Hamiltonian of the three-QDO system can be written as:

$$H = \sum_{i=1}^{3} \frac{\hbar\omega_i}{2}(X_i^2 + P_i^2) + \sum_{i<j}^{3} V_{Coul}(x_i, x_j) \qquad (3)$$

As, each Coulomb interaction is evaluated with its own distance dependence. Therefore, the interaction is written for the three independent pairs as:

$$V_{\text{Coul}} = V_{\text{Coul}}(x_1, x_2; d_{12}, \theta_{12}) + V_{\text{Coul}}(x_1, x_3; d_{13}, \theta_{13}) + V_{\text{Coul}}(x_2, x_3; d_{23}, \theta_{23})$$

Here, d_{ij} represents the fixed nuclear separation between the ith and jth QDOs, while θ_{ij} represents the angle between the Drude displacement direction and the inter-nuclear axis. Since the three-QDO system is considered in a general triangular configuration, d_{12}, d_{13}, and d_{23} may take different values.

The dimensionless oscillator variables can now be connected with the creation and annihilation operators. The Hamiltonian can be written as:

$$H_{(\theta_{ij}, d_{ij})} = \sum_{i=1}^{3} \hbar\,\omega_i \left(a_i^{\dagger} a_i + \frac{1}{2}\right) + \sum_{i<j}^{3} V_{\text{Coul}}^{(\theta_{ij}, d_{ij})} \left(\sqrt{\frac{\hbar}{2m_i\omega_i}}\,(a_i + a_i^{\dagger}), \sqrt{\frac{\hbar}{2m_j\omega_j}}\,(a_j + a_j^{\dagger})\right) \tag{4}$$

where a_i is the annihilation operator and $a_i^{\dagger}$ is the creation operator, this expression shows that the Coulomb interaction depends on the quantum displacement operators of the Drude particles

$$V_{\text{Coul}} = \sum_{i<j}^{3} V_{\text{Coul}}\left(\theta_{ij}, d_{ij}, x_i, x_j\right)$$

$$= \sum_{i<j}^{3} \frac{q_i q_j}{4\pi\varepsilon_0} \left[\frac{1}{d_{ij}} - \frac{1}{\sqrt{d_{ij}^2 - 2d_{ij}x_j\cos\theta_{ij} + x_j^2}} - \frac{1}{\sqrt{d_{ij}^2 - 2d_{ij}x_j\cos\theta_{ij} + x_j^2}} + \frac{1}{\sqrt{d_{ij}^2 + 2d_{ij}(x_i - x_j)\cos\theta_{ij} + (x_i - x_j)^2}}\right] \tag{5}$$

The first term represents nucleus–nucleus repulsion. The second and third terms represent attractive nucleus–Drude particle interactions, and the last term represents Drude particle–Drude particle repulsion. This form is applied to each of the three QDO pairs: (1,2), (1,3), and (2,3).

For the numerical simulation, we set $\hbar = \omega_i = q_i = m_i = 1$ and $k_{eff} = \frac{q_i q_j}{4\pi\varepsilon_0}$

For the dimensionless simulations, the charges and permittivity are normalized by taking $q_i = q_j = 1$ and $\varepsilon_0 = 1$. Consequently, the electrostatic prefactor reduces to

$$k_{eff} = \frac{1}{4\pi} \approx 0.08,$$

which is used throughout the simulations.

The resulting dimensionless Hamiltonian provides the theoretical basis for the photonic implementation described in the following section.

3. Photonic Quantum Circuit Representation of the Three-QDO Model

The three-QDO system is represented by a three-mode photonic quantum circuit, where each optical mode corresponds to one Quantum Drude Oscillator. The circuit prepares a three-mode quantum state for evaluating the expectation value of the 3-QDO Hamiltonian. It consists of Gaussian operations, including beam splitters, rotation, squeezing, and displacement gates, followed by non-Gaussian Kerr gates, as illustrated in Fig. 3.

