

Superconductivity, final stages

We had:

$$\begin{aligned} \text{- 'Cooper pairs': } \psi_0(\underline{r}_1, \underline{r}_2) &= \sum_{\underline{k}} g_{\underline{k}} e^{-i\underline{k}\cdot\underline{r}_1} e^{i\underline{k}\cdot\underline{r}_2} \\ &= \sum_{\underline{k}} \tilde{g}_{\underline{k}} \cos(\underline{k}(\underline{r}_1 - \underline{r}_2)) \end{aligned}$$

• extended in \underline{k} -space

• any however weakly attractive $V_{\underline{k}, \underline{k}'}$ will bind such pairs -

$$\text{BUT } E = 2\varepsilon_F - 2\hbar\omega_D e^{-\frac{2}{N(\varepsilon_F)V}}$$

NOT ANALYTIC \Leftrightarrow no perturb. theory

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

Hamiltonian:

$$\sum_{\underline{k}\sigma} \xi_{\underline{k}} c_{\underline{k}\sigma}^{\dagger} c_{\underline{k}\sigma} + \sum_{\underline{k}, \underline{k}'} c_{-\underline{k}}^{\dagger} c_{\underline{k}} V(\underline{k}, \underline{k}') c_{-\underline{k}'} c_{\underline{k}'}$$

$$\xi_{\underline{k}} = \varepsilon_{\underline{k}} - \varepsilon_F$$

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

Mean-field approximation:

$$\text{Set } \Delta_k = -V \sum_{\underline{k}'} \Theta(\hbar\omega_0 - |\xi_{\underline{k}'}|) \underline{b}_{\underline{k}'}$$

$$\underline{b}_{\underline{k}} = \langle c_{-\underline{k}\downarrow} c_{\underline{k}\uparrow} \rangle_{av} \quad \text{is the statistical average}$$

Can rewrite:

$$H_M = \sum_{\underline{k}\sigma} \xi_{\underline{k}} c_{\underline{k}\sigma}^\dagger c_{\underline{k}\sigma} - \sum_{\underline{k}} (\Delta_{\underline{k}} c_{\underline{k}\uparrow}^\dagger c_{-\underline{k}\downarrow}^\dagger + \Delta_{\underline{k}}^\dagger c_{-\underline{k}\downarrow} c_{\underline{k}\uparrow} - \Delta_{\underline{k}} b_{\underline{k}})$$

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

General transformation can be found

$$c_{\underline{k}\uparrow} = u_{\underline{k}} \alpha_{\underline{k}} + v_{\underline{k}} \beta_{\underline{k}}^\dagger$$

$$c_{-\underline{k}\downarrow} = u_{\underline{k}} \beta_{\underline{k}} - v_{\underline{k}} \alpha_{\underline{k}}^\dagger$$

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

$$H_M \rightarrow \tilde{H}_M = E_0 + \sum_{\underline{k}} E_{\underline{k}} (\alpha_{\underline{k}}^\dagger \alpha_{\underline{k}} + \beta_{\underline{k}}^\dagger \beta_{\underline{k}})$$

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

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

$$v_k^2 = \frac{1}{2} \left(1 - \frac{f_k}{E_k} \right)$$

$$u_k \cdot v_k = - \frac{\Delta_k}{2E_k}$$

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

if $\Delta = 0$

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

$$\Delta = -V \sum_{\underline{k}'} \Theta(\omega_0 - |f_{\underline{k}'}|) \langle c_{\underline{k}'}^\dagger c_{\underline{k}'} \rangle_{av}$$

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

↑
replace

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

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

0 at $T=0$

Find non-trivial solution

$\Delta = 0$ to (*)

$$\Rightarrow E_c = E_0(\Delta \neq 0) - E_0(\Delta = 0)$$

$$= \dots = \left(2 \sum_{\underline{k}} f_{\underline{k}} - \frac{1}{2} N(\epsilon_F) \Delta^2 \right) - 2 \sum_{\underline{k}} f_{\underline{k}}$$

< 0 ✓

I. Green function theory.

① warm up

② what message can be obtained?

③ $\Sigma \rightarrow v$.

④ Hedin's eqn.

⑤ Quasiparticle

II. EW approximation

① EWA.

② Current status.

