Superconductivity – final stages

We had:

- 'Cooper pairs': ∘ $\Psi_0(\underline{r}_1, \underline{r}_2) = \sum_{\underline{k}} g_{\underline{k}}\, e^{-i\underline{k}\underline{r}_1} e^{i\underline{k}\underline{r}_2}$

$$= \sum_{\underline{k}} \tilde{g}_{\underline{k}} \cos\left(\underline{k}(\underline{r}_1 - \underline{r}_2)\right)$$

  - extended in $\underline{k}$-space
  - any however weakly attractive $V_{\underline{k},\underline{k}'}$ will bind such pairs –

    BUT $E = 2\epsilon_F - 2\hbar\omega_D\, e^{-\frac{2}{N(0)\cdot V}}$

    NOT ANALYTIC ⟺ no perturb. theory

- BCS: Extend Cooper pairs to an N-electron pairing Hamiltonian

Hamiltonian:

$$\sum_{\underline{k}\sigma} \xi_{\underline{k}}\, c^+_{\underline{k}\sigma} c_{\underline{k}\sigma} + \sum_{\underline{k},\underline{k}'} c^+_{-\uparrow\underline{k}}\, c_{\underline{k}\downarrow}\, V(\underline{k},\underline{k}')\, c_{-\underline{k}'\downarrow}\, c_{\underline{k}'\uparrow}$$

$$\xi_{\underline{k}} = \epsilon_{\underline{k}} - \epsilon_F$$

Cooper: $V_{\underline{k},\underline{k}'} = \begin{cases} -V & \text{if } 0 < |\xi(\underline{k})| < \hbar\omega_D \\ & \underline{\text{and}}\ 0 < |\xi(\underline{k}')| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$

Mean-field approximation:

Set $\Delta := -V \sum_{\underline{k}'} \Theta(\hbar\omega_D - |\xi_{\underline{k}'}|)\, b_{\underline{k}'}$

$b_{\underline{k}'} = \langle c_{-\underline{k}'\downarrow} c_{\underline{k}'\uparrow} \rangle_{av}$ is the statistical average

Can rewrite:

$$H_M = \sum_{\underline{k}\sigma} \xi_{\underline{k}} c^{+}_{\underline{k}\sigma} c_{\underline{k}\sigma} - \sum_{\underline{k}} \left(\Delta_{\underline{k}} c^{+}_{\underline{k}\uparrow} c^{+}_{-\underline{k}\downarrow} + \Delta^{+}_{\underline{k}} c_{\underline{k}\downarrow} c_{\underline{k}\uparrow} - \Delta_{\underline{k}} b_{\underline{k}} \right)$$

$$\Delta_{\underline{k}} = \Theta(\hbar\omega_0 - |\xi_{\underline{k}}|) \cdot \Delta$$

General transformation can be found

$$c_{\underline{k}\uparrow} = u_{\underline{k}} \alpha_{\underline{k}} + v_{\underline{k}} \beta^{+}_{\underline{k}}$$

$$c_{-\underline{k}\downarrow} = u_{\underline{k}} \beta_{\underline{k}} - v_{\underline{k}} \alpha^{+}_{\underline{k}}$$

$\Longrightarrow$ can find $u_{\underline{k}}$, $v_{\underline{k}}$ to yield

$$H_M \longrightarrow \tilde{H}_M = E_0 + \sum_{\underline{k}} \varepsilon_{\underline{k}} \left(\alpha^{+}_{\underline{k}} \alpha_{\underline{k}} + \beta^{+}_{\underline{k}} \beta_{\underline{k}} \right)$$

by setting $\varepsilon_{\underline{k}} = \sqrt{\xi_{\underline{k}}^2 + |\Delta_{\underline{k}}|^2}$

$$u_{\underline{k}}^2 = \frac{1}{2} \left(1 + \frac{\xi_{\underline{k}}}{\varepsilon_{\underline{k}}} \right)$$

$$v_{\underline{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\underline{k}}}{E_{\underline{k}}}\right)$$

$$u_{\underline{k}} \cdot v_{\underline{k}} = -\frac{\Delta_{\underline{k}}}{2E_{\underline{k}}}$$

