

ENR-MOD.02.NCSRD (Final Reporting of 2024 – 2025 activities)

Application of Quantum Computing to Plasma Fusion

presented by

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on behalf of

QC Project Team*



This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

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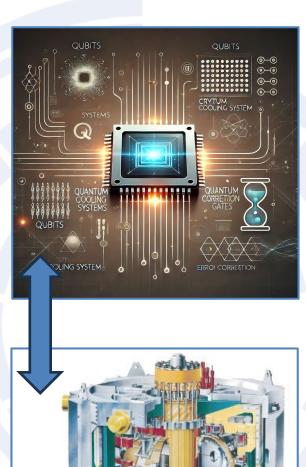


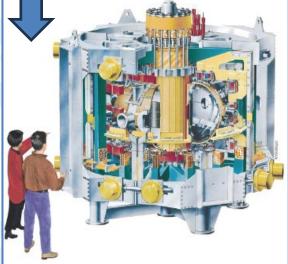
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Our Enabling Research Project's overview

- <u>Objective</u>: Highlight potential impact of quantum computing to plasma fusion in computational & theoretical level.
 - Quantum computing offers processing capabilities beyond classical HPC!
 - **►** Superposition, entanglement, quantum parallelism, ...
 - ► Already applied to the field of Quantum Information Science (QIS).
 - Plasma demonstrates complicated processes with high computational demands!
 - ▶ Propagation phenomena that require full-wave description (e.g. scattering).
 - ► Kinetic phenomena with nonlinearities (e.g. wave-wave interaction).
- Opportunity for relative fields of magnetic & inertial plasmas to establish synergies in fusion research!
 - Project implementation based on multidisciplinary team structure & collaboration.
- Research work spanning over different parts and goals.
 - <u>NTUA contributions</u>: QC formulation & simulation of Maxwell's equations for electromagnetic waves in cold & thermal inhomogeneous magnetized plasma.
 - <u>IPFN contributions</u>: QC formulation & simulation of 0D 3-wave interactions with variational error correction & quantum representation of the 1D problem.







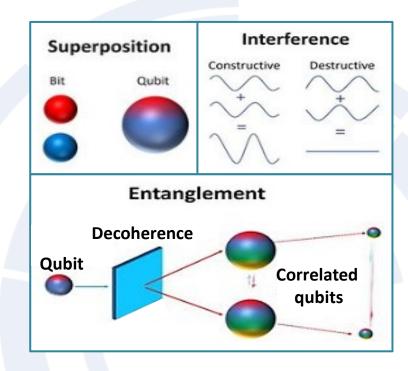
Basics of quantum computing

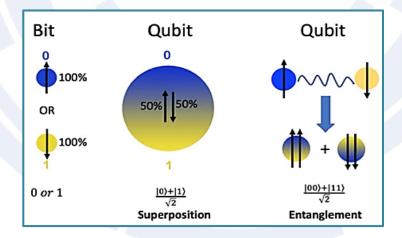
- Quantum Computing (QC) relies on many fundamental principles of quantum mechanics.
 - **Superposition** Decoherence Entanglement Interference.
 - Schrödinger's equation: $i\frac{\partial |\psi\rangle}{\partial t} = \hat{H} |\psi\rangle$, $\hat{H} = \hat{H}^{\dagger} \rightarrow$ unitary evolution operator
 - A system may possess one of a number of states $|\psi_i\rangle$ with probability p_i .

Probability density matrix formalism
$$i\frac{\partial \rho(t)}{\partial t} = [\hat{H}, \rho], \ \rho(t) = \hat{U}\rho_0 \hat{U}^\dagger \qquad \sum_i p_i = 1$$

- **Qubits: The fundamental carriers of information in QC!**
 - Qubits can behave like binary bits or weighted combinations of 0 & 1, but output a single bit of information at the end of the computation.
 - Superposed & entangled qubits can scale exponentially & create multi dimensional spaces (\rightarrow complex problems represented in new ways).

$$|\psi\rangle = \sum_{k=0}^{2^{n}-1} c_{k} |k\rangle, \quad k = j_{n-1}2^{n-1} + j_{n-2}2^{n-2} + \dots + j_{1}2^{1} + j_{0}2^{0} \quad |\psi\rangle_{entangled} \neq \bigotimes_{i=1}^{n} |qubit\rangle_{i}$$







Computer implementation of quantum states

Probabilistic nature (viewed as collection of measurement operators).

$$p(m) = \langle \psi | \hat{M}_{m}^{\dagger} \hat{M}_{m} | \psi \rangle, \quad |\psi\rangle' = \frac{\hat{M}_{m} |\psi\rangle}{\sqrt{p(m)}}.$$

- **1** Exponentially larger memory compared to classical machines, $dim(\mathcal{H}) = 2^n$
- Quantum parallelism
- Probabilistic and post-selective protocols
- Probability-preserving evolution is compatible with the use of logical "gates".

$$\hat{R}_x(\theta) = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix},$$

$$\hat{R}_{y}(\theta) = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix},$$

$$\hat{R}_z(\theta) = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$$

- Simplification in the representation by replacement of the multiple (groups) of gates with quantum circuits.
 - Quantum circuit: Collection of wires (\rightarrow qubits) & boxes (\rightarrow qubit gates).
 - **Input state** given on the left side, **outcome state** produced on the right side.
 - Control by **bit 1** \rightarrow solid black dot **vs** control by **bit 0** \rightarrow hollow white dot.
 - Advantage if the decomposition to qubit gates is simple (\rightarrow shallow circuit).

$$\begin{vmatrix}
0\rangle & \hat{H} \\
0\rangle & \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad \mathsf{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$



Quantum simulation of systems described by linear PDEs

• Schrödinger reformulation of classical PDE \rightarrow Quantum simulation of evolution operator.

$$i \frac{\partial |\boldsymbol{\psi}(\boldsymbol{r},t)\rangle}{\partial t} = \hat{D}(\boldsymbol{r},t) |\boldsymbol{\psi}(\boldsymbol{r},t)\rangle, \quad |\boldsymbol{\psi}\rangle \in \mathscr{H}$$
 Unitary evolution \rightarrow Hermitian tensor (characteristic of conservative systems) Non-unitary evolution \rightarrow anti-Hermitian part (connected to dissipation)

Quantum approach for Maxwell's equations (6-vector formalism for EM field).