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

\hat{C}_R^+ \hat{C}_R

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

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{\kappa}{2} \hat{\chi}^2$$

$$\hat{a}^\dagger = \left(\frac{m\omega}{2\hbar} \right)^{1/2} \left[\hat{\chi} + \frac{i\hat{p}}{m\omega} \right] \quad \omega = \sqrt{\frac{\kappa}{m}}$$

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

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

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

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

$|N\rangle \rightarrow$ ground state

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

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

$$G = \frac{1}{i} \langle N | \hat{T} \left[\hat{\psi}(\vec{r}, t) \hat{\psi}^\dagger(\vec{r}', t') \right] | N \rangle.$$

↪ time ordering.

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

$$\hat{H} = \int d^3r dt \hat{\psi}^\dagger(\vec{r}, t) \left[-\frac{1}{2} \nabla^2 + V_{\text{ext}}(\vec{r}) \right] \hat{\psi}(\vec{r}, t)$$

$$+ \frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 \hat{\Psi}^\dagger(\vec{r}_1, t) \hat{\Psi}^\dagger(\vec{r}_2, t) V(\vec{r}_1, \vec{r}_2) \delta(t-t) \hat{\Psi}(\vec{r}_3, t) \hat{\Psi}(\vec{r}_4, t)$$

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

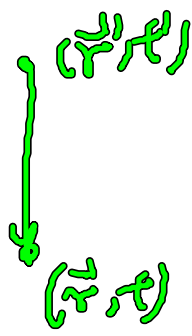
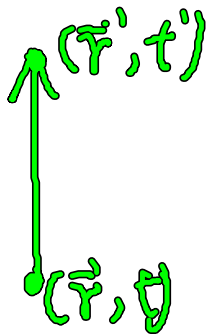
$$+ i \int d\vec{r}_i V(\vec{r}, \vec{r}_i) \langle N | \hat{T} \left\{ \hat{\Psi}^\dagger(\vec{r}_1, t) \hat{\Psi}^\dagger(\vec{r}_2, t) \hat{\Psi}(\vec{r}_3, t) \hat{\Psi}(\vec{r}_4, t) \right\} \rangle = \delta(\vec{r}-\vec{r}') \delta(t-t')$$

$$\int d\vec{r}, dt, M(\vec{r}, t, \vec{r}', t') G(\vec{r}, t, \vec{r}', t')$$

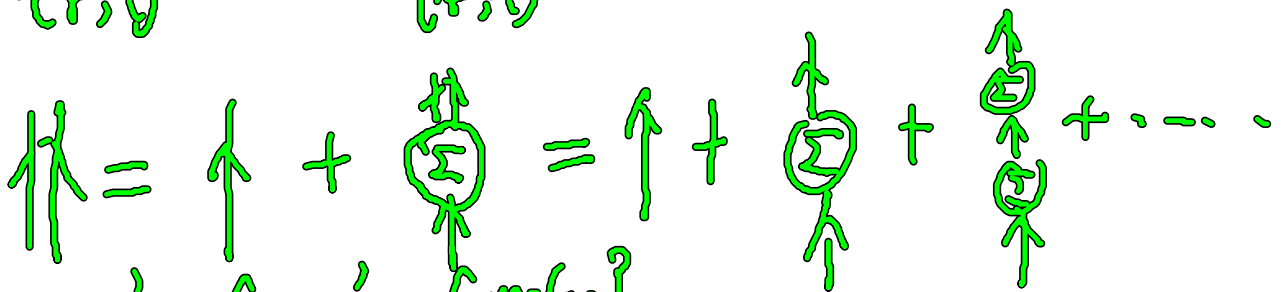
$$\Sigma = M - V^H$$

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

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



\Rightarrow Feynman.



2. Why Green's function?

⊙ expectation value of any single particle operator.

