First principle electronic state calculation

出発ハミルトニアン

$$H = \sum_{\mathbf{p}\sigma} \epsilon_{\mathbf{p}} c^{+}_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma} + \frac{1}{2} \sum_{\mathbf{q}} \sum_{\mathbf{p}\sigma} \sum_{\mathbf{p}'\sigma'} V(\mathbf{q}) c^{+}_{\mathbf{p}+\mathbf{q}\sigma} c^{+}_{\mathbf{p}'-\mathbf{q}\sigma'} c_{\mathbf{p}'\sigma'} c_{\mathbf{p}\sigma}$$

↓ Field operator 形式

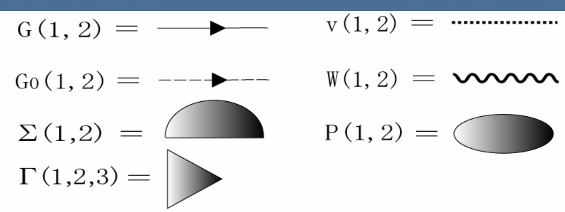
$$H = \int \hat{\psi}^{\dagger}(x) T(x) \hat{\psi}(x) dx + \frac{1}{2} \int \int \hat{\psi}^{\dagger}(x) \hat{\psi}^{\dagger}(x') v(x,x') \hat{\psi}(x') \hat{\psi}(x) dx dx'$$

↓ Green関数の導入

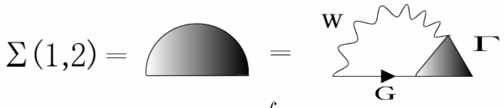
1 粒子 Green 関数を定義する。

$$iG(x,t,x',t') \equiv \langle N | T[\hat{\psi}(x,t)\hat{\psi}^{\dagger}(x',t')] | N \rangle \equiv \begin{cases} \langle N|\hat{\psi}(x,t)\hat{\psi}^{\dagger}(x',t')|N\rangle & \text{for } t > t' \\ -\langle N|\hat{\psi}^{\dagger}(x',t')\hat{\psi}(x,t)|N\rangle & \text{for } t < t' \end{cases}$$

ここで、$\hat{\psi}^{\dagger}(x,t), \hat{\psi}(x,t)$ は電子の生成消滅演算子。$|N\rangle$ は N 電子基底状態。

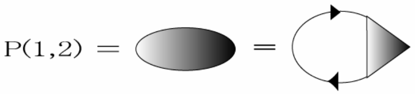


$$G(1,2) = G_0(1,2) + \int G_0(1,3)\Sigma(3,4)G(4,2)d[34]$$

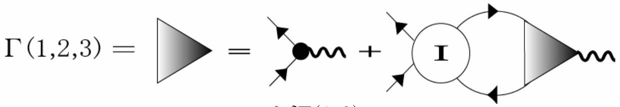


$$\hbar\Sigma(1,2) = i \int G(1,3)\Gamma(3,4;2)W(4,1)d[34]$$

$$W(1,2) = v(1,2) + \int v(1,3)P(3,4)W(4,2)d[34]$$



$$\hbar P(1,2) = -i \int G(1,3)\Gamma(3,4;2)G(4,1)d[34]$$



$$\Gamma(1,2;3) = \delta(1,2)\delta(1,3) + \int \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)\Gamma(6,7;3)G(7,5)d[4567]$$

Hedin's equations

$$G(1,2) = G_0(1,2) + \int G_0(1,3)\Sigma(3,4)G(4,2)d[34]$$

$$\hbar\Sigma(1,2) = i \int G(1,3)\Gamma(3,4;2)W(4,1)d[34]$$

$$\hbar P(1,2) = -i \int G(1,3)\Gamma(3,4;2)G(4,1)d[34]$$

$$\Gamma(1,2;3) = \delta(1,2)\delta(1,3) + \int \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)\Gamma(6,7;3)G(7,5)d[4567]$$

$$W(1,2) = v(1,2) + \int v(1,3)P(3,4)W(4,2)d[34]$$