

GW and BSE methods

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1 Diagrammatics

1.1 Infinitesimals

Note that here we need to do some “mini-regularization”. The first is about the value of the propagator to ensure that when $t = 0$, $\mathcal{T} \langle c(t)c^\dagger(0) \rangle$ is the particle number (so that if we evaluate the tadpole diagram, we get the Hartree term), the contribution of an electron line is actually

$$\mathcal{T} \langle c_{\mathbf{k}}(t)c_{\mathbf{k}}^\dagger(0) \rangle = \int \frac{d\omega}{2\pi} e^{-i\omega(t-0^+)} \frac{i}{\omega - \varepsilon_{\mathbf{k}} + \mu} = \int \frac{d\omega}{2\pi} e^{i\omega 0^+} iG_0(\omega, \mathbf{k}). \quad (1)$$

Another mini-regularization is when necessary, in the real space, we should assume the “out-time” is the “in-time” plus 0^+ , because the Coulomb interaction isn’t really spontaneous and there is a small time retardation. In the frequency space, we need to assume that there is an infinite amount of energy on the interaction line, and

$$V(q) = \frac{4\pi e^2}{q^2 - \omega^2 - i0^+}. \quad (2)$$

2 Overview of *GW*

2.1 One-shot *GW*

In practice, one-shot *GW* is usually preferred over self-consistent schemes. The point here is that *GW* neglects the vertex, so iterative *GW* only leads us towards the more and more inaccurate way. Still, this only explains why iterative *GW* is bad but doesn’t explain why one-shot *GW* is good. In other words, we need to know how certain factors in the one-shot *GW* scheme somehow makes up for the missing vertex correction.

One possible form of the vertex is the electron-hole interaction, which is calculated by solving the BSE. Now an empirical fact is LDA tends to give the same band gap as BSE, leading to a pretty good one-shot approximation.

The question, then, is why LDA in some cases works as well as BSE. The reason for this is because of the relation between the derivative discontinuity in DFT and electron-hole interaction kernel TODO: the relation with [1]

2.2 Deriving formulas

2.3 Discussion: what’s missing in the Hartree-Fock approximation, then?

3 Accuracy of *GW*

3.1 On so-called failure of *GW*

Some (weak-correlated, of course) materials are claimed to be impossible to be characterized correctly using *GW*, or at least G^0W^0 . [2] refutes such a claim, at least for ZnO.

3.2 Convergence issues

See <https://www.nersc.gov/assets/Uploads/ConvergenceinBGW.pdf>

References

- [1] John P Perdew, Robert G Parr, Mel Levy, and Jose L Balduz Jr. Density-functional theory for fractional particle number: derivative discontinuities of the energy. *Physical Review Letters*, 49(23):1691, 1982.
- [2] Bi-Ching Shih, Yu Xue, Peihong Zhang, Marvin L Cohen, and Steven G Louie. Quasiparticle band gap of zno: High accuracy from the conventional g₀ w₀ approach. *Physical review letters*, 105(14):146401, 2010.