GW and BSE methods

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1 Overview of GW

1.1 Diagrammatics

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

$$\mathcal{T} \langle c_{\boldsymbol{k}}(t) c_{\boldsymbol{k}}^\dagger(0) \rangle = \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-\mathrm{i}\omega(t-0^+)} \frac{\mathrm{i}}{\omega - \varepsilon_{\boldsymbol{k}} + \mu} = \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{\mathrm{i}\omega 0^+} \mathrm{i} G_0(\omega, \boldsymbol{k}). \tag{1}$$

Another mini-regularization is when necessary, we should assume there is a positive infinite amount of energy on the interaction line, because the Coulomb interaction isn't really spontaneous: there is a small time retardation.

1.1.1 Discussion: what is Hartree-Fock approximation, then?

1.2 Deriving formulas

2 Accuracy of GW

2.1 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 $G^0 W^0$. [1] refutes such a claim, at least for ZnO.

2.2 Convergence issues

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

References

[1] Bi-Ching Shih, Yu Xue, Peihong Zhang, Marvin L Cohen, and Steven G Louie. Quasiparticle band gap of zno: High accuracy from the conventional g 0 w 0 approach. *Physical review letters*, 105(14):146401, 2010.