$$E_0 = 2\sum_{\underline{k}} \left(\xi_{\underline{k}} v_{\underline{k}}^2 + \Delta_{\underline{k}} u_{\underline{k}} v_{\underline{k}}\right) + \frac{\Delta^2}{V}$$

if $\Delta = 0$

$$\longrightarrow \quad v_{\underline{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\underline{k}}}{|\xi_{\underline{k}}|}\right) \rightarrow E_0 = 2\sum_{\underline{k}} \xi_{\underline{k}}$$

$$\Delta = -V \sum_{\underline{k}'} \Theta(\omega_0 - |\xi_{\underline{k}'}|) \langle c_{-\underline{k}'\downarrow} c_{\underline{k}'\uparrow} \rangle_{av}$$

$$= \ldots = \frac{V}{2} \sum_{\underline{k}'} \frac{\Delta}{E_{\underline{k}'}} (1 - 2f_{\underline{k}'}) \qquad (*)$$

replacing $c_{\underline{k}}$ by $\alpha_{\underline{k}}, \beta_{\underline{k}}$

where $f_{\underline{k}'} = \dfrac{1}{e^{\frac{E_{k'}}{kT}} + 1}$

0 at $T = 0$

Find non-trivial solution $\Delta \neq 0$ to $(*)$

$$\Longrightarrow \quad E_c = E_0(\Delta \neq 0) - E_0(\Delta = 0)$$

$$= \ldots = \left(2\sum_{\underline{k}} \xi_{\underline{k}} - \frac{1}{2} N(\epsilon_F) \Delta^2\right) - 2\sum_{\underline{k}} \xi_{\underline{k}} < 0 \checkmark$$

I. Green function theory

① warm up

② what message can be obtained?

③ $\Sigma \longrightarrow v$.

④ Hedin's equation.

⑤ Quasiparticle

II. GW approximation

① GWA.

② Current status.

Part I. $\hat{\psi}^{+}(\vec{r},t)$ $\hat{\psi}(\vec{r},t)$

$\hat{C}_k^{+}$ $\hat{C}_k$

Harmonic oscillator. $[\hat{x}, \hat{P}_x] = i\hbar$ $E \to i\hbar\frac{\partial}{\partial t}$

$$\hat{H} = \frac{\hat{p}}{2m} + \frac{k}{2}\hat{x}$$

$$\hat{a}^{+} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left[\hat{x} + \frac{i\hat{p}}{m\omega}\right] \qquad \omega = \sqrt{\frac{k}{m}}$$

$$\hat{a} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left[\hat{x} - \frac{i\hat{p}}{m\omega}\right]$$

$$\hat{H} = \hbar\omega\left[\hat{a}^{+}\hat{a} + \frac{1}{2}\right]$$

$$\hat{a}^{+}|n\rangle = (n+1)^{1/2}|n+1\rangle \qquad \hat{a}|n\rangle = n^{1/2}|n-1\rangle$$

$$[\hat{a}, \hat{a}^{+}] = 1.$$

$|N\rangle \longrightarrow$ ground state

$$\langle N|\hat{\psi}(\vec{r},t)\,\hat{\psi}^{+}(\vec{r}',t')|N\rangle \quad t > t'$$

$$\langle N|\hat{\psi}^{+}(\vec{r}',t')\,\hat{\psi}(\vec{r},t)|N\rangle \quad t' > t$$

$$G = \frac{-1}{i}\langle N|\hat{T}\{\hat{\psi}(\vec{r},t)\,\hat{\psi}^{+}(\vec{r}',t')\}|N\rangle.$$

$\hat{T} \rightarrow$ time ordering.

$$i\frac{\partial\hat{\psi}(\vec{r},t)}{\partial t} = [\hat{\psi}(\vec{r},t), \hat{H}]$$

$$\hat{H} = \int d\vec{r}\,dt\,\hat{\psi}^{+}(\vec{r},t)\left[-\frac{1}{2}\nabla^2 + V_{ext}(\vec{r})\right]\hat{\psi}(\vec{r},t)$$

$$+\frac{1}{2}\iint d\vec{r}\,dt\,d\vec{r}'\,dt'\,\hat{\psi}^\dagger(\vec{r},t)\,\hat{\psi}^\dagger(\vec{r}',t')\,V(\vec{r},\vec{r}')\,\delta(t-t')\,\hat{\psi}(\vec{r}',t')\,\hat{\psi}(\vec{r},t)$$