$$\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t} = -\nabla \times \mathbf{E}(\mathbf{r},t), \quad \frac{\partial \mathbf{D}(\mathbf{r},t)}{\partial t} = \nabla \times \mathbf{H}(\mathbf{r},t),$$

$$\mathbf{v} \cdot \mathbf{D}(\mathbf{r},t) = 0, \quad \nabla \cdot \mathbf{B}(\mathbf{r},t) = 0.$$

$$i\frac{\partial \mathbf{d}}{\partial t} = \hat{\mathbf{M}}\mathbf{u}, \quad \nabla \cdot \mathbf{d} = 0, \quad \mathbf{d} = \begin{bmatrix} \mathbf{D} \\ \mathbf{B} \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} \mathbf{E} \\ \mathbf{H} \end{bmatrix}, \quad \hat{\mathbf{M}} = i\begin{bmatrix} 0 & \nabla \times \mathbf{X} \\ -\nabla \times & 0 \end{bmatrix}.$$

$$\mathbf{d}(\mathbf{r},t) = \hat{\mathbf{W}}(\mathbf{r})\mathbf{u}(\mathbf{r},t) + \int_{0}^{t} \hat{G}(\mathbf{r},t-\tau)\mathbf{u}(\mathbf{r},\tau)d\tau, \quad \hat{\mathbf{W}} = \begin{bmatrix} \epsilon(\mathbf{r}) & 0 \\ 0 & \mu(\mathbf{r}) \end{bmatrix}.$$

Quantum approach for wave-wave interaction problem (Hamiltonian formalism).

$$H = igA_1^{\dagger}A_2A_3 - ig^*A_1A_2^{\dagger}A_3^{\dagger}$$

$$COUPLING \\ COEFFICIENT$$

$$[A_j, A_l^{\dagger}] = \delta_{jl}$$

$$d_tA_1 = gA_2A_3$$

$$d_tA_2 = -g^*A_1A_3^{\dagger}$$

$$d_tA_3 = -g^*A_1A_2^{\dagger}$$

$$number operator$$

$$n_j = A_j^{\dagger}A_j$$

$$s_2 = n_1 + n_3, \ S_3 = n_1 + n_2$$

$$number operator$$

$$n_j = A_j^{\dagger}A_j$$
representation

^{*}On the basis $|n_1, n_2, n_3\rangle$, any state of the D-dimensional subspace V is represented by $|\psi\rangle = \sum_{j=0}^{\infty} \alpha_j |s_2 - j, s_3 - s_2 + j, j\rangle$



Principles followed by quantum computing algorithms

Quantum algorithms break down to the following stages:

- **▶** Qubit encoding & superposition of computational states.
- ► Generation of **entanglement** within the **quantum circuit**.
- ▶ Occurrence of **interference** between (some of) the different states.
- ➤ Some probable outcomes are canceled out, while others are amplified.
- ▶ The remaining outcomes are the computed solutions of the problem.

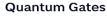


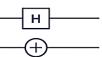


Entangelment













Qubit encoding: Representation of classical states as quantum superpositions.

• First step: Finite spatial discretization of the continuous (classical) state in configuration space.

$$\psi(\mathbf{r},t) = \sum_{i=0}^{s-1} \psi_i(\mathbf{r},t)e_i, \quad \mathcal{V} = [x_0, x_0 + L_x] \times [y_0, y_0 + L_y] \times [z_0, z_0 + L_z]$$

- Second step: Definition of amplitude & spatial qubit registers $\rightarrow |p_i\rangle = |i_0 + p_i\delta_i\rangle$, $p_i = 0, 1, ..., N_i 1$, for i = x, y, z. $\{|p\rangle\}$, $n_p = \log_2(N) = \log_2(N_x) + \log_2(N_y) + \log_2(N_z) = n_{px} + n_{py} + n_{pz}$ qubits $\{|q\rangle\}$, q = 0, 1, ..., s 1, $n_q = \log_2(d)$ qubits
- Third step: Discretization of configuration space on 3D lattice $\to N = N_x N_y N_z$ nodes, $\delta_i = L_i/N_i$, for i = x, y, z
- <u>Final result</u>: Classical state translates to $n=n_q+n_p-$ qubits quantum state $\rightarrow \psi(\mathbf{r},t) \leftrightarrow |\psi(t)\rangle = \sum_{q=0}^{q} \sum_{p=0}^{q} \psi_{qp}(t) |q\rangle |p\rangle$



Overview of our (dynamic) project workplan

	Project phases	Scientific milestones	
2	QC implementation for scattering & propagation of EM structures in cold magnetized plasma	Simulation of EM scattering in cold inhomogeneous magnetized plasma with QLA method	N
		Implementation of quantum-walk-based QLA algorithm for Maxwell's equations in cold magnetized plasma	U
U		Comparison of QLA computation with classical methods (scaling & accuracy vs FDTD computations)	Α
2	Optimization of variational circuits for 0D setup of 3-wave interaction	Characterization of decoherence errors for different QC parameters in the 0D 3-wave mixing problem	
Δ		Quantitative comparisons of decoherence errors for different quantum implementations of variational wavefunction ansatzes (parameterized circuit architectures)	P F
	in laser plasmas	Investigation on an optimal combination of quantum circuit depth & accuracy for 3-wave simulations	N
2	Quantum representation & QC implementation of Maxwell's equations in hot magnetized plasma	Theoretical reformulation of Maxwell's equations for dissipative plasmas in Schrödinger-Dirac form	N
_		Quantum circuit implementation for scattering & propagation of EM waves in hot magnetized plasma	U
0		[ADDITIONAL ACTIVITY] Theoretical QC framework for complex/nonlinear plasma physics problems	Α
2	Implementation of wave interaction scenarios in QC environment based on lower-dimensional simulations	Classical/Quantum simulations of lower-dimensional wave interaction problems in different parameter regimes for benchmark and diagnostic purposes	I
5		Implementation of wave interaction scenarios with different system parameters & circuit depths on IBM Qiskit and on quantum computer (if available)	P F N
		[ADDITIONAL ACTIVITY] Variational QC methods for the simulation of plasma instabilities	



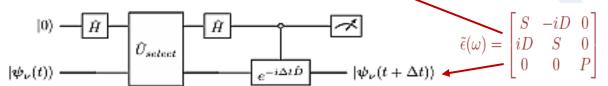
QC implementation for EM waves in cold magnetized plasma



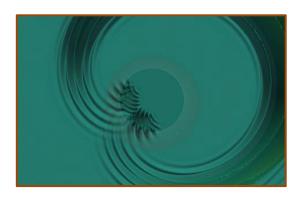
- QLA simulations of EM propagation & scattering in cold magnetized plasmas.
 - Quantum Lattice Algorithm (QLA) decomposes unitary evolution to product of simple unitary operators.

