The Connection between Diagrams and Electrodynamics in the Long-Range Dispersion Energy

RAHUL MAITRA, ROBERT DISTASIO, Cornell University — In this talk, we will discuss the different avenues that lead to the complete treatment of the long-range dispersion interaction energy between isolated fragments that are located outside the area of orbital (or electron density) overlap. By analyzing the higher-order terms in the perturbative expansion of the dispersion energy via a dipole response function formalism, we show that each of these terms can be expressed as physically meaningful quantities in classical electrodynamics. Based on this approach, we generalize the connection between the higher-order perturbative contributions to the dispersion energy, the different classes of diagrams (e.g. rings, ladders, etc.), and the aforementioned electrodynamical response functions.