$$\left[i\frac{\partial}{\partial t}+\frac{1}{2}\nabla^2-V_{ext}(\vec{r})\right]\underline{G(\vec{r},t,\vec{r}',t')}$$

$$+\,i\int d\vec{r}_1\,V(\vec{r},\vec{r}_1)\,\langle N|\hat{T}\{\hat{\psi}^\dagger(\vec{r}_1,t)\,\hat{\psi}(\vec{r}_1,t)\,\hat{\psi}(\vec{r},t)\,\hat{\psi}^\dagger(\vec{r}',t')\}|N\rangle$$

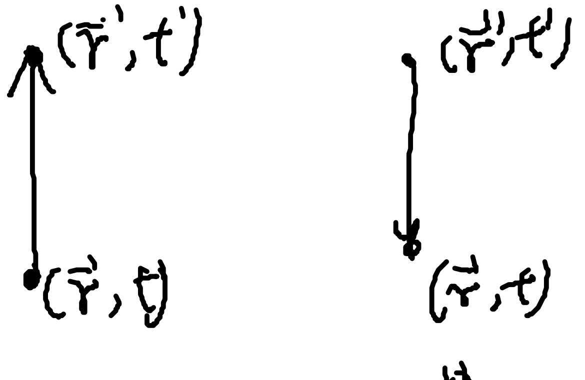
$$=\delta(\vec{r}-\vec{r}')\,\delta(t-t')$$

$$\int d\vec{r}_1\,dt_1\,M(\vec{r},t,\vec{r}_1,t_1)\,G(\vec{r}_1,t_1,\vec{r}',t')$$

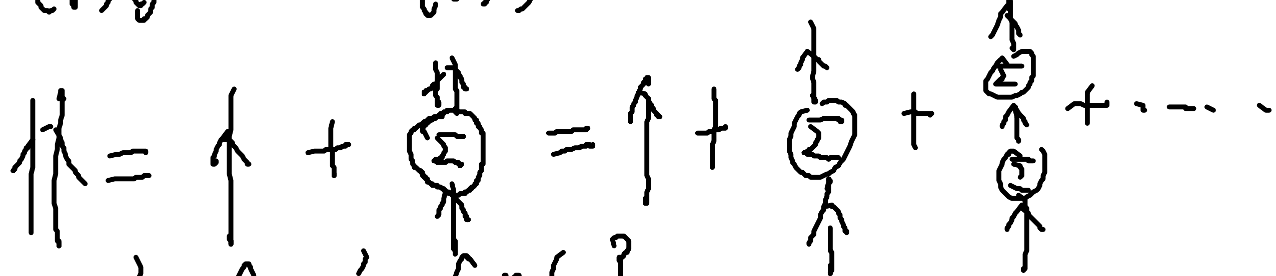
$$\Sigma = M - V^H$$

Non-interacting: $\left[i\frac{\partial}{\partial t}+\frac{1}{2}\nabla^2-V_{ext}(\vec{r})+V^H(\vec{r})\right]G_0 = \delta(\vec{r}-\vec{r}')\,\delta(t-t')$

$$\underline{G = G_0 + G_0\Sigma G} \quad \text{Dyson equation.}$$



$\Longrightarrow$ Feynman.



2. Why Green's function?

① expectation value of any single particle operator.

② Total energy.

③ Excitation spectrum.

①. $\hat{J}(\vec{r}) = \hat{\psi}^{+}(\vec{r})\, \hat{j}(r)\, \hat{\psi}(\vec{r})$

$\hat{J}(\vec{r})$ → second quantized.

$\hat{j}(r)$ → first quantized

Density. first quantized $= 1$

second: $\hat{\psi}^{+}(\vec{r})\, \hat{\psi}(\vec{r})$

$$\langle \hat{J}(x) \rangle = \langle N | \hat{\psi}^{+}(\vec{r})\, \hat{j}(x)\, \hat{\psi}(\vec{r}) | N \rangle$$

$$= \lim_{\vec{r}' \to \vec{r}} \hat{j}(x) \underline{\langle N | \hat{\psi}^{+}(\vec{r}')\, \hat{\psi}(\vec{r}) | N \rangle}$$

$$= \lim_{t' \to t} \lim_{\vec{r}' \to \vec{r}} \underset{\sigma}{\hat{j}(x)}\, i\, G(\vec{r}, t, \vec{r}', t')$$

$\vec{r}' \to \vec{r}$ is taken after $\hat{j}(x)$ act on G.