$$\begin{split} & \psi(\boldsymbol{r},\delta t) = \hat{C}_{vac} \hat{S} \hat{C}_{vac} \hat{C}_{\omega_{pi}} (\hat{\mathcal{R}}_{z}^{(pi)} \otimes I_{3\times3}) \hat{C}_{\omega_{pi}} \hat{C}_{\omega_{pe}}^{(1)} (\hat{\mathcal{R}}_{z}^{(pe)} \otimes I_{3\times3}) \hat{C}_{\omega_{pe}}^{(1)} \hat{C}_{\omega_{pe}}^{(2)} (\hat{\mathcal{R}}_{z}^{(pe)} \otimes I_{3\times3}) \hat{C}_{\omega_{pe}}^{(2)} \hat{C}_{\omega_{ei}}^{(2)} [I_{4\times4} \otimes \hat{R}_{z}^{(z)} (\theta_{ci}/2)] \\ & \times [I_{2\times2} \otimes \hat{R}_{z} (\hat{\sigma}_{z}^{(z)} \theta_{ci}/2)] \hat{\mathcal{R}}_{z}^{(1),(ci)\dagger} \hat{\mathcal{R}}_{z}^{(2),(ci)\dagger} \hat{C}_{\omega_{ci}} \hat{C}_{\omega_{ce}} [I_{4\times4} \otimes \hat{R}_{z}^{(z)} (\theta_{ce}/2)] [I_{2\times2} \otimes \hat{R}_{z}^{\dagger} (\hat{\sigma}_{z}^{(z)} \theta_{ce}/2)] \hat{\mathcal{R}}_{z}^{(1),(ce)\dagger} \hat{\mathcal{R}}_{z}^{(2),(ce)} \hat{C}_{\omega_{ci}} \psi_{0}. \end{split}$$

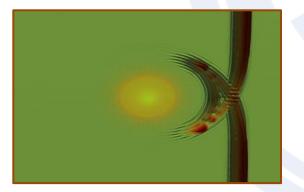
 Quantum circuit implementation for estimating the state vector (using 2-qubit registers).

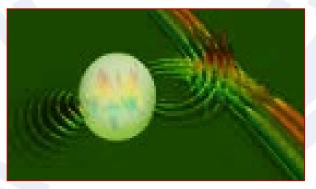


• QLA simulations of Gaussian wave-packet scattering by scalar inhomogeneous dielectrics (corresponding to turbulent plasma "blob" structures) test the capabilities of the spatio-temporal initial value simulators.









Visualization of the wave electric field's z-component in QLA simulation of electromagnetic wave-packet scattering off a dielectric inhomogeneity in the shape of a cylinder (left), ellipse (middle left), cone (middle right) and sphere (right).



QC implementation for EM waves in cold magnetized plasma



- Development of quantum-walk QLA algorithm for cold magnetized plasmas.
 - Explicit quantum algorithm by encoding QLA as a quantum-walk Hamiltonian simulation process.
 - Sequence of streaming, coin & simple unitary operators $\rightarrow |\psi(t+\Delta t)\rangle = \hat{V}_{pe}\hat{V}_{pi}\hat{V}_{ce}\hat{V}_{ci}\hat{U}_{QLA}|\psi(t)\rangle$

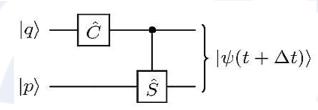
$$\hat{U}_{QLA} = \hat{U}_{Y}\hat{U}_{X}$$

$$\hat{U}_{X} = \hat{S}_{25}^{+x}\hat{C}_{X}^{\dagger}\hat{S}_{25}^{-x}\hat{C}_{X}\hat{S}_{14}^{-x}\hat{C}_{X}^{\dagger}\hat{S}_{14}^{+x}\hat{C}_{X}\hat{S}_{25}^{-x}\hat{C}_{X}\hat{S}_{25}^{+x}\hat{C}_{X}^{\dagger}\hat{S}_{14}^{+x}\hat{C}_{X}\hat{S}_{14}^{-x}\hat{C}_{X}^{\dagger}$$

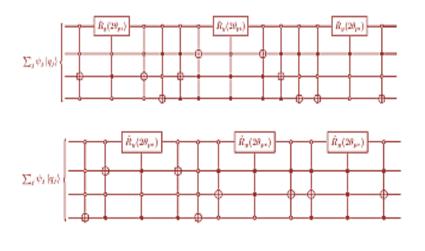
$$\hat{U}_{Y} = \hat{S}_{25}^{+y}\hat{C}_{Y}^{\dagger}\hat{S}_{25}^{-y}\hat{C}_{Y}\hat{S}_{03}^{-y}\hat{C}_{Y}^{\dagger}\hat{S}_{03}^{+y}\hat{C}_{Y}\hat{S}_{25}^{-y}\hat{C}_{Y}\hat{S}_{25}^{+y}\hat{C}_{Y}^{\dagger}\hat{S}_{03}^{+y}\hat{C}_{Y}\hat{S}_{03}^{-y}\hat{C}_{Y}^{\dagger}$$

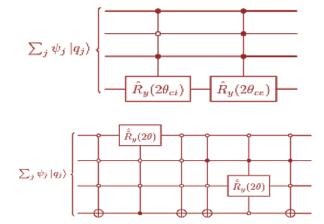
$$\hat{S}_{ij}^{+x,y} = (|q_i\rangle \langle q_i| + |q_j\rangle \langle q_j|) \otimes \hat{S}^{+x,y}.$$

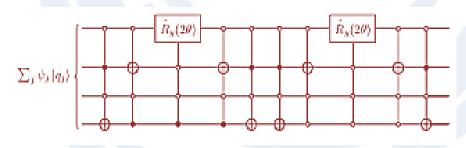
$$+ \sum_{k-\{i,j\}} |q_k\rangle \langle q_k| \otimes I_{2_{P\times 2_P}}.$$



- Quantum walks have been prioritized over relevant Hamiltonian algorithms (QHS) due to their natural alignment with QLA procedure, as well as due to simpler/explicit quantum encoding.
- Quantum circuit implementation of all operators (→ application envisaged using 2-qubit registers).









Algorithm ready to port to quantum hardware



QC implementation for EM waves in cold magnetized plasma

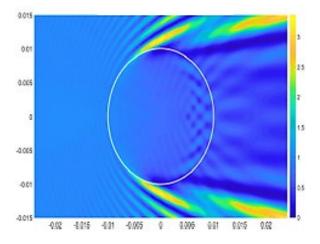


- Comparison with FDTD & investigation of limitations & advantages of each method.
 - Challenges in computationally defining appropriate initial conditions for simulations in Qiskit.
 - ► Traditional response theory is not formulated as an initial value problem!
 - Resource-efficiency in the asymptotic limit for the quantum walk algorithm over (3D) FDTD method.
 - <u>Case study</u>: EM scattering in 3D lattice with N nodes.
 - ► QLA *poly[log(N)]* logical gates vs FDTD *O(N)* operations.
 - ► Supported by QLA data in reduced non-dispersive cases.