- ② Total energy.
- ③ Excitation spectrum.

$$\textcircled{1}. \hat{J}(\vec{r}) = \hat{\psi}^\dagger(\vec{r}) \hat{j}(\alpha) \hat{\psi}(\vec{r})$$

\downarrow second quantized. \downarrow first quantized

Density. first quantized = 1

$$\begin{aligned} \langle \hat{J}(\alpha) \rangle &= \langle N | \hat{\psi}^\dagger(\vec{r}) \hat{j}(\alpha) \hat{\psi}(\vec{r}) | N \rangle \\ &= \lim_{\vec{r}' \rightarrow \vec{r}} \hat{j}(\alpha) \langle N | \hat{\psi}^\dagger(\vec{r}') \hat{\psi}(\vec{r}) | N \rangle \\ &= \lim_{t \rightarrow t'} \lim_{\vec{r}' \rightarrow \vec{r}} \hat{j}(\alpha) \hat{G}(\vec{r}, t, \vec{r}', t') \end{aligned}$$

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

Density: $\langle \hat{\psi}^\dagger(\vec{r}') \hat{\psi}(\vec{r}) \rangle = i \hat{G}(\vec{r}, t, \vec{r}', t')$

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

- ② Total energy.
- ③ excitation spectrum.

$$\sum_{N_0} \langle N, s \rangle \langle N, s \rangle = 1.$$

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

Fourier transform

$$G(\vec{r}, \vec{r}', \omega) = \lim_{T \rightarrow \infty} \int_{-T}^T \hat{\psi}^s(\vec{r}) \hat{\psi}^{s*}(\vec{r}') \left[\frac{\theta(\epsilon - \mu)}{\omega - \epsilon + i\eta} + \frac{\theta(\mu - \epsilon)}{\omega - \epsilon - i\eta} \right]$$

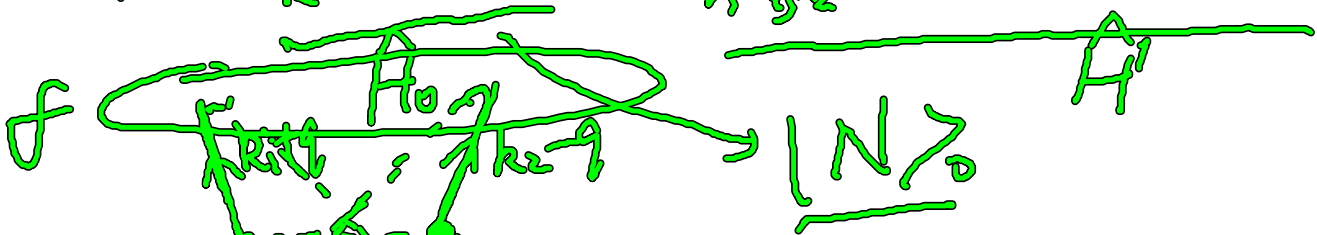
$\mu \rightarrow$ chemical potential

$$G_s = \bar{E}_{N+1}^s - E_N \quad \hat{\psi}^s(\vec{r}) = \langle N | \hat{\psi}(\vec{r}) | N+1, s \rangle \quad \text{for } \epsilon > \mu$$

$$G_s = \bar{E}_N - \bar{E}_{N-1}^s \quad \hat{\psi}^s(\vec{r}) = \langle N-1, s | \hat{\psi}(\vec{r}) | N \rangle \quad \text{for } \epsilon < \mu.$$

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

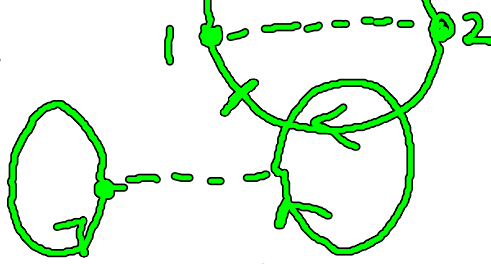
$$\hat{H} = \sum_k \epsilon_k \hat{c}_k^\dagger \hat{c}_k + \sum_{i, k_1, k_2} V_{ij} \hat{c}_{i+q}^\dagger \hat{c}_{j+q}^\dagger \hat{c}_{k_2} \hat{c}_{k_1}$$