Density: $\langle \hat{\psi}^{+}(\vec{r})\, \hat{\psi}(\vec{r}) \rangle = i\, G(\vec{r}, t, \vec{r}, t^{+})$

kinetic energy: $\underline{\langle \hat{T} \rangle = i \int d\vec{r} \lim_{\vec{r}' \to \vec{r}} \left[-\frac{\hbar^2 \nabla^2}{2m} G(\vec{r}, t, \vec{r}', t^{+}) \right]}$

② Total energy.

③ excitation spectrum.

$$\sum_{N,s} |N,s\rangle\langle N,s| = 1.$$

$$\hat{\psi}^{+}(\vec{r},t) = e^{i\hat{H}t}\,\psi(\vec{r})\,e^{-i\hat{H}t}$$

Fourier transform

$$G(\vec{r},\vec{r}',\omega) = \lim_{\eta\to 0^+}\sum_s \psi^s(\vec{r})\,\psi^{s*}(\vec{r}')\left[\frac{\theta(\epsilon_s-\mu)}{\omega-\epsilon_s+i\eta}+\frac{\theta(\mu-\epsilon_s)}{\omega-\epsilon_s-i\eta}\right]$$

$\mu \rightarrow$ chemical. potential

$$\epsilon_s = E^s_{N+1} - E_N \qquad \hat{\psi}^s(\vec{r}) = \langle N|\hat{\psi}(\vec{r})|N+1,s\rangle$$

for $\epsilon_s > \mu$

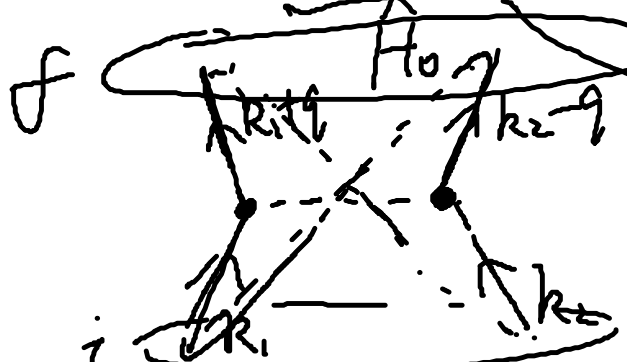
$$\epsilon_s = E_N - E^s_{N-1} \qquad \hat{\psi}^s(\vec{r}) = \langle N-1,s|\hat{\psi}(\vec{r})|N\rangle$$

for $\epsilon_s < \mu$.

3. $\Sigma \rightarrow$ expanded $\rightarrow$ Homogeneous.

$$\hat{H} = \underbrace{\sum_k \epsilon_k \hat{C}^+_k \hat{C}_k}_{\hat{H}_0} + \underbrace{\sum_{q,k_1,k_2} V_q\, \hat{C}^+_{k_1+q}\, \hat{C}^+_{k_2-q}\, \hat{C}_{k_2}\, \hat{C}_{k_1}}_{\hat{H}'}$$

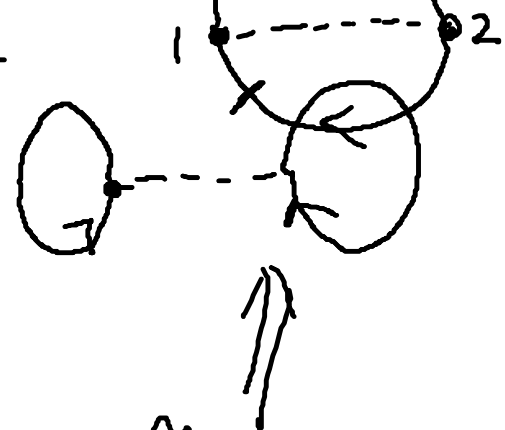
$\rightarrow |N\rangle_0$



$$\Delta E = \langle N_0|\hat{H}'|N_0\rangle \Rightarrow \langle N_0|\hat{C}^+_{k_1+q}\hat{C}^+_{k_2-q}\hat{C}_{k_1}\hat{C}_{k_2}|N_0\rangle$$

