GW and BSE methods

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1 Diagrammatics

1.1 Infinitesimals

Note that here we need to add some convergence factors. 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

$$\begin{aligned}\mathcal{T}\,\langle c_{\boldsymbol{k}}(t)c^\dagger_{\boldsymbol{k}}(0)\rangle &:= \mathcal{T}\,\langle c_{\boldsymbol{k}}(t-0^+)c^\dagger_{\boldsymbol{k}}(0)\rangle \\ &= \int \frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-\mathrm{i}\omega(t-0^+)}\underbrace{\frac{\mathrm{i}}{\omega-\xi_{\boldsymbol{k}}+\mathrm{i}0^+\,\mathrm{sgn}(\xi_{\boldsymbol{k}})}}_{\mathrm{i}G_0(\omega,\boldsymbol{k})} = \int\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}\omega 0^+}\mathrm{i}G_0(\omega,\boldsymbol{k}).\end{aligned} \tag{1}$$

The necessity of this $\mathrm{e}^{\mathrm{i}\omega 0^+}$ factor can also be seen by explicitly doing the integration: when $t=0$, if we ignore the $\mathrm{e}^{\mathrm{i}\omega 0^+}$ factor, we get

$$\int\frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{i}}{\omega-\xi_{\boldsymbol{k}}+\mathrm{i}0^+\,\mathrm{sgn}(\xi_{\boldsymbol{k}})}.$$

This integral is not zero, but we want it to be zero when $\xi_{\boldsymbol{k}} > 0$, so we have to add a $\mathrm{e}^{\mathrm{i}\omega 0^+}$ factor to make the integrand approaches zero quickly enough in the upper plane, so we can construct an integration contour in the upper plane, in which there is no pole, and

$$\int_{|\omega|=R\gg 1}\frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{i}}{\omega-\xi_{\boldsymbol{k}}+\mathrm{i}0^+\,\mathrm{sgn}(\xi_{\boldsymbol{k}})} = 0.$$

Another mini-regularization is when necessary, for a real space interaction line – screened or unscreened – 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,

For bare Coulomb interaction this is rarely needed, because we don't have ω dependence in the potential, and it makes no sense to discuss the poles when we change ω. It does make sense to talk about retardation in the relativistic origin of Coulomb interaction: the Coulomb interaction is mediated by virtual photons, and is therefore proportional to the off-shell (i.e. $\omega \to 0$) limit of the photon propagator, which has $\omega^2 - \boldsymbol{q}^2 + \mathrm{i}0^+$ as the denominator, and we get

$$V(q) = \frac{4\pi e^2}{\boldsymbol{q}^2 - \omega^2 - \mathrm{i}0^+}. \tag{2}$$

For screened Coulomb interaction, however, the correct retardation is important, because now something looking like (2) appears again.

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 band 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 g 0 w 0 approach. *Physical review letters*, 105(14):146401, 2010.