Method	$\mathcal{N}_{gate}(N)$	$N_{gate}^{T}(N)$	$N_{gate}^{T}(\varepsilon)$
FDTD	O[poly(N)]	$O[N^{1/\kappa}poly(N)]$	$O[(T^2/\varepsilon)poly(T^2/\varepsilon)^{\kappa}]$
QLA	$O(\log^2 N) - O(N)$	$O(N^{2/\kappa} \log^2 N) - O(N^{\frac{2+\kappa}{\kappa}})$	$O[(T^2/\varepsilon)\log^2(T^2/\varepsilon)^{\kappa/2}] - O[(T^2/\varepsilon)^{\frac{2+\kappa}{2}}]$

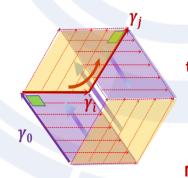
- Setup similar FDTD simulations of EM wave propagation in cold plasma to benchmark with QC method.
 - ► First results show sufficient agreement.

$$\begin{split} H_{sq}|_{i,j,k}^{n+\frac{1}{2}} &= H_{sq}|_{i,j,k}^{n-\frac{1}{2}} - \frac{\Delta t}{\mu_0 \Delta r} \Psi_q(E_s|_{i,j,k}^n). \\ E_{sq}|_{i,j,k}^{n+1} &= \sum_{l=1}^3 \sum_{m=1}^3 \vartheta_{ql} \left[\xi_{lm} E_{sm}|_{i,j,k}^n + \Psi_q(H_s|_{i,j,k}^{n+\frac{1}{2}}) \right. \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. - \sigma_{lm} E_{im}|_{i,j,k}^{n+\frac{1}{2}} - (\varepsilon_{lm} - \delta_{lm} \varepsilon_0) \frac{\partial E_{im}}{\partial t} \right|_{i,j,k}^{n+\frac{1}{2}} \\ &\left. -$$



Pursue further improvement in scaling via geometric methods

- Geometric representation of cold magnetized plasmas using Clifford algebra (CLA).
- Offers a geometric invariant framework that benefits computations not only in QC but also in classical plasma simulation techniques.



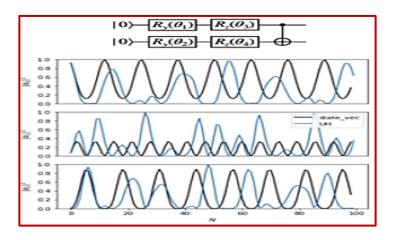
Geometric
representation of a
grade-3 trivector in
the framework of CLA
corresponding to
synthesis of spatial
rotations and time
translations in
Minkowski spacetime.

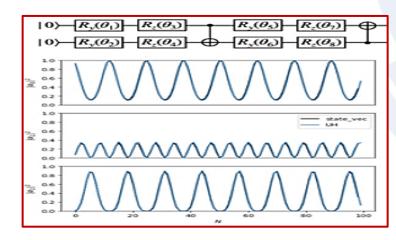


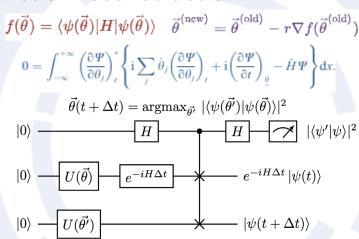
Optimization of variational circuits for 3-wave interaction



- VQE simulations of 0D 3-wave mixing scenarios under different QC parameters.
 - Study of OD setup: Mapping of the occupation probability of each wave to a 2-qubit system.
 - Variational approach has the advantage of shorter circuit depth & wavefunction reconstruction.
 - ► Standard QHS algorithm may accumulate errors after several time-steps.
 - ► Variational Quantum Eigensolver (VQE) is a hybrid quantum-classical method to model the system as a cost function minimization problem.
 - **Requires** variational principle to map QC states to the VQE parameters.
 - VQE noiseless simulation for 2 ansatzes of different expressibility.
 - ▶ Deeper circuits appear more robust than shallower circuits.
 - ► Optimal observable retrieval depends on robustness of ansatz to noise.







VQE ansatzes of 3-wave mixing problem for 2 different variational blocks.

(from top to bottom) The quantum circuit, with a block including the corresponding parametrized rotations, and simulation results. The 3 rows represent the time evolution of the relative probabilities or weights of each of the 3 waves.

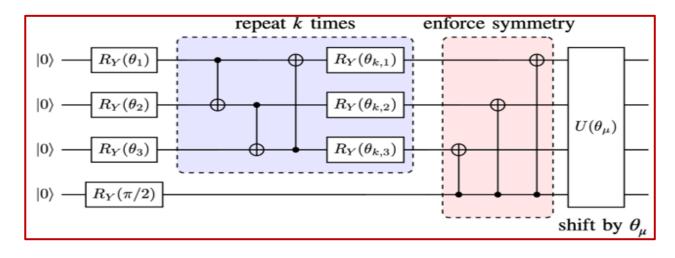


Optimization of variational circuits for 3-wave interaction

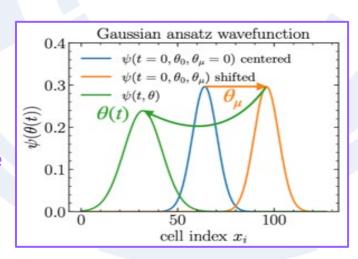


 $\psi_a(x,0) = \frac{1}{(2\pi)^{1/4}\sqrt{a}}e^{-x^2/4a^2}$

- Quantum implementation & analysis of 3-wave interaction scenarios.
 - Simulation results yield particular variational ansatz that allows for shallower & more robust circuits.
 - ► Support simulation input via Gaussian-like wavefunctions using only few parameters.
 - ► Provision of improved chances for efficient use in quantum hardware computers!
 - Quantum circuit implementation for the 0D version of the 3-wave system.
 - \blacktriangleright All the (first in sequence) n-1 qubits are based on a Y-rotation gate with a parameterized variable.
 - ► Employment of CNOT logical (gate) operations assuming a general (n-1)-qubit wavefunction.
 - ► Circuit depth minimization by enforcing mirror symmetry around the midpoint of the computational basis.
 - \blacktriangleright The last block introduces a series of advection operations which shift the wavefunction by ϑ_{μ} .



Shifting of the Gaussian variational ansatz and position of the wavefunction after time t.



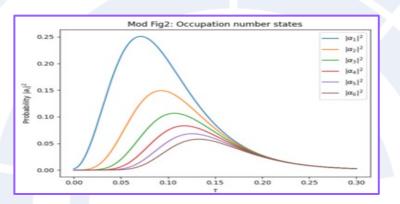


Optimization of variational circuits for 3-wave interaction



• Quantification of error reduction based on different variational algorithms.

- Optimal VQ circuits for scenarios mapped to physical problems.
 - ▶ Prediction of required resources for large-scale QC simulations.
 - ► Study expansions on analytic solutions to n-wave mixing problems.
 - ► Calculation of probabilities of occupation number states for n = 3.
- Gaussian-like ansatz shows possibility of efficiently reproducing symmetrical functions (to be used as simulation input).

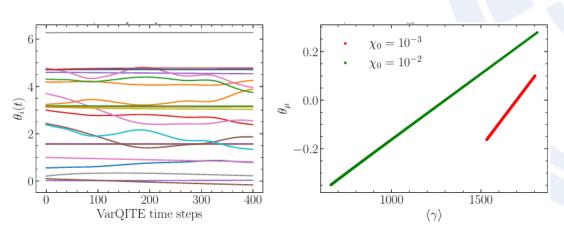


- ▶ Performed tests on robustness of the ansatz by varying the quantum circuit size & depth.
- ► Quantum circuit needs to have the same number of controlled rotations blocks as its number of qubits.
- ► <u>Caveat of method</u>: Fails to reproduce effects owed to asymmetry (like skewness).

