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Green's Functions in Nanoscience¹ MURILO L. TIAGO, Oak Ridge National Laboratory

Theoretical nanoscience is a fast growing area in physics. It gains momentum with the recent advances in related areas such as nanodevice design, synthesis and characterization of novel nanostructures, nanoscale imaging and spectroscopy. Several techniques common to quantum chemistry and condensed matter physics have been applied successfully to the modeling of nanoscale structures. In particular, methods based on many-body Green's functions (MBGF) are becoming more and more popular. One of the reasons for this success is that these methods have predicted several phenomena at nanoscale, for example the peculiar dimensional confinement of excitons in nanostructures. Further advances in quantum transport and exciton dynamics can be foreseen. Moreover, algorithms tailored to confined systems have made calculations of Green's functions in nanostructures much more manageable [1]. With those algorithms, we were able to investigate the properties of correlated excitations in clusters of semiconductors (CdSe and silicon)[1,2]. We were also able to explain the properties of electronic excitations in fullerenes and other organic compounds [1,3]. This talk will present an overview of the current stage of MBGF techniques, discuss the various approximations that have been proposed, and review recent advances.

References:

[1] M. L. Tiago and J. R. Chelikowsky, Phys. Rev. B 73, 205334 (2006)

[2] M. L. Del Puerto, M. L. Tiago and J. R. Chelikowsky, Phys. Rev. Lett. 97, 096401 (2006).

[3] M. L. Tiago, P. R. C. Kent, R. Q. Hood, and F. A. Reboredo, J. Chem. Phys. 129, 084311 (2008).

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