Simulating Disordered Many-Body Open Quantum Systems:
Modelling Organic Polariton Bose-Einstein Condensation

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Research Summary

The theory of open quantum systems describes the interaction between quantum systems (like molecules) and their environments. Computational methods were previously implemented in the Open Quantum Systems in Python (OQuPy) package to model a single open system[1,2]. These methods can simulate the dynamics of many organic molecules of a single type transitioning into a state of matter known as Bose-Einstein Condensate (BEC). In this project, these computational methods were expanded so that they can model multiple types of molecules undergoing condensation together. Focus was given to the case of disorder, where different types of molecules have different energies.

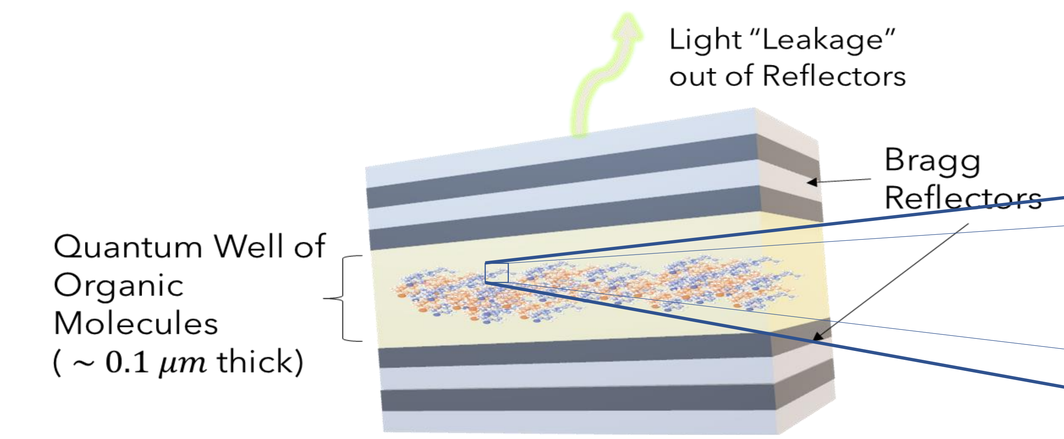

Figure 1: Diagram of reflective microcavity with organic molecules. Two types of systems (organic molecules) are depicted within a "quantum well", shown by orange and blue molecules. The molecules are excited, for instance by an external pump laser (not shown here). The excited molecules then emit light which is confined between two mirrors known as Bragg Reflectors. The reflected light is reabsorbed by the molecules, creating a cycle of emission and reabsorption.

Room Temperature Polariton Bose-Einstein Condensation

- **BEC is formed when a large number of particles have wavelengths which exceed interparticle spacing; the particles condense into a single matter wave.** All particles have a wavelength associated with them which is inversely proportional to their momenta (the product of mass and velocity). While not noticeable in everyday life, very small particles with low masses or low velocities, can have appreciable wavelengths.
- **Traditionally, BEC is made by cooling atomic gases to extremely cold temperatures** (around a billionth of a degree above absolute zero) so that particles all have low velocities and hence large wavelengths for BEC formation.
- **Recent advances have made it possible to form BEC even at room temperature.** Instead of particles with low velocities, "quasiparticles" with extremely small masses are created, which also have large wavelengths. These quasiparticles, known as polaritons, are formed by trapping light within a reflective microcavity containing organic molecules (see **Figures 1 & 2**).

Acknowledgements

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Expanding Open Quantum System Simulation

- **An open quantum system is one which interacts with its environment.** Simulating open systems requires a lot of memory to be stored about system-environment dynamics, which makes computation difficult.
- **Computational techniques based on the mathematical framework of tensor networks can efficiently simulate open system dynamics[3,4].** Code written for this project generalized pre-existing single-system-type techniques so that the interaction between any number of open systems and environments can now be simulated.
- This code **is well-suited to model polariton condensation of multiple types of organic molecules interacting with vibrational environments at room temperature.**