A "TEST-CASE" PROBLEM Quantum Radiation Reaction

$$\frac{\partial f(t,\gamma)}{\partial t} = \frac{\partial}{\partial \gamma} \left[-(Af) + \frac{1}{2} \frac{\partial}{\partial \gamma} \left(Bf \right) \right] \begin{array}{c} \text{Fokker-Planck} \\ \text{equation} \end{array}$$

$$A \sim \frac{2}{3} \frac{\alpha mc^2}{\hbar} \chi^2 \quad \mathcal{B} \sim \frac{55}{24\sqrt{3}} \frac{\alpha mc^2}{\hbar} \gamma \ \chi^3$$



(left) The evolution of variational parameters for nonlinearity parameter $\chi_0 = 10^{-3}$, (right) The linear correlation between the average energy from the wavefunction and the parameter of the wavefunction translation.

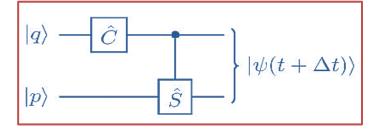


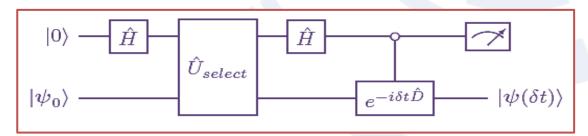
QC representation of Maxwell's equations in dissipative plasma



- Formulation of non-Hermitian plasma permittivity tensors for modeling dissipation.
 - Unitary evolution structure in Schrödinger representation of Maxwell's equations is broken!
 - ▶ Dissipation appears as a sparse diagonal operator occupying a multi-dimensional subspace.
 - ► Suzuki-Trotter approximation for the evolution operator enables isolation of its non-unitary part.
 - ▶ The unitary part is implemented with QLA on n qubits, whereas the non-unitary part needs more effort...
 - Example: Algorithmic approach to efficiently handle collisional dissipation effects in dispersive media.
 - ► Introducing a phenomenological collision frequency between the plasma species (ions & electrons).
 - ► Generalization of quantum-walk QLA formulation with post-selective time marching procedure.

$$\begin{split} |\psi_{\nu}(t+\Delta t)\rangle &= e^{-i\Delta t \hat{D}} e^{-\Delta t \hat{D}_{diss}} \, |\psi_{\nu}(t)\rangle + O(\Delta t^2) \\ p_{success}(T) &= \|\psi_{\nu}(t+\Delta t)\|^2 \cdot \frac{\|\psi_{\nu}(t+2\Delta t)\|^2}{\|\psi_{\nu}(t+\Delta t)\|^2} \cdots \frac{\|\psi_{\nu}(t+(N_t-1)\Delta t)\|^2}{\|\psi_{\nu}(t+(N_t-2)\Delta t)\|^2} \cdot \frac{\|\psi_{\nu}(t+T)\|^2}{\|\psi_{\nu}(t+(N_t-1)\Delta t)\|^2} \\ \hat{K} &= e^{-\Delta t \hat{D}_{diss}} = diag(I_{6N\times 6N}, e^{-\nu\Delta t}I_{6N\times N}) \\ \hat{U}(|0\rangle \otimes |\psi_{\nu}(t)\rangle) &= |0\rangle \, \hat{K} \, |\psi_{\nu}(t)\rangle + \frac{1}{2} \, |1\rangle \, (\hat{K}_z - \hat{K}_z^{\dagger}) \, |\psi_{\nu}(t)\rangle \\ &= \lim_{N_t \to \infty} p_{success}(T) = e^{\ln P} = e^{-a_0} \geq \frac{1}{e} \end{split}$$





QC circuits of the QLA-based unitary (left) and Trotterized non-unitary (right) evolution operators for collisionally dissipative systems.

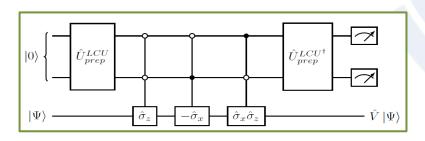


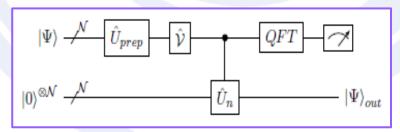
QC representation of Maxwell's equations in dissipative plasma



- Probabilistic dilation QC algorithms for plasma wave propagation including dissipation.
 - Algorithm #1: Linear damping-type, completely positive trace-preserving (CPTP) quantum channel.
 - ► An unspecified environment interacts with the system & produces the non-unitary evolution.
 - The unspecified environment is modeled by one ancillary qubit, resulting in implementation scaling of $O(2^{n-1}n^2)$ elementary gates for the (closed) system-environment evolution operator in the dilated space.
 - Algorithm #2: Approximation of non-unitary operators as a Linear Combination of Unitaries (LCU).
 - ▶ Diagonal structure of dissipation \rightarrow Optimized representation of non-unitary part over $O(2^n)$ gates.
 - ightharpoonup LCU method further reduces the implementation scaling into O[poly(n)] basic gates.
 - Algorithm #3: Biorthogonal representation of the non-unitary evolution operator.
 - ► Mapping non-unitary process to isomorphic unitary matrix in the orthonormal computational basis.
 - ▶ Option to implement non-unitary operators with eigenvalues > 1 (\rightarrow modeling of wave instabilities).
 - ▶ Implementation cost of the method scales as $O(N^22^N)$ using a single unitary oracle ("black box").

$$\begin{split} \hat{\mathcal{U}}_{diss} &= \prod_{l=1}^r \hat{\mathcal{R}}_y(\theta_l) \qquad \rho(\delta t) = \frac{e^{-i\delta t \hat{D}} \hat{K}_0 \rho(0) \hat{K}_0^\dagger e^{i\delta t \hat{D}}}{\langle \psi_0 | \hat{K}_0^2 | \psi_0 \rangle} \\ \hat{\mathcal{U}}_{diss} &\left. | 0 \right\rangle \left| \psi_0 \right\rangle = \left| 0 \right\rangle \hat{K}_0 \left| \psi_0 \right\rangle + \frac{1}{2} \left| 1 \right\rangle (\hat{K}_{0z} - \hat{K}_{0z}^\dagger) \left| \psi_0 \right\rangle \\ C^n \hat{U}_n (\hat{\mathcal{V}} \otimes \hat{1}) (\left| \bar{\psi} \right\rangle \otimes \left| 0 \right\rangle^{\otimes \mathcal{N}}) &= \frac{1}{c} \sum_{n,m} \left| n \right\rangle \otimes V_{nm} c_m \left| u_n \right\rangle \end{split}$$





QC implementations of the CPTP-based, LCU-based and biorthogonal-based evolution operators for waves in dissipative plasma.