The input state of the circuit is taken as the three-mode Fock vacuum state:

$$|0\rangle \otimes |0\rangle \otimes |0\rangle \qquad (6)$$

where each vacuum mode corresponds to one Quantum Drude Oscillator. The photonic circuit transforms this initial state into a three-mode quantum state through a sequence of Gaussian and non-Gaussian operations. A photonic circuit represented by the unitary operator U acts on this vacuum state and prepares the quantum state:

$$|\psi = U(|0\rangle \otimes |0\rangle \otimes |0\rangle) \qquad (7)$$

The prepared quantum state is subsequently used to evaluate the expectation value of the 3-QDO Hamiltonian, given by:

$$E = \langle\psi|H|\psi\rangle \qquad (8)$$

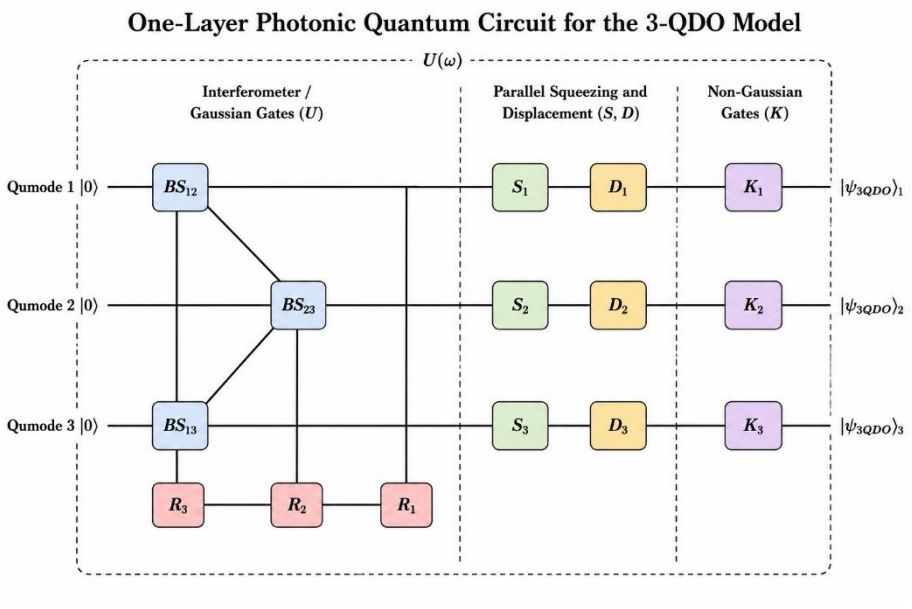


Fig. 2 One layer of the three-mode photonic quantum circuit for the 3-QDO model. Each optical mode corresponds to one Quantum Drude Oscillator, and the circuit comprises beam splitters (BS), rotation gates (R), squeezing gates (S), displacement gates (D), and Kerr gates (K).

Accordingly, the total energy expectation value can be evaluated as

$$\langle H \rangle = \langle H_1 \rangle + \langle H_2 \rangle + \langle H_3 \rangle + \langle V_{Coul}^{12} \rangle + \langle V_{Coul}^{13} \rangle + \langle V_{Coul}^{23} \rangle \quad (8)$$

The Coulomb contribution is position-dependent, so it is evaluated using the position quadrature statistics of the prepared photonic state. For the complete three-QDO system, the three-body expectation value can be written as:

$$\langle f(X_1, X_2, X_3) \rangle = \int f(X_1, X_2, X_3) \rho(X_1, X_2, X_3)\, dX_1\, dX_2\, dX_3 \quad (9)$$

Here, $\rho(X_1, X_2, X_3)$ is the joint probability density. In the Fock basis, the prepared three-mode state can be expanded as:

$$|\psi\rangle = \sum_{n_1,n_2,n_3=0}^{\infty} \alpha_{n_1 n_2 n_3} |n_1\rangle \otimes |n_2\rangle \otimes |n_3\rangle \quad (10)$$