① $k_1+q=k_2$

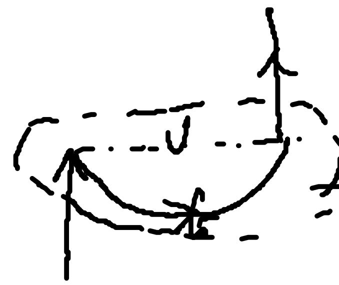
② $q=0$



$\Sigma \to$ 'v'.

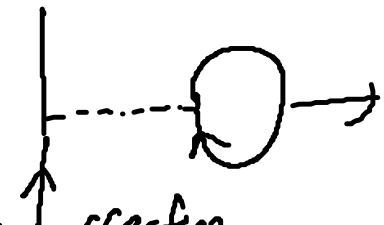
First order correction

①



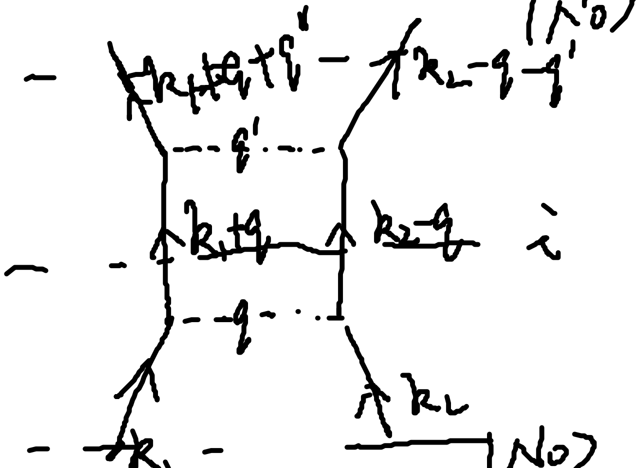
$\boxed{iGv=\Sigma}$

~~②~~



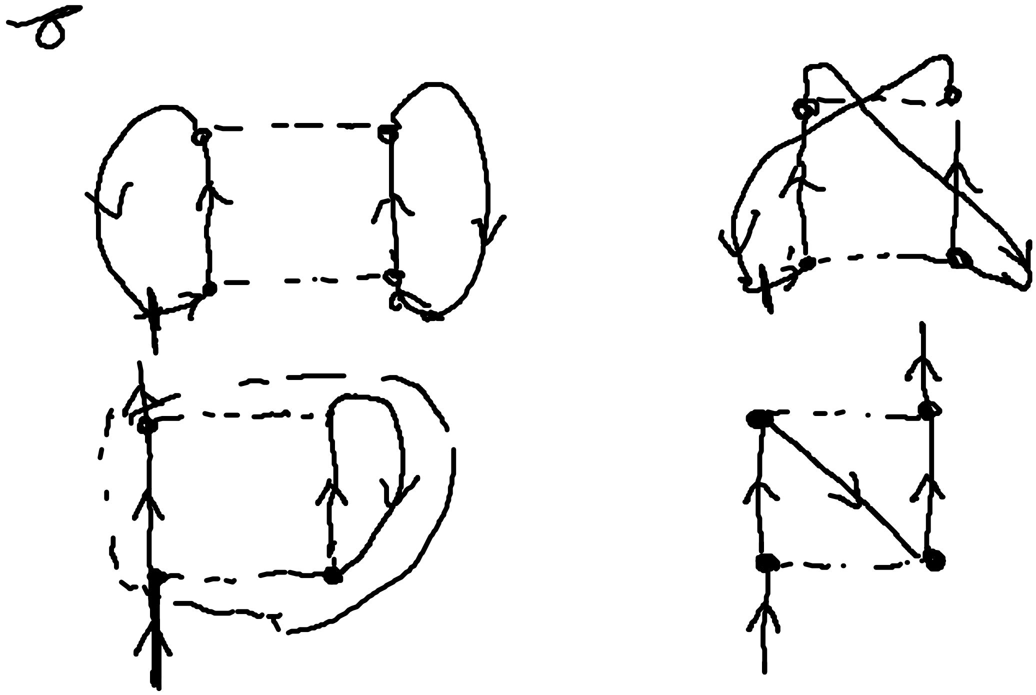
$\to$ doesn't contribute to Σ

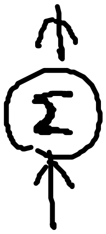
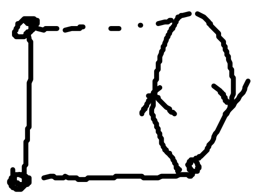