Additional activity on QC for complex/nonlinear plasma systems



- Transitioning to quantum algorithms for nonlinear physical problems and plasmas.
 - Problem #1: Classical fluid dynamics in the presence of nonlinearities.
 - ▶ QC reformulation via 2-stage generalized Madelung transformation on a scalar Gross-Pitaevski equation.

$$\frac{\partial \rho u_i}{\partial t} + \partial_j \left[\rho u_i u_j + p \delta_{i,j} \right] = -\partial_i \left[4 \, \partial_j \sqrt{\rho} \partial_i \sqrt{\rho} - \nabla^2 \rho \, \delta_{i_j} \right] \quad \blacksquare \psi = \sqrt{\rho} \, e^{i\theta/2} \quad \Longrightarrow \quad i \frac{\partial \psi}{\partial t} = \left(-\nabla^2 + V + g |\psi|^2 \right) \psi \quad \blacksquare |\nabla \mathbf{s}|^2 = 4 \rho_0 \left(|\nabla \psi_1|^2 + |\nabla \psi_2|^2 \right) - \rho_0 |\mathbf{u}|^2 \\ \Longrightarrow \quad i \frac{\partial \psi}{\partial t} = \left(-\nabla^2 + \frac{1}{4\rho^2} |\nabla \mathbf{s}|^2 \right) \psi \quad \blacksquare |\nabla \mathbf{s}|^2 = 4 \rho_0 \left(|\nabla \psi_1|^2 + |\nabla \psi_2|^2 \right) - \rho_0 |\mathbf{u}|^2 \\ \Longrightarrow \quad i \frac{\partial \psi}{\partial t} = \left(-\nabla^2 + \frac{1}{4\rho^2} |\nabla \mathbf{s}|^2 \right) \psi \quad \blacksquare |\nabla \mathbf{s}|^2 = 4 \rho_0 \left(|\nabla \psi_1|^2 + |\nabla \psi_2|^2 \right) - \rho_0 |\mathbf{u}|^2 \\ \Longrightarrow \quad i \frac{\partial \psi}{\partial t} = \left(-\nabla^2 + \frac{1}{4\rho^2} |\nabla \mathbf{s}|^2 \right) \psi \quad \blacksquare |\nabla \mathbf{s}|^2 = 4 \rho_0 \left(|\nabla \psi_1|^2 + |\nabla \psi_2|^2 \right) - \rho_0 |\mathbf{u}|^2 \\ \Longrightarrow \quad i \frac{\partial \psi}{\partial t} = \left(-\nabla^2 + \frac{1}{4\rho^2} |\nabla \mathbf{s}|^2 \right) \psi \quad \blacksquare |\nabla \mathbf{s}|^2 = 4 \rho_0 \left(|\nabla \psi_1|^2 + |\nabla \psi_2|^2 \right) - \rho_0 |\mathbf{u}|^2 \\ \Longrightarrow \quad i \frac{\partial \psi}{\partial t} = \left(-\nabla^2 + \frac{1}{4\rho^2} |\nabla \mathbf{s}|^2 \right) \psi \quad \blacksquare |\nabla \mathbf{s}|^2 + \rho_0 \left(|\nabla \psi_1|^2 + |\nabla \psi_2|^2 \right) - \rho_0 |\mathbf{u}|^2$$

► Unitary QLA determined as 2nd-order discrete representation.

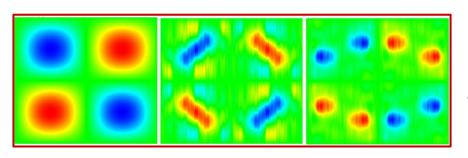
$$\psi(t + \Delta t) = \mathbf{U_Y} \, \mathbf{U_X} \psi(t)$$

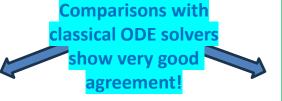
 $\mathbf{U_X} = S_2^{-x} C. S_2^{+x} C. S_2^{-x} C. S_2^{+x} C, S_1^{-x} C. S_1^{+x} C. S_1^{-x} C. S_1^{+x} C.$

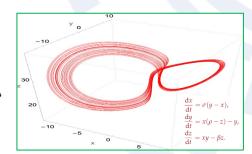
- Problem #2: Chaotic dynamics of the Lorentz attractor.
 - ► Time-marching algorithm combined with QC-arithmetic Hadamard model for constructing the nonlinear terms.

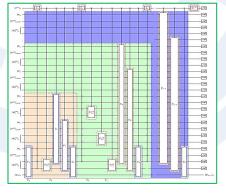
$$\begin{aligned} \hat{U}_{nl} \Big| \boldsymbol{\psi}^{\otimes K} \Big\rangle &= \sum_{j=1}^{K} a_{j} \Big| \odot^{j} \boldsymbol{\psi} \Big\rangle = \sum_{j=1}^{K} \sum_{i=0}^{2^{n}-1} a_{j} \psi_{i}^{j} | i \rangle. \qquad |\psi\rangle \\ \hat{U}_{select}^{h} &= \sum_{k=0}^{2^{n}-1} \hat{S}_{-}^{k} \otimes |k\rangle \langle k|, \quad \hat{S}_{-}^{0} = \hat{1}, \quad \hat{S}_{-} | k \rangle = |k-1\rangle \qquad |\phi\rangle \end{aligned} \qquad |\psi \odot \phi\rangle$$

Caveat: QNC theorem → Nested recursive structure scaling worse than RK solvers.









QLA computation of initial 2D Taylor-Green vortices, following the time evolution (left to right) of a nonlinear conservative fluid equation.

Lorentz attractor trajectory (left) as computed by a 2nd-order recursive QC algorithm (right)

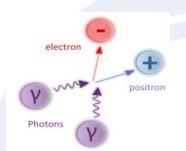


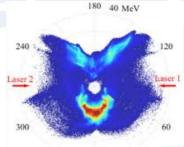
Simulation of lower-dimensional n-wave interaction problems



- QMC simulations of interacting photon beams in different parameter regimes.
 - Investigation of pair production via linear Breit-Wheeler mechanism.
 - ► Strong connection with applications envisaged in the current era of Noisy Intermediate-Scale Quantum (NISQ) computers.



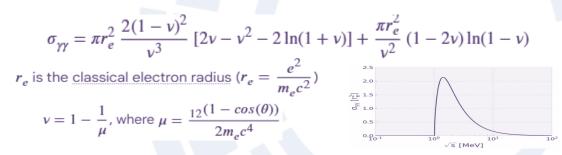


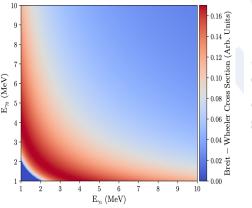


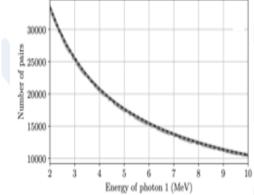
- Physics setup: Two photon beams with uniform & Gaussian-like energy distributions collide head-on.
 - ► Breit-Wheeler cross section & pair-production probability readily calculated from theory.
- Estimation of the pair production number.
 - ► Calculation via Quantum Monte Carlo (QMC) integration algorithm.

$$A|0
angle_n|0
angle = \sum_{i=0}^{2^n-1} \sqrt{f_i} \sqrt{p_i} |i
angle_n|1
angle + \sum_{i=0}^{2^n-1} \sqrt{1-f_i} \sqrt{p_i} |i
angle_n|0
angle$$

► Requires to construct a **Grover operator** & apply an **amplitude estimation algorithm**.