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

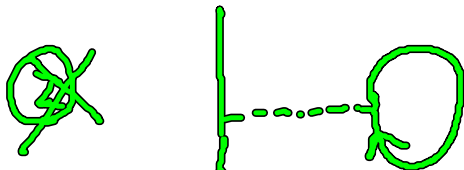
① $k_1 + q = k_2$

② $q = 0$



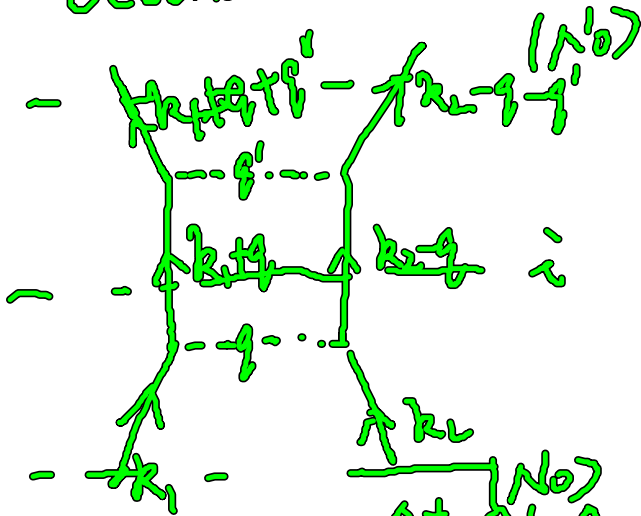
$\Sigma \rightarrow 'v'$

First order correction



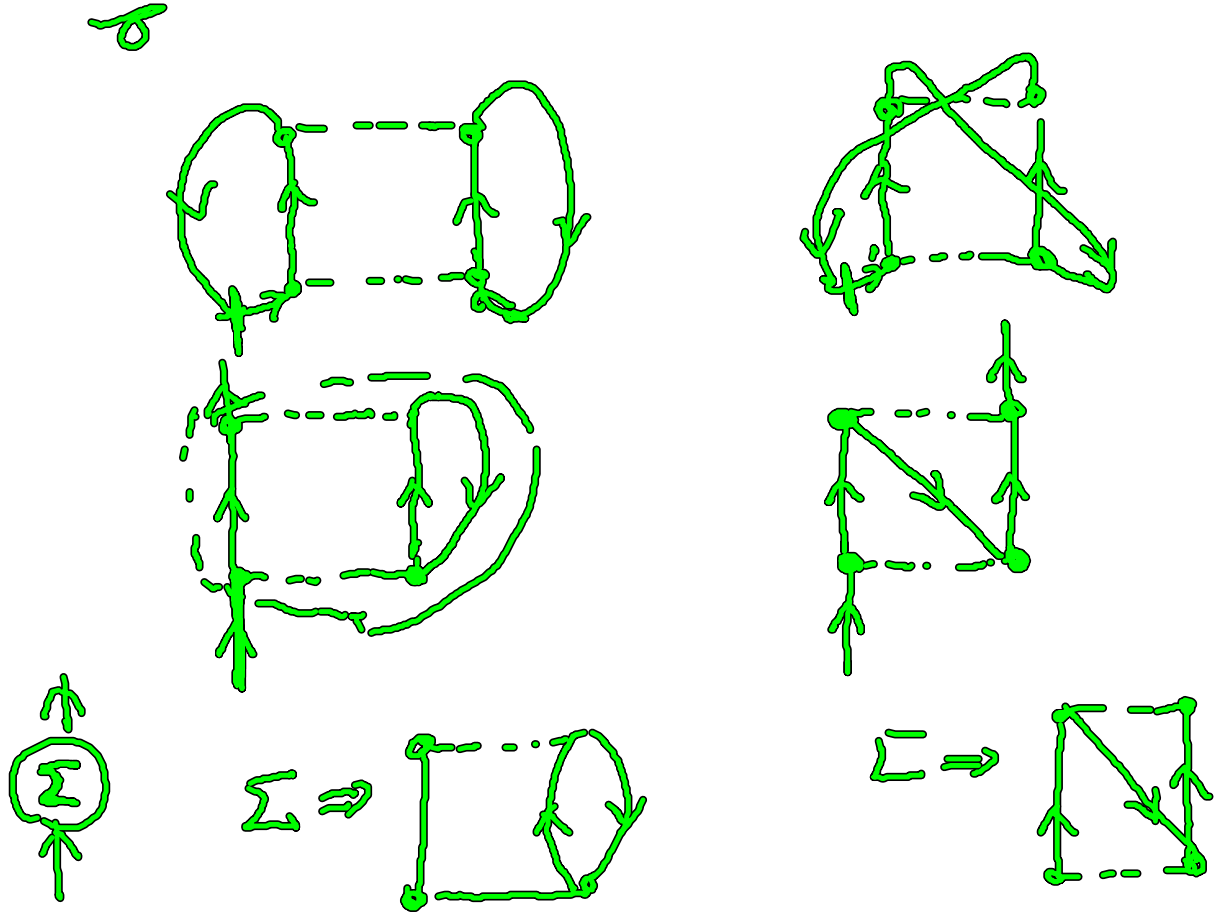
doesn't contribute to Σ

Second order correction:



