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META-GGA based time-dependent density-functional theory

Prof. Vladimir Nazarov

时间：3月15日（星期四）15:00—16:40
地点：北京大学物理楼中212教室

Prof. Vladimir Nazarov, Habilitation (Doctor of Phys.& Math. Sciences) in Solid State Physics, Far-Eastern National University (1998).; Ph.D. in Physics (Candidate of Phys.& Math.Sciences) from Institute for Automation, Russian Academy of Sciences (1990); July 2010 – present, Associate Research Fellow at Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan. Research Fields: Fundamentals and applications of time-dependent density-functional theory; Plasmonics

Recent Publications:

(1) V. U. Nazarov and G. Vignale, Optics of semiconductors from meta-GGA-based time-dependent density-functional theory, Phys. Rev. Lett. 107, 216402 (2011).
(2) E. E. Krasovskii, V. M. Silkin, V. U. Nazarov, P. M. Echenique, and E. V. Chulkov, Dielectric screening and band-structure effects in low-energy photoemission, Phys. Rev. B 82, 125102 (2010).
(3) V. U. Nazarov, G. Vignale, and Y.-C. Chang, On the relation between the scalar and tensor exchange-correlation kernels of the time-dependent density-functional theory, Journal of Chemical Physics 133, 021101 (2010).
(4) V. U. Nazarov, I. V. Tokatly, S. Pittalis, and G. Vignale, Antiadiabatic limit of the exchange-correlation kernel of an inhomogeneous electron gas, Phys. Rev. B 81, 245101 (2010)
(5) V. U. Nazarov, G. Vignale, and Y.-C. Chang, Exact dynamical exchange-correlation kernel of a weakly inhomogeneous electron gas, Phys. Rev. Lett. 102, 113001 (2009)
(6) V. U. Nazarov, J. M. Pitarke, Y. Takada, G. Vignale, and Y.-C. Chang, Including nonlocality in exchange-correlation kernel from time-dependent current density functional theory: Application to the stopping power of electron liquids, Phys. Rev. B 76, 205103 (2007)

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).

联系人：田光善 教授 ， 邮箱：tiangs@pku.edu.cn

北京大学物理学院凝聚态物理与材料物理所

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