Here, $\alpha_{n_1 n_2 n_3}$ are the probability amplitudes of the three-mode Fock state generated by the photonic circuit. In the numerical simulations, the infinite-dimensional Fock space is truncated to a finite cutoff dimension. The amplitude of the state in the position quadrature basis is obtained using Hermite polynomials. For the three-mode case, it can be written as:

$$\langle X_1, X_2, X_3 | \psi \rangle = \sum_{n_1,n_2,n_3=0}^{\infty} \alpha_{n_1 n_2 n_3} \prod_{i=1}^{3} \frac{e^{-X_i^2/2} H_{n_i}(X_i)}{\sqrt{\pi^{1/2} 2^{n_i} n_i!}} \quad (11)$$

Here, $H_{n_i}(X_i)$ represents the Hermite polynomial corresponding to the i^{th} mode. The joint probability density of the three-mode position quadrature is then given by:

$$\rho(X_1, X_2, X_3) = |\langle X_1, X_2, X_3 | \psi \rangle|\hat{}2 \quad (12)$$

The position quadrature probability distribution and the mean photon number of each mode are extracted from the simulated quantum state and used to evaluate the Hamiltonian expectation value given in Eq. (11). After preparing the three-mode photonic state, the position quadrature probability distribution and the mean photon number of each mode are extracted from the simulation. These quantities are used to evaluate the expectation value of the 3-QDO Hamiltonian, including both the harmonic oscillator energy and the Coulomb interaction. The interacting and non-interacting energies obtained from the photonic simulation are subsequently used to calculate the binding energy of the three-QDO system. The variation of the binding energy with intermolecular separation is then used to investigate the non-covalent interaction behavior for different molecular geometries.

4. Simulation Implementation of the Three-QDO Model

The photonic quantum circuit framework developed for the three-QDO model is implemented using the Strawberry Fields photonic quantum simulator. Although the circuit follows a variational photonic architecture, all gate parameters are kept fixed throughout the present study for computational simplicity. Consequently, only the molecular geometry parameters, namely the inter-QDO distances and angular configurations, are varied to evaluate the interacting energy, non-interacting energy, and the corresponding binding energy of the three-QDO system. The Gaussian and non-Gaussian gate parameters used throughout the simulations are listed in Table.1.

Parameter	**Symbol**	**Value**
Beam splitter angle	$\theta BS_{12} = \theta BS_{23} = \theta BS_{13}$	0.05
Beam splitter phase	$\varphi B_{S12} = \varphi BS_{23} = \varphi BS_{13}$	0.00
Rotation gate parameter	$R_1 = R_2 = R_3$	0.05
Squeezing gate parameter	$S_1 = S_2 = S_3$	0.10
Displacement gate parameter	$D_1 = D_2 = D_3$	0.02
Kerr gate parameter	$K_1 = K_2 = K_3$	0.01
Fock cutoff dimension	$N_{cut\ off}$	6
Quadrature grid range	X	−6 to 6
Number of quadrature grid points	N_x	81
Harmonic oscillator frequency	Ω	1.0
Reduced Planck constant	$\hbar$	1.0
Effective Coulomb constant	K_{eff}	0.08

Table. 1 Fixed photonic circuit and simulation parameters employed in the Strawberry Fields implementation of the three-QDO model. These parameters remain unchanged throughout all simulations, while only the inter-QDO distances and angular configurations are varied.