(No)

$\Delta \bar{E} \propto N \langle N | \hat{C}_{k_1}^{\dagger} \hat{C}_{k_2}^{\dagger} \hat{C}_{k_1} \hat{C}_{k_2} | i \rangle \langle i | \hat{C}_{k_1}^{\dagger} \hat{C}_{k_2}^{\dagger} \hat{C}_{k_1} \hat{C}_{k_2} | N_0 \rangle$



third order.

4. Hedén's eqn. (1965)

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

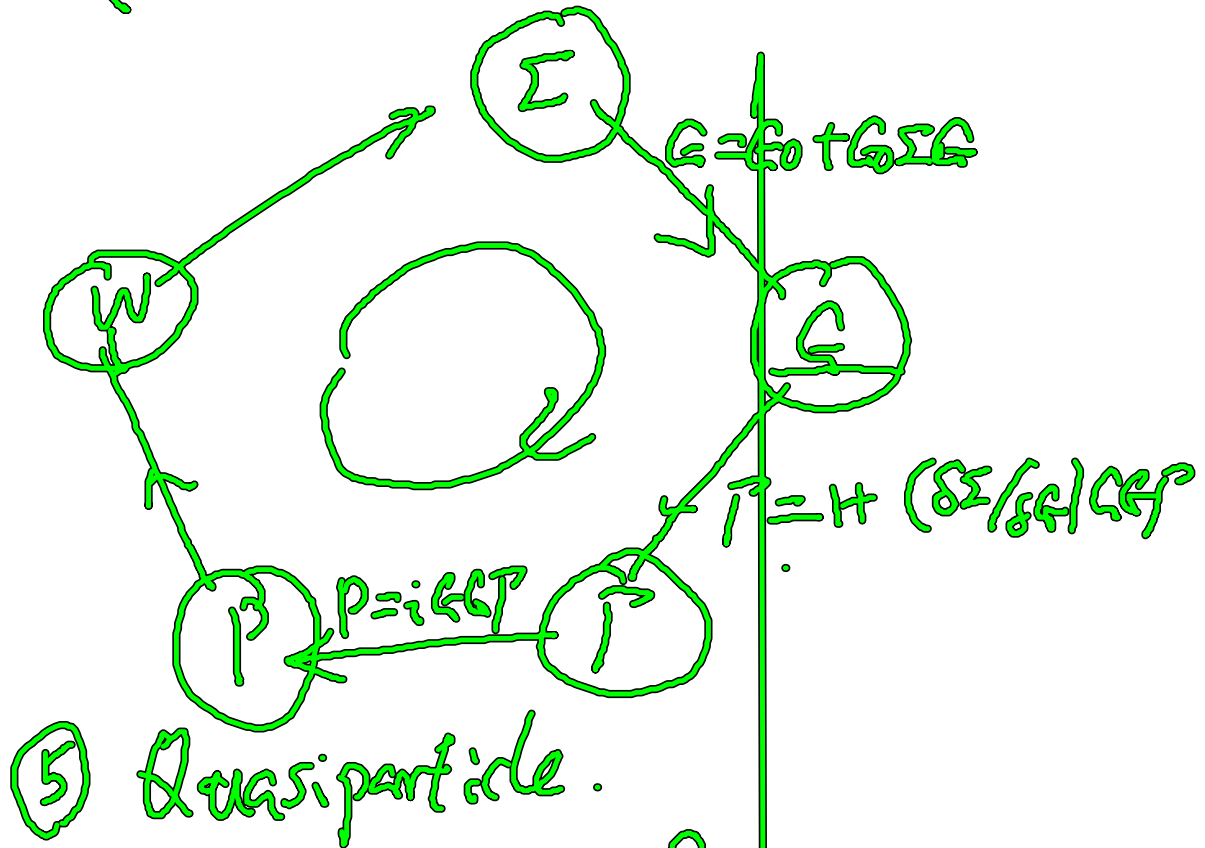
$$\Gamma(1, 2, 3) = \delta(1, 2) \delta(2, 3) + \int d(4, 5, 6, 7) \frac{\delta \Sigma(1, 2)}{\delta G(4, 5)} G(4, 6) G(7, 5) P(6, 7, 3)$$