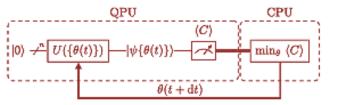
Breit-Wheeler cross section (left) and number of produced pairs (right) for head-on photon collision.

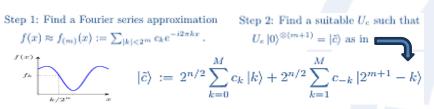


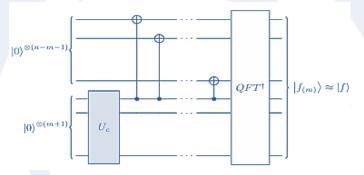
Simulation of lower-dimensional n-wave interaction problems



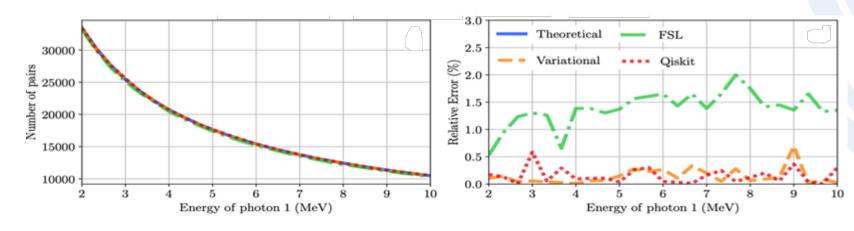
- Programming simulation algorithms for the 2-photon interaction in Qiskit emulator.
 - Overview of requirements for the quantum circuital structure towards QC simulations.
 - ► Beam energy initialization into quantum state → Variational approach + Fourier Series Loader (FSL).







- ightharpoonup Offline post-processing (\rightarrow avoid repeated simulations on real hardware).
- **►** Embedding of cross-sections using controlled rotations (via QC gates).
- Results of QC simulations compared for each initialization technique (Qiskit vs FSL vs variational).
 - ▶ Qiskit & variational method give better accuracy than FSL (below truncation number limit of *n-1* qubits).



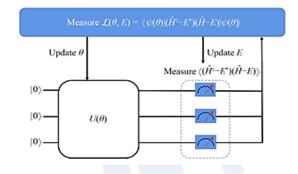
(left) Calculated number of pairs produced by 2 interacting photon beams by varying the energy of the monoenergetic photon beam, and (right) relative error of the results from FSL, variational and Qiskit's own initialization vs the theoretical results.

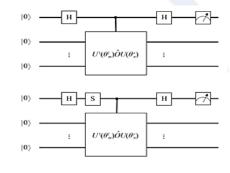


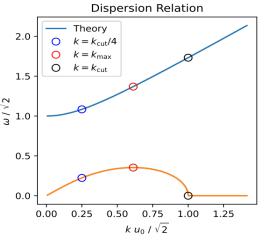
Additional activity on QC simulation of plasma instabilities

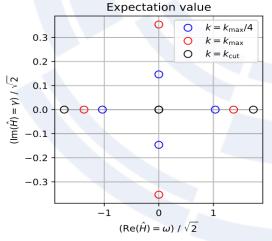


- Setup of variational QC models for simulating kinetic wave-plasma instabilities.
 - Quantum algorithms have the potential to efficiently solve certain classes of eigenvalue problems.
 - **▶** Quantum Phase Estimation (QPE) algorithm recovers real spectra of Hermitian Hamiltonians.
 - ► Characterization of instabilities require access to complex eigenvalue calculation!
 - Variational framework encodes non-Hermitian plasma
 Hamiltonians into measurable Hermitian cost functions.
 - ► Cost function's minima yield the desired eigenvalues.
 - ► Potential applications to kinetic plasma instabilities of complex nature (nonlinear, resistive, multi-branch, ...).
 - Proof of concept given over simple plasma dispersion problems!
 - ► Cold 2-stream instability dynamics encoded to 4x4 matrix of density & velocity beam perturbations.
 - ► QC algorithm recovers the wave's frequency & growth rate.
 - ightharpoonup Ran on present-day QC (\rightarrow IonQ)!









(left) Dispersion relation of the 2-stream instability for a cold plasma fluid and (right) expectation values of the dispersion equation roots.



Results published in peer-reviewed journals & book chapters

Authors	Title of manuscript	Journal/Book
E. Koukoutsis, K. Hizanidis, A. K. Ram, G. Vahala	Quantum simulation of dissipation for Maxwell's equations in dispersive media	Future Gener. Comput. Syst., vol. 159, pp. 221–229 (2024)
Ó. Amaro, L. I. Iñigo Gamiz, M. Vranic	Variational quantum simulation of the Fokker–Planck equation applied to quantum radiation reaction	J. Plasma Phys., vol. 91, pp. 122 (2025)
E. Koukoutsis, P. Papagiannis, K. Hizanidis, A. K. Ram, G. Vahala, Ó. Amaro, L. I. I. Gamiz, D. Vallis	Quantum implementation of non-unitary operations with biorthogonal representations	Quantum Inf. Comput., vol. 25, pp. 141–155 (2025)
M. Soe, G. Vahala, L. Vahala, A. K. Ram, E. Koukoutsis, K. Hizanidis	Quantum lattice representation of nonlinear classical physics	Radiat. Eff. Defects Solids, vol. 180, pp. 98–102 (2025)
A. K. Ram, E. Koukoutsis, G. Vahala, K. Hizanidis	Mathematical foundation for quantum computing of electromagnetic wave propagation in dielectric media	Emerging Applications of Ions & Plasmas, Springer Nature (2025)
K. Hizanidis, E. Koukoutsis, P. Papagiannis, A. K. Ram, G. Vahala	Spacetime algebra formulation of cold magnetized plasmas	Phys. Plasmas, vol. 32, art. 092110 (2025)
E. Koukoutsis, G. Vahala, M. Soe, K. Hizanidis, L. Vahala, A. K. Ram	Time-marching quantum algorithm for simulation of the nonlinear Lorenz dynamics	Entropy, vol. 27, p. 871 (2025)
E. Koukoutsis, K. Hizanidis, G. Vahala, C. Tsironis, A. K. Ram, M. Soe, L. Vahala	A quantum walk inspired algorithm for simulating wave propagation and scattering in conservative and dissipative magnetized plasma	arXiv, art. 2503.24211 (2025)

