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Excited state calculations in solids by auxiliary-field quantum Monte Carlo[1] FENGJIE MA, SHIWEI ZHANG, HENRY KRAKAUER, Dept. of Physics, College of William & Mary — We have studied electronic excitations in solid systems using the phaseless auxiliary-field quantum Monte Carlo (AFQMC) method.[2] Trial wave functions for excited states are simply constructed from the corresponding density functional theory (DFT) ground state orbitals by promoting electrons to conduction bands. The post-processing finite size (FS) correction method[3] is applied to remove the many-body FS effects. By fitting the calculated excitation energies at various crystal momentum values, a many-body electronic band structure is obtained. Our results for prototypical semiconductors such as silicon are compared to those from the GW approximation[4] and diffusion Monte Carlo calculations.[5]

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[2]S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003); W. Purwanto, S. Zhang, and H. Krakauer, J. Chem. Phys. **130**, 094107 (2009).
[3]F. Ma, S. Zhang, and H. Krakauer, Phys. Rev. B **84**, 155130 (2011); H. Kwee, S. Zhang, and H. Krakauer, Phys. Rev. Lett. **100**, 126404 (2008).
[4]M. Rohlfing, P. Krüger, and J. Pollmann, Phys. Rev B. **48**, 17791 (1993).
[5]A. J. Williamson, R. Q. Hood, R. J. Needs, and G. Rajagopal, Phys. Rev. B **57**, 12140 (1998).

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