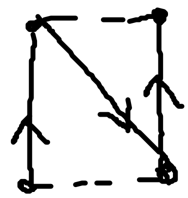
Second order correction:



$|N_0\rangle$

$$\Delta E \propto \langle N_0 | \hat{C}^\dagger_{k_2-q-q'} \hat{C}^\dagger_{k_1+q+q'} \hat{C}_{k_2-q} \hat{C}_{k_1+q} | i \rangle \langle i | \hat{C}^\dagger_{k_2-q} \hat{C}^\dagger_{k_1+q} \hat{C}_{k_2} \hat{C}_{k_1} | N_0 \rangle$$



 $\Sigma \Rightarrow$  $\Sigma \Rightarrow$ 

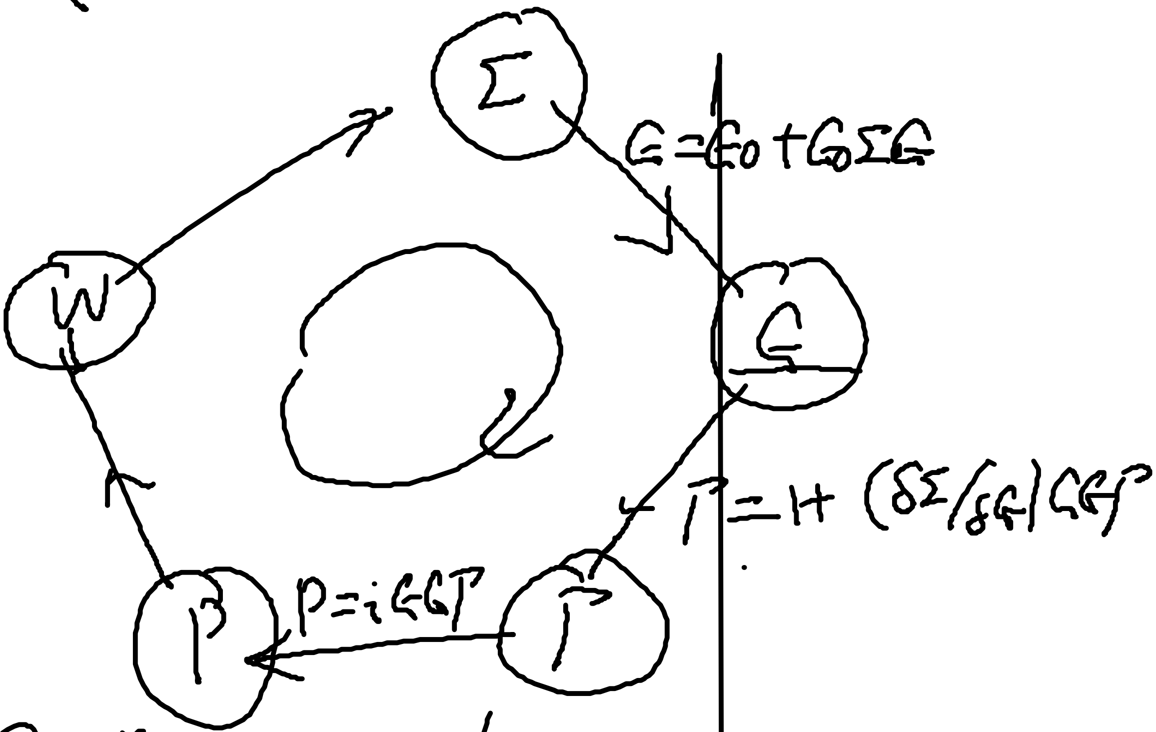
third order.

