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Time-Dependent Density Functional Theory of an Oscillating Electron Density around a Nanoparticle

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Abstract : A theoretical probe describing the excited energy states of the electron density surrounding a nanoparticle (NP) is presented. An electromagnetic (EM) wave interacts with a NP much smaller than the incident wavelength. The plasmon that oscillates locally around the NP comprises of excited conduction electrons. The system is based on the Jellium model of a cluster of metal atoms. Hohenberg-Kohn (HK) equations and the variational Kohn-Sham (SK) scheme have been used to obtain the NP electron density in the ground state. Furthermore, a time-dependent density functional (TDDFT) theory is used to treat the excited states in a density functional theory (DFT) framework. The non-interacting fermionic kinetic energy is shown to be a functional of the electron density. The time dependent potential is written as the sum of the nucleic potential and the incoming EM field. This view of the quantum oscillation of the electron density is a part of the localized surface plasmon resonance.

Keywords : electron density, energy, electromagnetic, DFT, TDDFT, plasmon, resonance
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