The prepared three-mode quantum state is first converted into the position-quadrature probability distribution. From this distribution, the expectation value of the pairwise Coulomb interaction is evaluated numerically for all three oscillator pairs,

$$\langle V_{\mathrm{Coul}}^{(3)} \rangle = \langle V_{12} + V_{13} + V_{23} \rangle$$

The non-interacting energy is obtained from the harmonic oscillator contribution,

$$E_{\mathrm{non}} = E_0$$

Whereas the interacting energy is calculated as

$$\mathrm{E_{int}} = \mathrm{E_0} + \langle \mathrm{V_{12}} + \mathrm{V_{13}} + \mathrm{V_{23}} \rangle$$

The binding energy of the three-QDO system is then evaluated as

$$\mathrm{E_b^{(3)}} = \mathrm{E_{int}} - \mathrm{E_{non}} \qquad (13)$$

To compare different molecular geometries, the binding energy is shifted relative to a reference configuration corresponding to the largest intermolecular separation,

$$\Delta \mathrm{E_b^{(3)}} = \mathrm{E_b^{(3)}} - \mathrm{E_{ref}} \qquad (14)$$

For comparison with the simulated binding-energy profile, a Morse type function is employed as a fitting model. The Morse potential is not used in the calculation of the Coulomb interaction or the binding energy; it is introduced only to reproduce the numerical binding-energy curve obtained from the photonic simulation. The pairwise Morse function is written as

$$f_{ij}(d_{ij}) = E_b^{\mathrm{pair}}\left[e^{-2(d_{ij}-d_b)/s} - 2e^{-(d_{ij}-d_b)/s}\right] \qquad (15)$$

The corresponding three-QDO Morse function is obtained by summing the three pairwise contributions,

$$f_{\mathrm{Morse}}^{(3)}(d_{12}, d_{13}, d_{23}) = \sum_{i<j} f_{ij}\,(d_{ij})$$

Since the numerical binding energies are referenced to large-distance geometry, the Morse curve is shifted using

$$f_{\mathrm{shifted}}^{(3)} = f_{\mathrm{Morse}}^{(3)} - f_{\mathrm{Morse}}^{(3)}(d_{12}^{\mathrm{ref}}, d_{13}^{\mathrm{ref}}, d_{23}^{\mathrm{ref}}) \qquad (16)$$

The fitting parameters, d_b, E_b^{pair}, and $s$are determined from the simulated binding-energy data. The same computational framework is employed for all simulation cases. Only the intermolecular distances (d_{12}, d_{13}, d_{23}) and angular parameters $(\theta_{12}, \theta_{13}, \theta_{23})$ are varied to investigate different three-body geometries. Accordingly, the implementation allows the study of equal-distance configurations, partially variable geometries, fully variable triangular geometries, angular dependence, and user-defined molecular arrangements using a single computational framework.

5. Results and Discussion

We investigate the effect of molecular geometry on the interaction energy of the three-QDO system using the proposed photonic quantum circuit. By considering six representative simulation cases, the intermolecular distances and angular parameters are varied systematically. For the distance-dependent simulations (Cases I–IV), the angular parameters are kept fixed at $\theta_{12} = \theta_{13} = \theta_{23} = 0.58$ to isolate the influence of intermolecular separation

on the interaction energy, whereas Case V examines the effect of angular variation and Case VI demonstrates the flexibility of the framework for arbitrary user-defined geometries. The corresponding binding-energy curves are then used to examine the interaction behavior and identify the influence of molecular geometry on the interacting and binding energies of the three-QDO system.

Case I: Symmetric Geometry ($d_{12} = d_{13} = d_{23} = d$,)

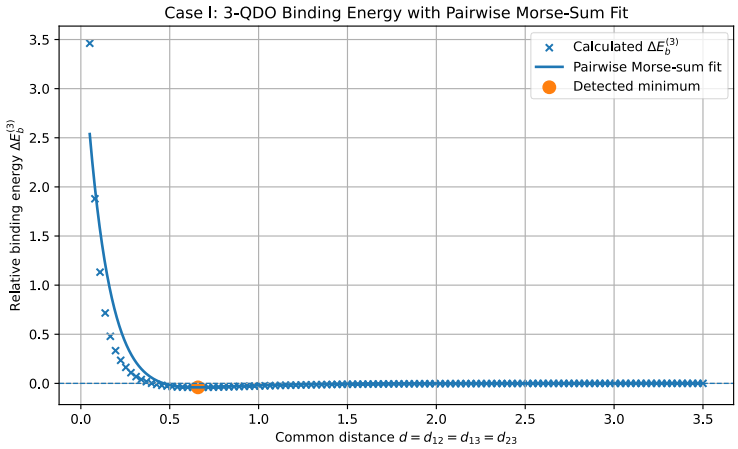


Fig.3. Binding energy for the symmetric 3-QDO system with equal intermolecular distances.

