Joint CQSE and CASTS Seminar

Weekly Seminar
May 11, 2012 (Friday)

TIME   May 11, 14:30 ~ 15:30

TITLE   Optics of semiconductors from meta-GGA-based
time-dependent density-functional theory

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PLACE   Rm716, CCMS & New Physics Building, NTU

Abstract

The local-density approximation (LDA) to the ground-state density functional theory (DFT) is well known to allow for a generalization to the time-dependent case [1].

The assumption of the adiabaticity of the process greatly simplifies the theory. The further extension of the time-dependent DFT (TDDFT) to the generalized gradient approximation (GGA) is trivial.

Here we address lifting the adiabatic TDDFT to the third rung of the 'Jacobs ladder' [2] : We work out the kinetic energy density dependent (meta-GGA) TDDFT formalism.

The new theory possesses remarkable properties not present in LDA and GGA:

(i) It is non-local with respect to the particle density;

(ii) In the case of bulk semiconductors, it supports the $1/q^2$ singularity of the exchange-correlation kernel, where q is the wave-vector, the latter being important to reproduce the excitonic effect. We also present illustrative calculations of the optical absorption in semiconductors [3].

[1] A. Zangwill and P. Soven, Phys. Rev. A, 21, 1561 (1980).

[2] J. Tao, J. P. Perdew, V. N. Staroverov, and G. E. Scuseria, Phys. Rev. Lett. 91, 146401 (2003).

[3] V. U. Nazarov and G. Vignale, Phys. Rev. Lett. 107, 216402 (2011).