Finite temperature cumulant Green's function approach for exchange, correlation, and thermodynamic properties of electronic systems

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The cumulant expansion approach for the one-electron Green’s function has been shown to give improved excited state properties in comparison to those based on the usual GW-Dyson approach. In addition, a cumulant expansion of the retarded Green’s function yielded improved ground state energies in comparison to those with the G0W0self energy.1,2

Here we discuss some more recent developments of the cumulant approach for the finite temperature Green’s function,3 including its application to thermodynamic properties such as free-energies, entropies and heat capacities. The approach is found to give reasonable agreement with available QMC data, and allows for an analysis of the temperature dependence of exchange and correlation in terms of physical quantities such as the screened coulomb interaction and the density of states. Comparisons to Fermi liquid theory are also made at the T=0 limit.

Finally, a finite temperature extension to TDDFT is discussed, where the TDLDA exchange-correlation kernel is extracted from the cumulant Greeen’s function and thermodynamic properties. Calculations of optical properties of the homogeneous electron gas show appreciable temperature dependence, especially at high momentum transfer.

1. Guzzo et al., Phys. Rev. Lett. **107**, 166401 (2011).

2. J. J. Kas, J. J. Rehr, and L. Reining, Phys. Rev. B **90**, 085112 (2014).

3. J. J. Kas and J. J. Rehr, Phys. Rev. Lett. **119**, 176403 (2017)