Intra-system derivative discontinuities in static DFT and correlated

photon-electron wavefunctions in cavity QED

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Standard local and semi-local functionals in DFT are known for their shortcomingsin describing

correct charge transfer and level alignment. In the first part ofour presentation we show how to

construct the exact Hohenberg-Kohn energy functionaland density-to-wavefunction mapping for

a lattice system. The exact functional exhibitsintra-system derivative discontinuities in the lowdensity

limit. These intra-systemderivative discontinuities are shown to be generic for all

observables and besidesthe ground-state energy also excited-state energies, the partition

function, and S^2 are shown as examples [1]. Experimental progress in recent years has

enabled the fabrication of Fabry-Perotresonators with high optical quality factors (high-Q). Such

cavities allow to studythe interaction of matter with quantized light at the single-photon level.In

the second part of the presentation we investigate the real-time evolution ofcorrelated photonelectron

wavefunctions during spontaneous emission in high-Qcavities. Implications for a multicomponent

density functional theory based onthe time-dependent electron density and the

photon energy density are drawn [2].

[1] T. Dimitrov et al, to be submitted

[2] H. Appel et al, to be submitted