Interplay between photon condensation and electron-electron interaction in molecular systems.

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Abstract: We investigate a minimal model describing an ensemble of square molecules hosting multiple interacting electrons and coupled to a spatially uniform magnetic cavity mode. We demonstrated the system can display a superradiant phase and analyse how the Coulomb repulsion impacts the phase transition.

We consider an ensemble of small planar molecules, each modelled as square plaquettes hosting multiple electrons and described by a tight-binding Hamiltonian with an on-site repulsion term. In each molecular plaquette, one of the hopping energies (τ) is assumed to be different from the other (t), a condition under which the system's ground state can exhibit a degeneracy and show an enhanced paramagnetic response[1]. The system interacts with a nonuniform quantized vector potential which describes a uniform magnetic field. Using exact diagonalization for the electron system and a mean-field treatment of the cavity field, we explored the effect the electron-electron repulsion has on the phase transition.

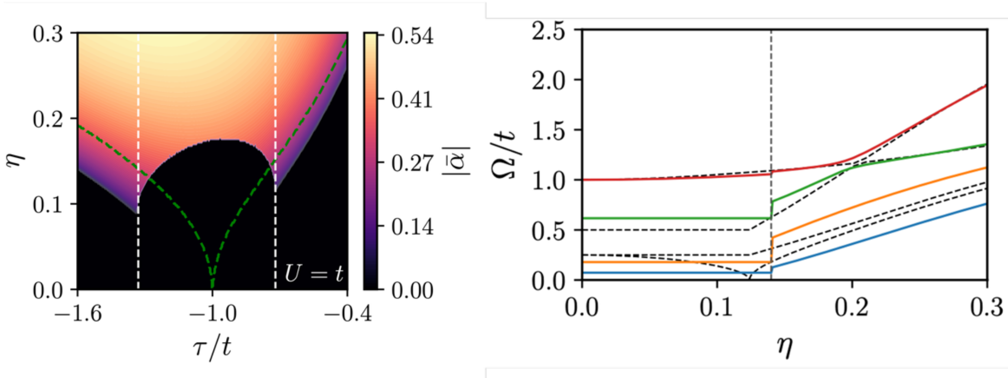

Fig. 1 Left: Photonic order parameter as a function of the inequivalent hopping parameter τ and the light-matter coupling strength η, at fixed electrostatic energy $U = t$. The green dashed lines marks critical values of parameters at which the transition takes place in the noninteracting case. Right: polaritonic spectrum of the system as a function of the light-matter coupling strength. The dashed vertical line marks the coupling at which the photon condensation occurs, and the abrupt change in the polaritons energies enlighten the first-order nature of the phase transition.

We demonstrated that, depending on electron filling and interaction strength, photon condensation may occur either as a continuous second-order transition or as a discontinuous first-order one. Specifically, for one electron and at half-filling, the transition remains continuous whenever it occurs, whereas for intermediate fillings the Hubbard interaction can generate discontinuous, first-order transitions because of the structure of the low-energy spectrum of the electron system[2]. We further interpret these effects in terms of the magnetic response of the molecular ground state, which shows a crossover from Van Vleck paramagnetism toward diamagnetic behaviour. We also examined the Van Vleck–type magnetic response and the polaritonic spectrum, identifying spectroscopic signatures that can be used to detect the magnetostatic instability[3].

References

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