$$P(1, 2) = -i \int G(2, 3) G(3, 4) P(3, 4) d(3, 4)$$

$$W(1, 2) = V(1, 2) + \int W(1, 3) P(3, 4) V(4, 3) d(3, 4)$$

$$\Sigma(1, 2) = i \int d(3, 4) G(1, 3^+) W(1, 4) P(3, 2, 4)$$

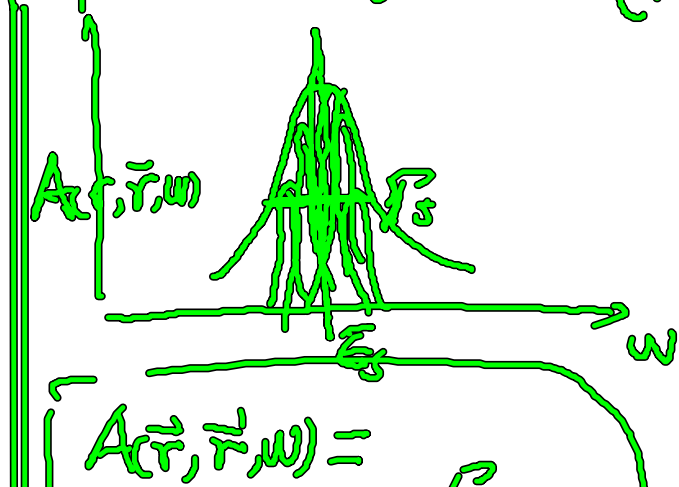
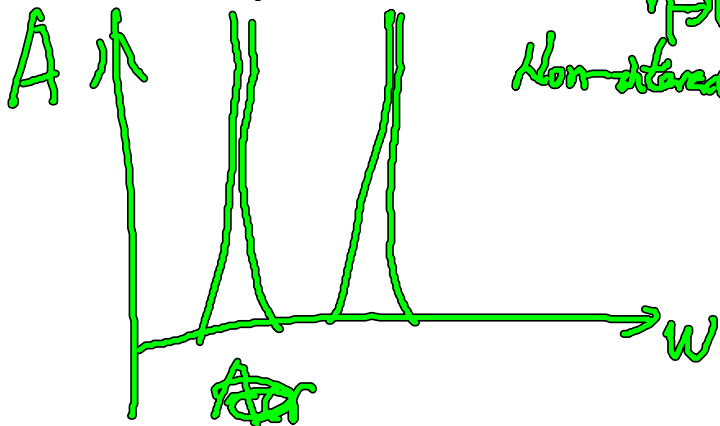
$$\epsilon = \epsilon_0 + \epsilon_0 \sum \epsilon$$



$$|N\rangle_0 \quad \frac{\sum_s \delta(\omega - \epsilon_s)}$$

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

$$G(\vec{r}, \vec{r}', \omega) = \lim_{\eta \rightarrow 0^+} \int d\omega' \frac{A(\vec{r}, \vec{r}', \omega')}{\omega - \omega' + i \text{sign}(\omega - \omega') \eta}$$



$$E_S = \bar{E}_S + i\Gamma_S$$

$$\left[-\frac{\nabla^2}{2} + V_{ext}(\vec{r}) + V_{int}(\vec{r}) \right] \psi(\vec{r}) = E_S \psi(\vec{r})$$

$$\int \frac{\psi(\vec{r}) \psi^*(\vec{r}')}{|\vec{r} - \vec{r}'|} \frac{1}{(E_S - E_S')^2 + \Gamma_S^2} \psi_S(\vec{r}') = E_S \psi_S(\vec{r})$$

