Solution of the Bethe-Salpeter equation without empty electronic states*

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We present an approach to compute optical absorption spectra of solids and molecules from first principles, which is suitable for the study of large systems and gives access to spectra within a wide energy range. In this approach, the quantum Liouville equation is solved iteratively within first order perturbation theory, with a Hamiltonian containing a static self-energy operator[1]. This is equivalent to solving the Bethe-Salpeter equation. Explicit calculations of single particle excited states and inversion of dielectric matrices are avoided using techniques based on Density Functional Perturbation Theory[1−2]. The calculation and inclusion of GW quasi-particle corrections within this framework are discussed. The efficiency and accuracy of the new approach are demonstrated by computing optical spectra of nanostructures, bulk crystals and charge transfer excitations.

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[2] H. Wilson, F. Gygi and G. Galli, Phys. Rev. B , **78**, 113303, 2008;H. Wilson, D. Lu, F. Gygi and G. Galli, Phys. Rev. B, **79**, 245106,2009.

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