4. Hedin's equation. (1965)

functional derivative method. $1 = (\vec{r}, t)$

$$\begin{cases} \underbrace{\Gamma(1,2,3)}_{0} = \delta(1,2)\,\delta(2,3) + \int d(4,5,6,7)\, \dfrac{\delta\Sigma(1,2)}{\delta G(4,5)}\, G(4,6)\, G(7,5)\, \Gamma(6,7,3) \\ P(1,2) = -i \int G(2,3)\, G(4,2)\, \Gamma(3,4,1)\, d(3,4) \\ W(1,2) = V(1,2) + \int W(1,3)\, P(3,4)\, V(4,3)\, d(3,4) \\ \Sigma(1,2) = i \int d(3,4)\, G(1,3^{+})\, W(1,4)\, \Gamma(3,2,4) \end{cases}$$

$G = G_0 + G_0 \Sigma G$

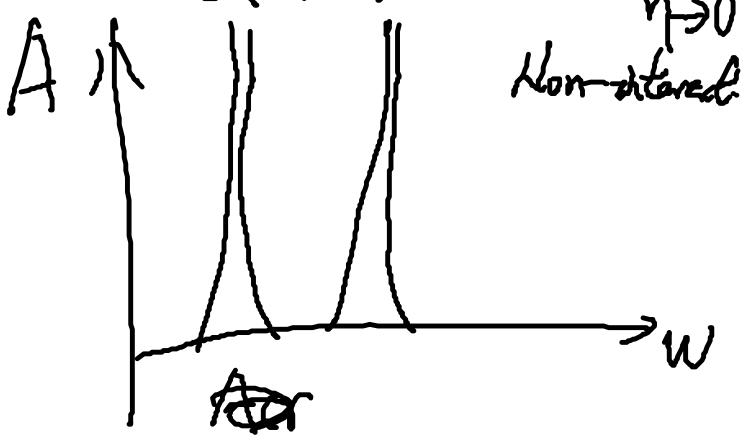


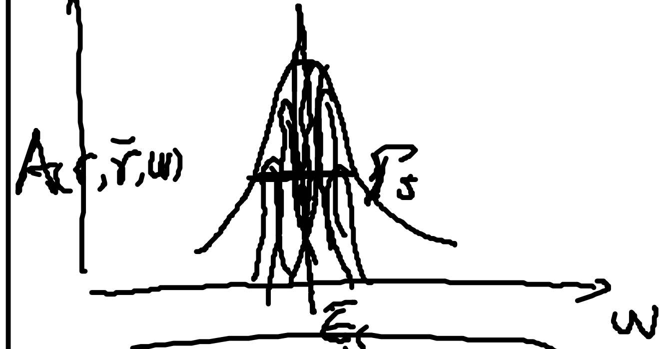
⑤ Quasiparticle.

$|N\rangle_0$ $\qquad \underline{\sum_s \delta(\omega - \epsilon_s)}$

$$A(\vec{r}, \vec{r}', \omega) = \sum_s \varphi_s(\vec{r}) \varphi_s^*(\vec{r}') \delta(\omega - \epsilon_s)$$

$$G(\vec{r}, \vec{r}', \omega) = \lim_{\eta \to 0^+} \int d\omega' \frac{A(\vec{r}, \vec{r}', \omega)}{\omega - \omega' + i\,\mathrm{sgn}(\omega' - \mu)\eta}.$$





$A(\vec{r}, \vec{r}', \omega) =$

$\epsilon_s = \bar{\epsilon}_s + i\Gamma_s$

$\sum_s \varphi_s(r)\,\varphi^*(r)\,\frac{\Gamma_s}{(w-\bar{\epsilon}_s)^2+\Gamma_s^2}$

