Abstract Submitted
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Ab initio calculations of optical spectra by solving the Bethe-Salpeter equation without empty states.Work[1] DARIO ROCCA, DEYU LU, GIULIA GALLI, University of California, Davis — We present a novel first principle approach to solve the Bethe-Salpeter equation (BSE) that builds on recent progress in time-dependent density functional perturbation theory [1], and uses an eigenvalue decomposition representation of the dielectric matrix [2]. This approach does not require the explicit calculation of excited single particle electronic states, making it suitable for calculations involving large basis sets and/or a large number of transitions. The numerical solution of the BSE is obtained through a generalized, non-Hermitian Lanczos iterative algorithm and does not require the use of the Tamm-Dancoff approximation. Furthermore, since Lanczos coefficients are frequency independent, optical spectra may be obtained in a very broad energy range. The efficiency and accuracy of the new approach are demonstrated by calculating the optical properties of silicon nanoclusters with up to 1 nm diameter. [1] D. Rocca, R. Gebauer, Y Saad, and S. Baroni, J. Chem. Phys. 128, 154105 (2008). [2] H.Wilson, F.Gygi and G.Galli, Phys. Rev. B 78, 113303 (2008).

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