As illustrated in Fig.3, we found that the symmetric 3-QDO geometry produces a well-defined attractive region with a minimum binding energy of approximately $E_{\min} = -0.0406$ at an equilibrium distance of $d_b \approx 0.6588$. The obtained negative binding energy confirms the formation of a stable bound configuration when all three pairwise distances are equals. We further observed that the calculated binding-energy curve is accurately reproduced by the pairwise Morse-sum approximation, yielding an effective pair binding depth of $E_b^{\text{pair}} \approx 0.0135$. This agreement indicates that the proposed photonic 3-QDO framework successfully captures the equilibrium interaction of the symmetric geometry while preserving the essential pairwise interaction characteristics.

Case II: One-variable-distance simulation (d_{12} varied, $d_{13}$and d_{23}fixed)

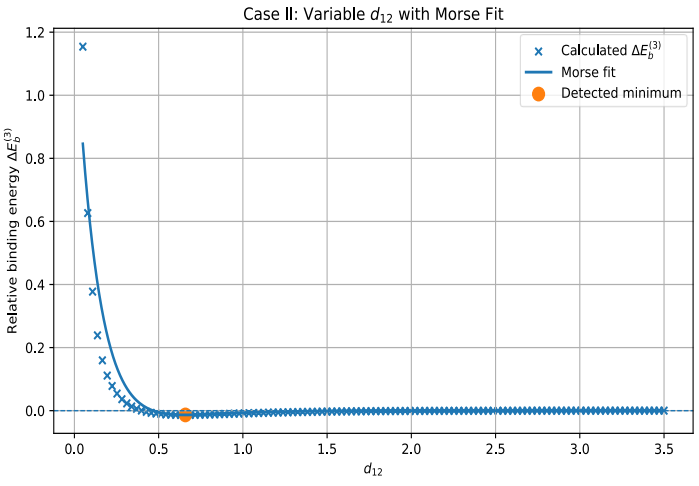


Fig.4. Binding energy variation with d_{12} while keeping d_{23} and d_{13} fixed.

To examine the effect of an individual intermolecular separation on the binding behavior, we varied only the distance d_{12} while keeping d_{13} and d_{23} fixed. We found that the relative binding energy decreases continuously with increasing d_{12} until it reaches a minimum value of $E_{\min} \approx -0.01353$ at the equilibrium distance $d_b \approx 0.6588$.

Beyond this point, the binding energy gradually increases, indicating that the attractive interaction weakens as the oscillators move further apart. As illustrated in **Fig.4,** this behavior corresponds to the characteristic potential-energy well of a bound system. The obtained pair binding depth ($E_b^{\text{pair}} \approx 0.01353$) and the fitted Morse parameter ($s \approx 0.2775$) further confirm that varying a single intermolecular distance is sufficient to produce a stable attractive configuration, although the interaction remains weaker than in the fully symmetric geometry.

Case III: Two-variable-distance simulation (d_{12} and d_{13}varied, $d_{23} = 2.5$)

