Green's function approach to ab initio band structures

Christian Buth*

Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38,
01187 Dresden, Germany

Correlated ground state wave functions and energies of crystals and large molecules can be obtained routinely by employing, for example, the incremental scheme [1, 2], yet excited states are still conceptually challenging. Several schemes using, e.g. the effective Hamiltonians [1, 3] or Green's functions [4], have been formulated to establish a long sought-after method which allows to calculate correlated band structures without relying on density functional theory.

We propose a new Green's function approach to correlated band structures [5]. It is based on the well-established algebraic diagrammatic construction scheme (ADC) for molecules which we extended to localized crystal orbitals (CO-ADC). Band structures are obtained directly by diagonalizing the band structure matrix which incorporates all correlation effects. ADC has been proven to be highly reliable, being able to describe strong correlation, occurring for ionization from the inner valence of molecules, and electronic resonances [6]. The band structures of $(HF)_\infty$ chains and bulk LiF are presently studied.

References

[1] P. Fulde, Adv. Phys. **51** 909 (2002)

[2] C. Buth, B. Paulus, Chem. Phys. Lett., **398** 44 (2004), arXiv:cond-mat/0408243

[3] V. Bezugly, U. Birkenheuer, Chem. Phys. Lett. **399** 57 (2004), arXiv:cond-mat/0407382

[4] J. J. Ladik, Phys. Rep. **313** 171–235 (1999)

[5] C. Buth, U. Birkenheuer, M. Albrecht, and P. Fulde, manuscript submitted to Phys. Rev. B, arXiv:cond-mat/0409078

[6] C. Buth, R. Santra, and L. S. Cederbaum, J. Chem. Phys., **119** 7763 (2003), arXiv:physics/0306123; J. Chem. Phys., **119** 10575 (2003), arXiv:physics/0303100

*Correspondence to cbuth@mpipks-dresden.mpg.de