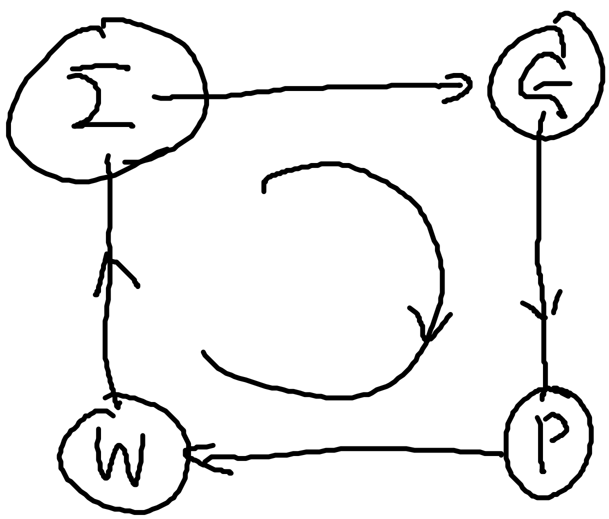
$\left[-\frac{\nabla^2}{2} + V_{ext}(\vec{r}) + V_H(\vec{r})\right]\varphi_s(\vec{r}) + \int dr' \,\underline{\Sigma(\vec{r},\vec{r}',\epsilon_s)}\,\varphi_s(\vec{r}') = \epsilon_s\,\varphi_s(\vec{r})$

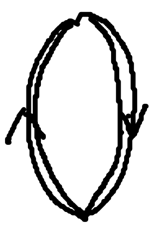
Part II. GW approximation

$\Gamma(1,2,3) = \delta(1,2)\,\delta(2,3)$

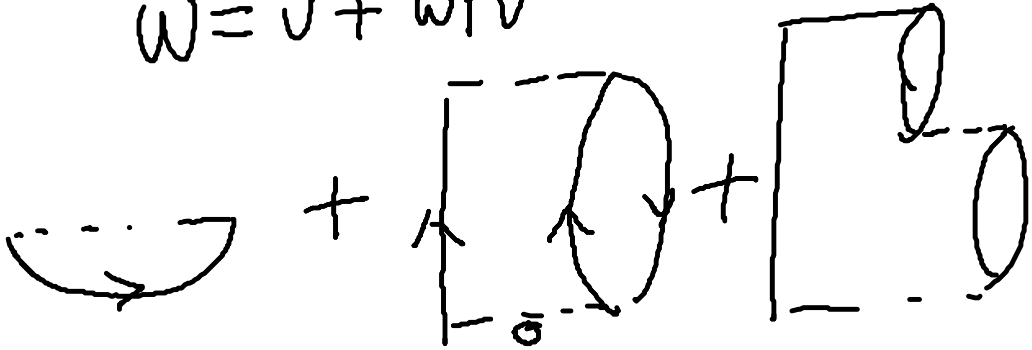
$$
\begin{cases}
P(1,2) = -i\,G(1,2)\,G(2,1) \\
W(1,2) = V(1,2) + \int d(3,4)\; W(1,3)\,P(3,4)\,V(4,2) \\
\Sigma(1,2) = i\,G(1,2)\; W(1^+,2)
\end{cases}
$$

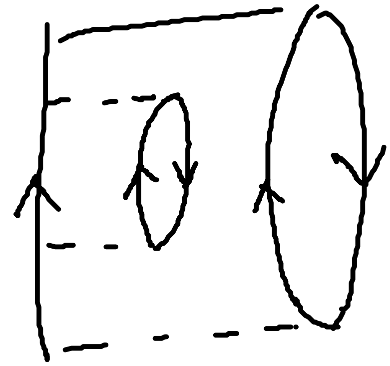
$G = G_0 + G_0 \Sigma G$



P = 

W = v + wPv

Σ : 

$+$  $+ \cdots$

2. Current status of study.

$$\Sigma(1,2) = i\, \underline{G_0(1,2)}\, \underline{W_0(1^+,2)}$$

$$\Sigma(\vec{r},\vec{r}',w) = \frac{i}{2\pi}\int \underline{G_0(\vec{r},\vec{r}',w+w')}\, W_0\underline{(\vec{r},\vec{r}',w')}\, dw'$$

$$\Delta\Sigma(\vec{r},\vec{r}',w) = \Sigma(\vec{r},\vec{r}',w) - V^{xc}(\vec{r})\,\delta(\vec{r}-\vec{r}')$$

$$G^{QP}_{nk} = G^{KS}_{nk} + \langle \varphi^{KS}_{nk}(\vec{r}) | \Delta\Sigma(\vec{r},\vec{r}',w) | \varphi^{KS}_{nk}(\vec{r}')\rangle$$

G_0W_0 method.