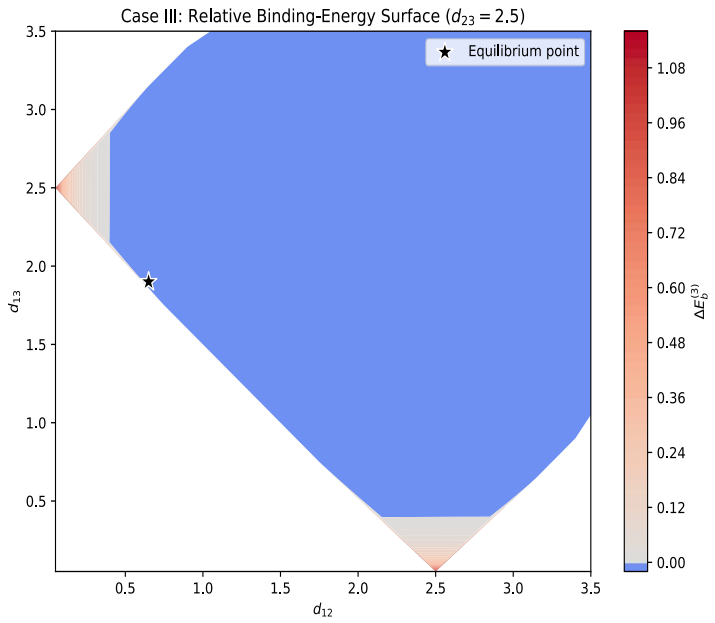


Fig.5. Two dimensional binding energy surface obtained by varying d_{12} and d_{13} with fixed d_{23}.

To investigate the combined effect of two intermolecular separations on the binding behavior, we simultaneously varied d_{12} and d_{13} while maintaining the third distance at $d_{23} = 2.5$. We found that the interaction energy depends on the coupled variation of both distances rather than on either distance individually. The minimum relative binding energy obtained in this case is $E_{\min} \approx -0.01473$, corresponding to the equilibrium configuration $d_{12,b} \approx$

0.6500 and $d_{13,b} \approx 1.9000$. The average equilibrium separation is $d_b \approx 1.6833$, with a pair binding depth of $E_b^{\text{pair}} \approx 0.00491$.

As illustrated in **Fig.5,** the two-dimensional binding-energy surface exhibits a localized energy minimum, indicating that stable binding is achieved only for a specific combination of $d_{12}$and d_{13}. Compared with the symmetric geometry of Case 1, the interaction becomes shallower, demonstrating that asymmetric variations in intermolecular distances reduce the overall binding strength. The fitted Morse parameter $s \approx 0.8475$ further suggests a broader and less localized potential well for this configuration.

Case IV: All Variable Distances

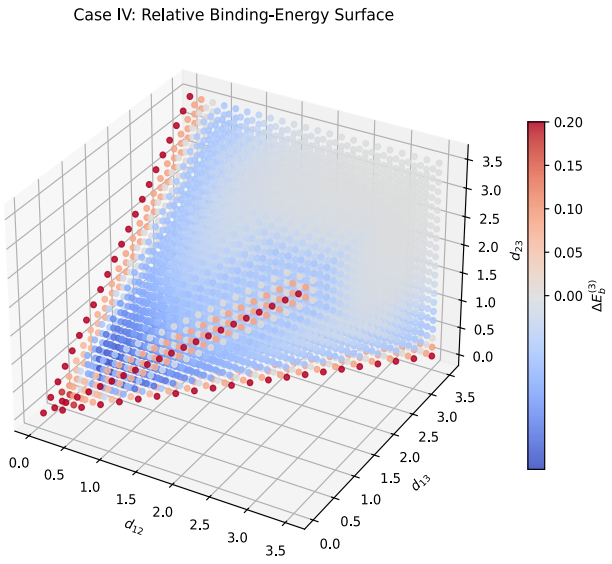


Fig.6. Three dimensional binding-energy landscape obtained by varying all intermolecular separations simultaneously.

Our objective in this case was to investigate the complete distance-dependent behavior of the proposed 3-QDO model by allowing all three intermolecular distances to vary simultaneously. Unlike the previous cases, where one or two pairwise distances were constrained, this simulation explores the full triangular configuration space to identify the global equilibrium geometry and understand how the combined variation of all three pairwise interactions influences the binding energy.

