How Biexcitons Systems Interact in a Quantized Radiation Field

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Background

Frenkel excitons are quasiparticles that possess momentum, energy, and a center of mass. Excitons are the product of an electron jumping up from the valence band of molecules to the conducting band. The exciton is the relationship between the excited electron and the hole. The electron-hole is the space in the valence band that the electron leaves behind. Biexcitons are two bound exciton systems found in a wide range of matter from DNA to organic semiconductors and are used as sophisticated probes for spectroscopy.

Motivation

Biexcitons have not been fully understood within organic solids and lattices. Theoretical physics work states, however, that it should be possible. This study sought to numerically quantify the interactions between the excitons in the biexciton system. The purpose of which is to pave new paths toward understanding many-body electric structures. These structures are in a plethora of molecular excitonic systems, leading to many technological advances and touching many other fields.

Methodology

Quantum simulations as well as theoretical quantum physics and organic chemistry were used to explore biexciton behavior. Quantum trajectory simulations make it possible to study how photon pairs become entangled. This is done by interacting quantum emitters that can form biexciton states and predict the experimental signatures of biexciton formation. By applying Schrödinger's equation to the matrix produced by these simulations, the probability of the exciton systems' location within an artificial box can be calculated.

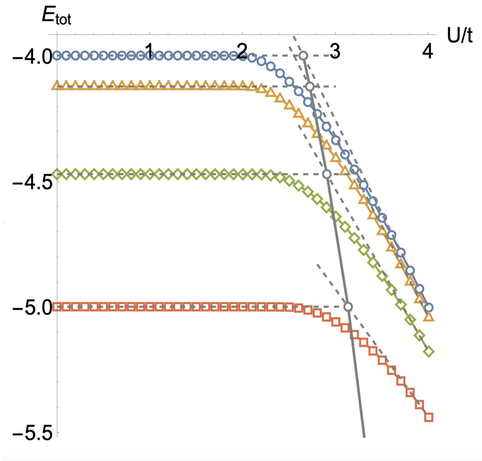

Figure 1: Note bound biexcitons reach stability when $E_B < E_{Free}$

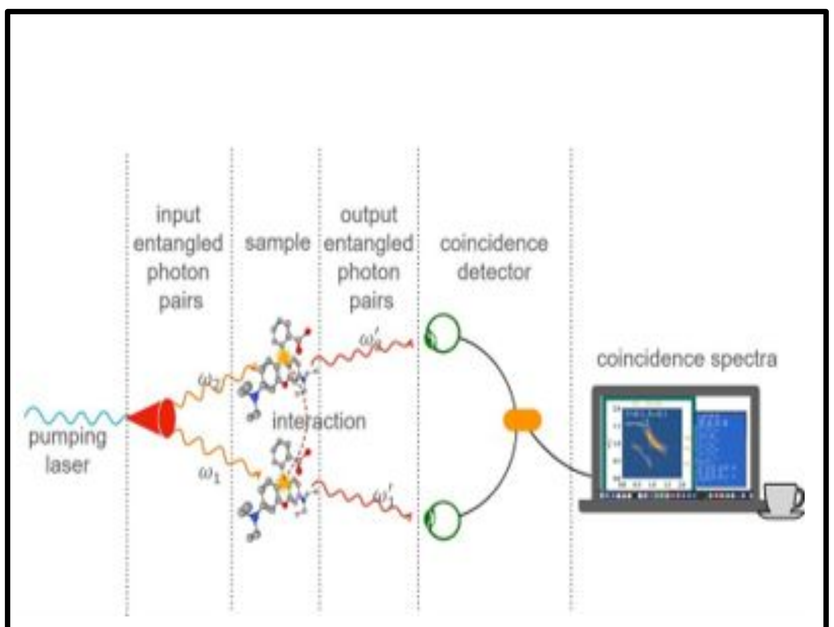

Figure 2: Visualization of how we use quantum trajectory simulations to probe biexcitons

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In[•]:= Hubbard[2, 2, 1] / matrix form

        Hubbard model

        Number of sites: 2
        Number of particles: 2
        spin-up particles= 1

        Calculating the Hamiltonian matrix

        The dimension of this matrix is 4 x 4.

Out[•]= {{-2 form w / matrix, -2 form t / matrix, -2 form t / matrix, 0},
         {-2 form t / matrix, 0, 0, -2 form t / matrix},
         {-2 form t / matrix, 0, 0, -2 form t / matrix},
         {0, -2 form t / matrix, -2 form t / matrix, 2 form w / matrix}}
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Figure 3: Sample of the matrix generated by the quantum trajectory simulations

Results

Results suggest that molecular geometries and the interaction energies between the two bound excitons govern the behaviors of biexciton systems, resulting in their stability within the organic solids. Additionally, the measurements reveal a set of microscopic criteria for the attractive or repulsive nature of biexciton binding in macromolecular semiconductors. Both types of interactions (attractive and repulsive) have the ability to produce the bound states required for the biexciton system. Biexciton behavior greatly depends on their interaction energy as well as their molecular geometry.

Conclusion & Future Studies

Different mathematical approaches and changes to the simulations can bring about new info in the future. Understanding biexcitons will lead to advances in quantum computing, medicine, and many-body electric structures. This will benefit not only the field of physics, but technology and knowledge across all fields. Biexcitons are a result of photoexcitations that happen in our everyday lives. Understanding biexcitons is important for understanding the world around us.

References

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[2] Meza, Elizabeth & Malatesta, Ravyn & Li, Hongmo & Bargigia, Ilaria & Kandada, Ajay & Valverde-Chávez, David & Stingelin, Natalie & Tretiak, Sergei & Bittner, Eric & Silva, Carlos. (2021). The molecular origin of Frenkel biexciton binding.

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