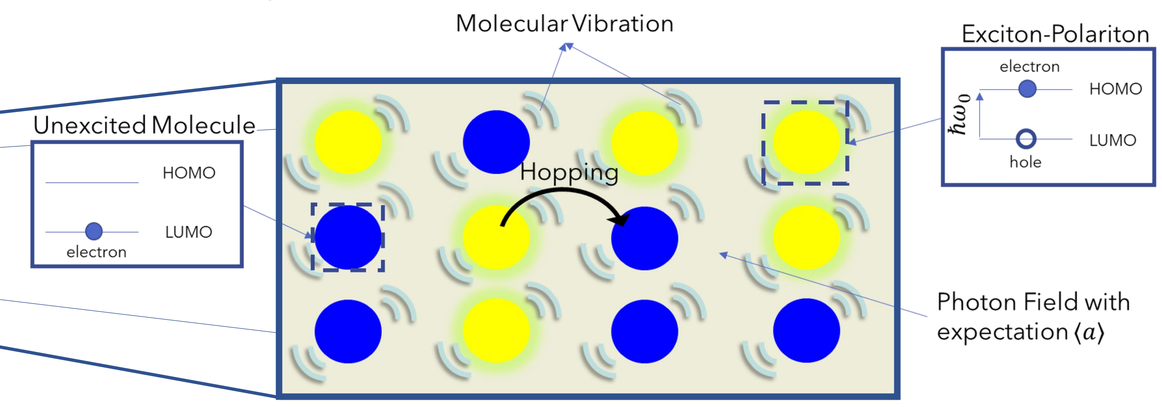

Figure 2: Simplified illustration of molecular excitation in the microcavity. A zoomed in section of the lattice of some blue molecules in **Figure 1** (shown by the small rectangle in the quantum well) is shown. The molecules are vibrating in the presence of the photon field confined in the microcavity. Light can excite an electron in a molecule from the Lowest Unoccupied Molecular Orbital (LUMO) to the Highest Occupied Molecular Orbital (HOMO). Excitations may hop from one place to another within the lattice.

Results and Potential Applications

- Building on the approach taken by Ref. [1], this project **successfully modelled polariton condensation for multiple types of organic molecules** interacting with one another via a photon field.
- **Basic tests were successfully run to simulate disordered systems**, where different molecule types have different excitation energies. **Figure 3** shows results of one such test.
- It is hoped that this code will be used with more realistic values for simulation parameters to model phenomena like the energy exchange between two types of molecular polaritons. This is of **practical interest to fields such as lasing and organic chemistry**.

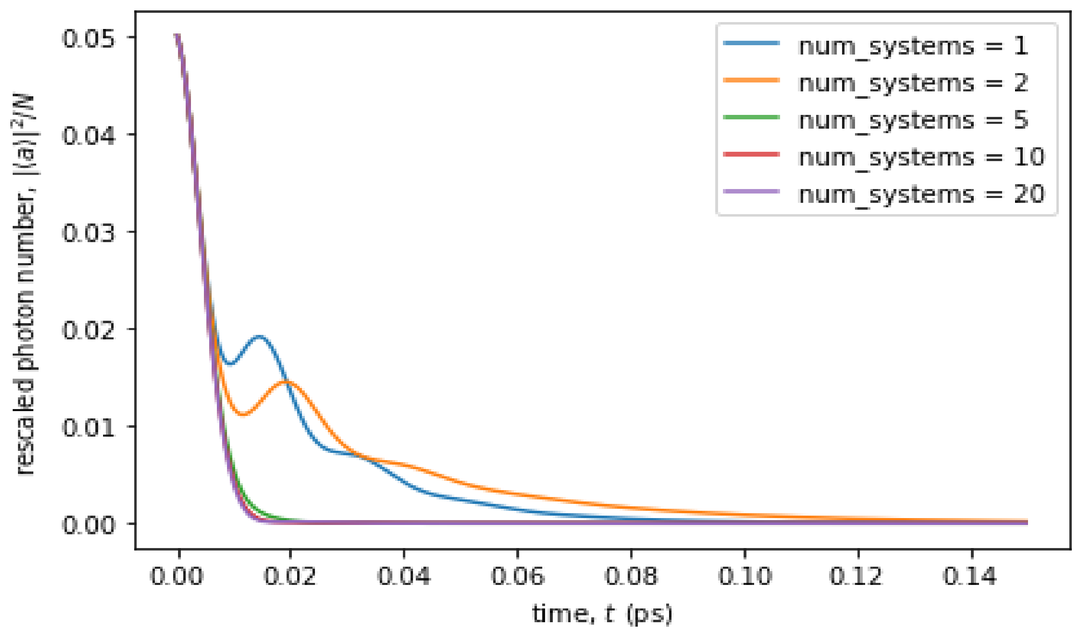

Figure 3: Plot of rescaled photon number ($|\langle a \rangle|^2/N$) against time (t) for a fixed variance value of molecular excitation energies ($\hbar\omega_0$) and different numbers of systems (molecule types). This data was generated using the new code written. As was expected, results converge as the number of systems increases.

References

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