As illustrated in **Fig.6,** the three-dimensional binding-energy surface exhibits a well-defined dark-colored region corresponding to the stable attractive basin, whereas the lighter-colored regions represent weakly interacting or non-binding configurations with higher relative energy. We found that the global minimum occurs at $d_{12} = d_{13} = d_{23} \approx 0.7071$, with $E_{\min} \approx -0.03983$. The appearance of the minimum at equal pairwise distances indicates that

the symmetric triangular geometry remains the energetically preferred configuration even when all three distances are allowed to vary freely. This result confirms that the equilibrium binding of the 3-QDO system is governed by the collective optimization of all three pairwise interactions rather than by any individual intermolecular separation.

Case V: Symmetric geometry, different θ values

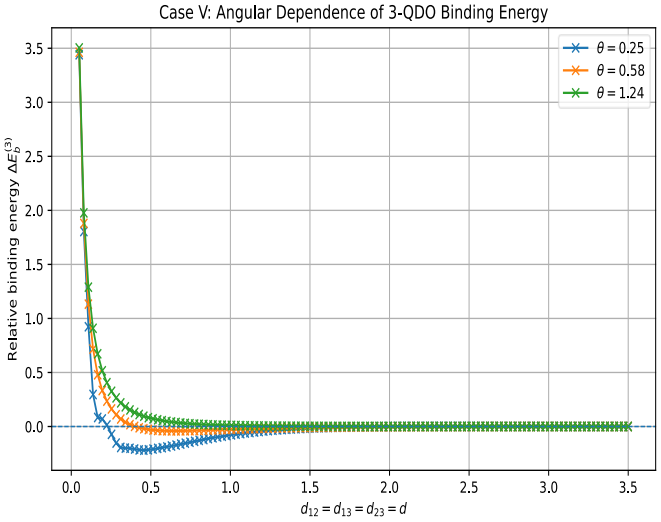


Fig.7. *Binding energy curves for the symmetric-geometry at different angular values* $\theta =$ 0.25,0.58,1.24

Case V was included to investigate the influence of the angular parameter while keeping the intermolecular separations equal($d_{12} = d_{13} = d_{23} = d$). As illustrated in **Fig.7, we** found that the binding-energy depth depends strongly on the angular arrangement of the three QDOs. The deepest attractive minimum is obtained for $\theta = 0.25$, where $d_b = 0.4559$ and $E_{\min} = -0.2192$, indicating the strongest binding among the three angular configurations. For the reference angle $\theta = 0.58$, the minimum shifts to $d_b = 0.6588$ with a much smaller binding energy $E_{\min} = -0.0406$,while for $\theta = 1.24$ the curve does not show a negative minimum within the scanned range and approaches zero at the largest distance. These results show that, even when the pairwise distances remain fixed, the angular orientation significantly controls the strength of the Coulomb interaction and can suppress the formation of a bound state.

Case VI: User-defined geometry

To demonstrate the flexibility of the proposed 3-QDO framework, we considered a user-defined geometry in which all intermolecular distances and angular parameters were specified independently. This case verifies that the developed photonic circuit can evaluate the interaction energy for any prescribed three-QDO configuration without modifying the

computational implementation. For the representative geometry $d_{12} = 0.55$, $d_{13} = 0.85$, $d_{23} = 1.00$with $\theta_{12} = \theta_{13} = \theta_{23} = 0.25$, the simulation produced $V_{\text{Coul}}^{(3)} = -0.13117$, $E_{\text{int}} = 1.40012$, $E_{\text{non}} = 1.53129$, and a binding energy of $E_b^{(3)} = -0.13117$. The probability density remained properly normalized ($\rho \approx 1.0000$), confirming the numerical consistency of the calculation. These results demonstrate that the proposed framework can directly evaluate the binding energy for any user-specified three-QDO geometry.

