The Bethe-Salpeter Equation (BSE)

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Linear Response Theory

- **Random Phase Approximation** tells us that[1]

$$\hat{\mathcal{O}}^\dagger = \sum_{i,a} a^\dagger i X_{ia} + \sum_{i,a} i^\dagger a Y_{ia}, \tag{1}$$

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- **Problem**: only describes the linear response of single-particle transitions. It does not work well for excitons, where a hole is interacting with an electron, *after* the transition has taken place
- **Solution**: BSE within the Green's function *formalism*

Green's Functions

The single-particle Green's function $\mathcal{D}$ is given as

$$\mathcal{D}\left(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2\right) = -i\left\langle \Psi_0 \middle| T\left[\hat{\psi}\left(\mathbf{r}_1, t_1\right)\hat{\psi}^\dagger\left(\mathbf{r}_2, t_2\right)\right] \middle| \Psi_0 \right\rangle, \qquad (2)$$

where $\hat{\psi}$ is the second quantization field operator, the spacetime coordinates are $\mathbf{r}_1, t_1$ and $\mathbf{r}_2, t_2$, T is the time-ordering operator, and Ψ_0 is the ground state wave function.

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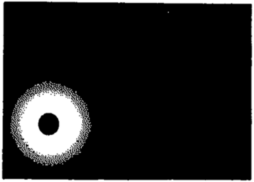
Distinction: Noninteracting G_0 (think mean field i.e. DFT) versus interacting G Green's functions

Self-Energy

Dyson equation[2]: $\Sigma = G^{-1} - G_0^{-1}$, where Σ is the self-energy.

Figure: Electron gas propagation[3]

(a) The electron is shot into the gas



(b) The electron creates holes as it moves along

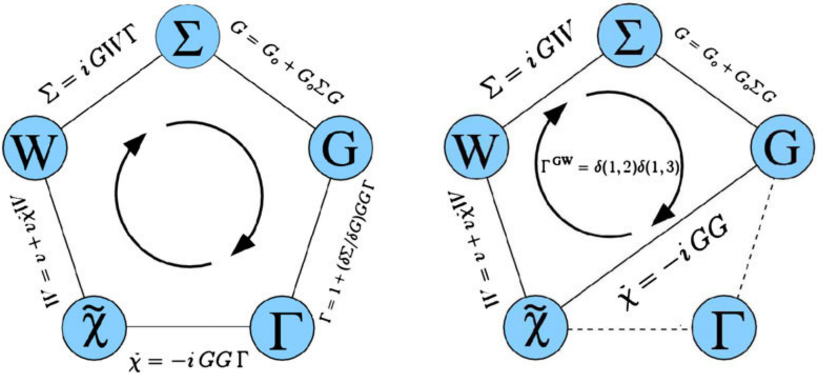
Analogous to

$$\epsilon_{\text{self}} = \epsilon_{\text{quasi}} - \epsilon_{\text{bare}}, \tag{3}$$

So Σ is the difference between the quasi-particle and bare energies; an electron's "clothing."

GW Approximation

Hedin's equations[4] define a self-consistent procedure, schematically[5] as



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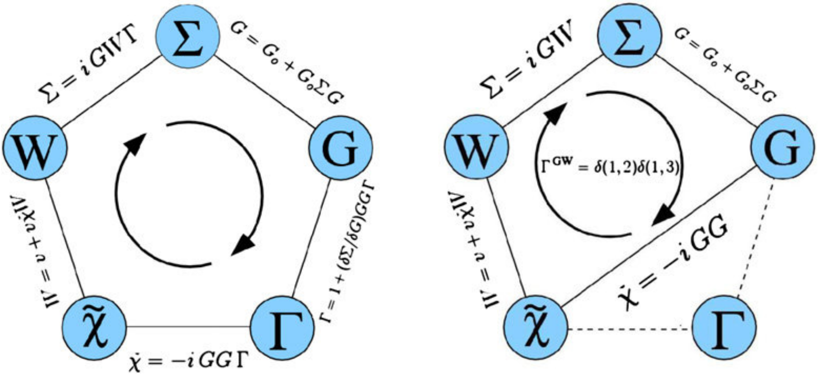

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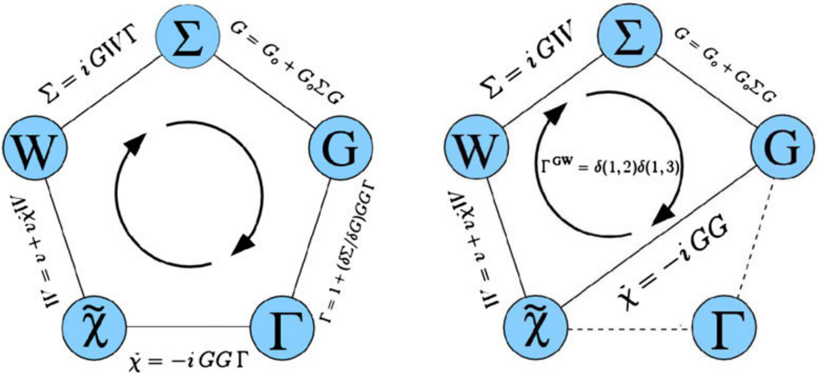

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Right diagram constitutes the *GW* approximation, whereas for the BSE we need to consider the left diagram.

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$$\boxed{L\left(1,2;1',2'\right) = -G_2\left(1,2;1',2'\right) + G\left(1,1'\right)G\left(2,2'\right)} \qquad (4)$$

where we have defined a two-particle Green's function G_2.

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- Now we are able to describe the interaction between an electron and a hole because this is inherently a two-particle process.

Bibliography

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