2 articles in preparation: QMC Simulations for Strong Field QED (Gamiz et al) QC Framework for Transient Scattering of EM Waves by Dielectric Structures (Ram et al)



Results presented in conferences, workshops & meetings

Presenters	Type of contribution	Conference
E. Koukoutsis	Oral contribution	NTUA Young Minds Physics Day 2024 (Greece, 17/5/2024)
E. Koukoutsis	Poster presentation	50 th EPS Conference on Plasma Physics (Spain, 8 – 12/7/2024)
Ó. Amaro	Poster presentation	37 th European Conference on Laser Interaction with Matter (Portugal, 16 – 20/9/2024)
E. Koukoutsis	Poster presentation	66 th APS Division of Plasma Physics Meeting (United States, 7 – 11/10/2024)
E. Koukoutsis	Poster presentation	European Quantum Technologies Conference 2024 (Portugal, 18 – 20/11/2024)
Ó. Amaro	Poster presentation	European Quantum Technologies Conference 2024 (Portugal, 18 – 20/11/2024)
E. Koukoutsis	Oral contribution	Quantum Science & Technology Activities @ NTUA (Greece, 17/3/2005)
Ó. Amaro	Poster presentation	Quantum Day @ PT (Portugal, 14/4/2025)
L. I. Iñigo Gamiz	Poster presentation	Quantum Day @ PT (Portugal, 14/4/2025)
Ó. Amaro	Poster presentation	2 nd FoQaCiA Workshop (Portugal, 2 – 6//2025)
Ó. Amaro	Oral contribution	51st EPS Conference on Plasma Physics (Lithuania, 7 – 11/7/2025)
E. Koukoutsis	Poster presentation	51st EPS Conference on Plasma Physics (Lithuania, 7 – 11/7/2025)
K. Hizanidis	Invited lecture	21st European Fusion Theory Conference (France, 23 – 26/9/2025)
K. Hizanidis	Poster presentation	21st European Fusion Theory Conference (France, 23 – 26/9/2025)



Scientific events organized for project dissemination

Satellite meeting "Quantum Computing for Plasma Physics" (part of the 2025 EPS Plasma Conference at Lithuania)



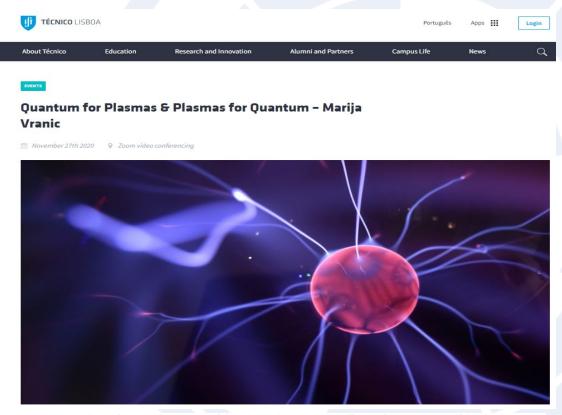




Harnessing the microscopic quantum particles and phenomena as powerful information carriers and computational microprocessors for breakthrough advancements in large-scale plasma fusion research.

Guest Editors Efstratios Koukoutsis Lucas I. Inigo Gamiz Marija Vranic

Colloquium "Quantum for Plasmas & Plasmas for Quantum" (series of lectures on QC organized regularly by IPFN)



Everyone is welcomed to attend (registration required). Each session will include a summary or review talk of 30 minutes followed by a discussion of 30 minutes. The discussion sessions will run once per month, and will be hosted by Técnico Professors Yasser Omar (DM/IST & IT) and Luís Oliveira e Silva (GoLP/IPFN/IST).



Summary of project outcome

- QC algorithms for various problems relevant to plasma fusion.
 - QC implementation for EM waves in cold magnetized plasma.
 - ▶ QLA simulations of EM propagation & scattering in cold magnetized plasmas.
 - ▶ Implementation of quantum-walk QLA & comparison with classical methods.
 - QC representation of Maxwell's equations in dissipative plasma.
 - ► Formulation of non-Hermitian plasma permittivity tensors for modeling dissipation.
 - ▶ Probabilistic dilation algorithms for plasma wave propagation including dissipation.
 - ► Transitioning to quantum algorithms for nonlinear physical problems and plasmas.
 - Optimization of variational circuits for 3-wave interaction.
 - ▶ VQE simulations of 0D 3-wave mixing scenarios under different QC parameters.
 - ▶ Quantum implementation & analysis of 3-wave interaction scenarios.
 - Simulation of lower-dimensional n-wave interaction problems.
 - ▶ QMC simulations of interacting photon beams in different parameter regimes.
 - ▶ Programming algorithms for the 2-photon interaction in Qiskit emulator.
 - ► Setup of variational QC models for simulating kinetic wave-plasma instabilities.

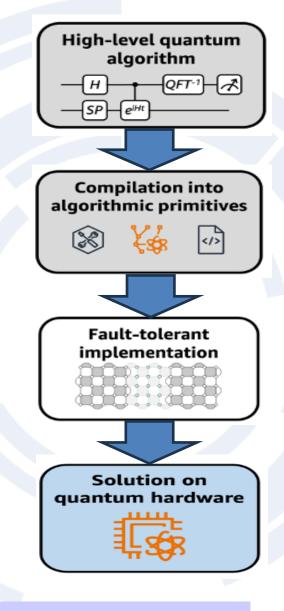
Project dissemination 7 articles in peerreviewed journals (+2 in preparation) 1 chapter in books 14 presentations in conferences **Organization of 1** conference satellite meeting (+ special issue in peerreviewed journal)

Built fruitful collaboration between NTUA & IST teams on various topics in plasma physics within the QC umbrella!!!



Challenges for the future

- Pursue QC developments in problems relevant to plasma fusion.
 - QC implementation for EM waves in magnetized plasma.
 - ► Program QC algorithms for plasma EM wave propagation in Qiskit emulator.
 - ► Further explore geometric representation of cold magnetized plasmas.
 - ► NTUA QCLab acquired 4 2-qubit NMR QCs from SPINQ → Hands-on training.
 - Transitioning to quantum algorithms for nonlinear plasma physics problems.
 - ► Redefining **key questions** surrounding the use of QC for **nonlinear systems**.
 - ► Work on microscopic, first-principles Hamiltonian frameworks that integrate canonical perturbation methods with geometric quantum description.
 - ► Allow transition from dense phase-space portraits to n-qubit QC states.
 - Variational QC models for simulating kinetic wave-plasma instabilities.
 - ▶ Develop **QMC framework** for studying **collisions in plasmas**.
 - ► Employ more advanced algorithms (like QSVT) to increase problem dimensions.
 - ► Investigate more complex scenarios (like nonlinear MHD & kinetic instabilities).



Simulation in hardware QC may include inherent noise → Error mitigation techniques (e.g. Pauli twirling)

The journey of a QUANTUM ALGORITHM