6. Conclusion

This study introduces a generalized three-body Quantum Drude Oscillator (3-QDO) model aimed at simulating non-covalent interactions in photonics using the Strawberry Fields continuous-variable platform. By broadening the traditional two-body QDO framework to accommodate any triangular molecular configurations, this new model allows for effective exploration of geometry-dependent many-body dispersion interactions. Simulations conducted on configurations that are symmetric, asymmetric, angle-dependent, and user-defined indicate that both the distances between molecules and their angular orientation significantly affect the equilibrium binding energy, with symmetric structures demonstrating the highest stability. These findings establish the proposed 3-QDO model as a scalable and physically valid approach for examining many-body dispersion interactions, laying a solid groundwork for advancing photonic quantum simulations into larger molecular systems and more complex quantum chemical applications.

Funding: This study has been carried out without any funding

Data availability: The data that support the findings of this study are available from the corresponding author upon reasonable request.

Declarations of competing interests: The authors declare no competing interests.

References

1. Israelachvili JN (2011) Intermolecular and surface forces, 3rd edn. Academic Press, London. https://doi.org/10.1016/C2011-0-05119-0

2. Stone AJ (2013) The theory of intermolecular forces, 2nd edn. Oxford University Press, Oxford. https://doi.org/10.1093/acprof:oso/9780199672394.001.0001

3. Dobson JF, White A, Rubio A (2006) Asymptotics of the dispersion interaction: analytic benchmarks for van der Waals energy functionals. Phys Rev Lett 96(7):073201. https://doi.org/10.1103/PhysRevLett.96.073201

4. Tkatchenko A, Scheffler M (2009) Accurate molecular van der Waals interactions from ground-state electron density and free-atom reference data. Phys Rev Lett 102(7):073005. https://doi.org/10.1103/PhysRevLett.102.073005

5. Ambrosetti A, Reilly AM, DiStasio RA Jr, Tkatchenko A (2014) Long-range correlation energy calculated from coupled atomic response functions. J Chem Phys 140(18):18A508. https://doi.org/10.1063/1.4865104

6. Burke K (2012) Perspective on density functional theory. J Chem Phys 136(15):150901. https://doi.org/10.1063/1.4704546

7. Møller C, Plesset MS (1934) Note on an approximation treatment for many-electron systems. Phys Rev 46(7):618–622. https://doi.org/10.1103/PhysRev.46.618

8. Purvis GD III, Bartlett RJ (1982) A full coupled-cluster singles and doubles model: the inclusion of disconnected triples. J Chem Phys 76(4):1910–1918. https://doi.org/10.1063/1.443164

9. Tkatchenko A, DiStasio RA Jr, Car R, Scheffler M (2012) Accurate and efficient method for many-body van der Waals interactions. Phys Rev Lett 108(23):236402. https://doi.org/10.1103/PhysRevLett.108.236402

10. Jones AP, Crain J, Sokhan VP, Whitfield TW, Martyna GJ (2013) Quantum Drude oscillator model of atoms and molecules: many-body polarization and dispersion interactions for atomistic simulation. Phys Rev B 87(14):144103. https://doi.org/10.1103/PhysRevB.87.144103

11. Willby C, Kiffner M, Tindall J, Crain J, Jaksch D (2025) Quantum information perspective on many-body dispersive forces. Phys Rev Lett 135(11):110403. https://doi.org/10.1103/f7yf-mxd5

12. Killoran N, Izaac J, Quesada N, Bergholm V, Amy M, Weedbrook C (2019) Strawberry Fields: a software platform for photonic quantum computing. Quantum 3:129. https://doi.org/10.22331/q-2019-03-11-129

13. Weedbrook C, Pirandola S, García-Patrón R, Cerf NJ, Ralph TC, Shapiro JH, Lloyd S (2012) Gaussian quantum information. Rev Mod Phys 84(2):621–669. https://doi.org/10.1103/RevModPhys.84.621

14. Sarkis M, Fallani A, Tkatchenko A (2023) Modeling noncovalent interatomic interactions on a photonic quantum computer. Phys Rev Res 5(4):043072. https://doi.org/10.1103/PhysRevResearch.5.043072