Part II. EW approximation

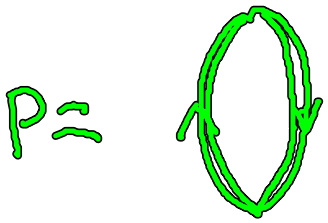
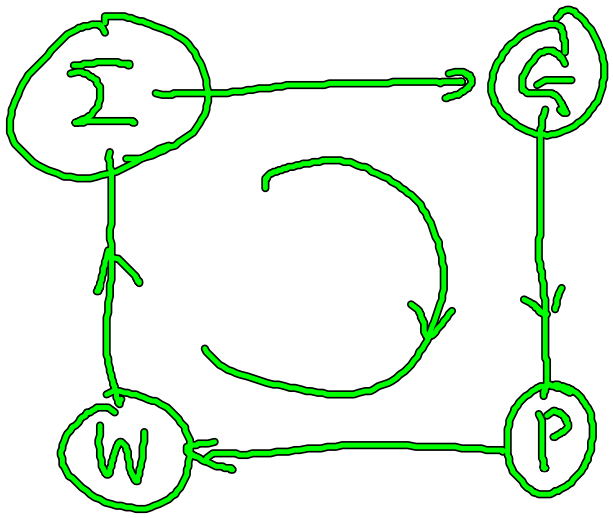
$$\overline{P}_{(1,2,3)} \delta(1,2) \delta(2,3)$$

$$P(1,2) = -i G(1,2) K(2,1)$$

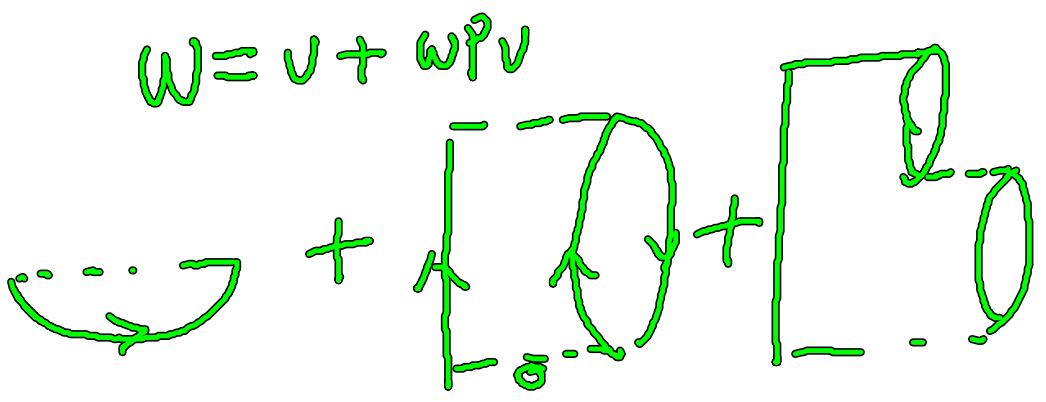
$$W(1,2) = V(1,2) + \int d(3,4) W(1,3) P(3,4) V(4,2)$$

$$\Sigma(1,2) = i K(1,2) W(\tau, 2)$$

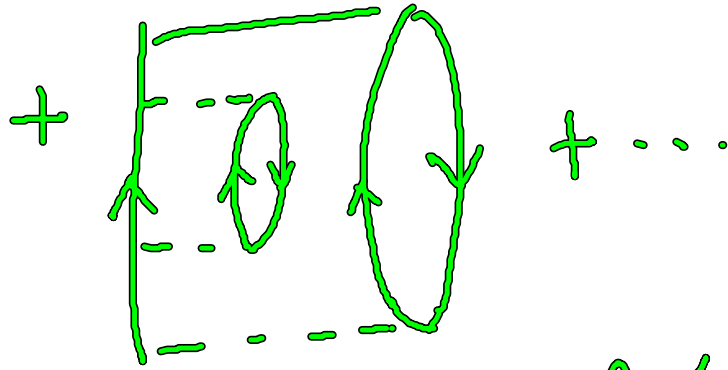
$$G = G_0 + \Sigma G$$



$\Sigma :=$



$$W = V + W P V$$



2. Current status of study.

$$\Sigma(1, 2) = i \underline{\epsilon_0(1, 2)} \underline{U_0(1^+, 2)}$$

$$\Sigma(\vec{r}, \vec{r}', \omega) = \frac{i}{2\pi} \int \underline{\epsilon_0(\vec{r}, \vec{r}', \omega + \omega')} \underline{U_0(\vec{r}, \vec{r}', \omega')} d\omega'$$

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

$$\epsilon_{nk}^{QP} = \epsilon_{nk}^{KS} + \langle \varphi_{nk}^{KS}(\vec{r}) | \Delta \Sigma(\vec{r}, \vec{r}', \omega) | \varphi_{nk}^{KS}(\vec{r}') \rangle$$

$\epsilon_0 U_0$ method.