Trieste 6 août 2012

1) Second quantization
- Creation operators
- Change of basis
- One and two-body operators

2) Hubbard model
- Simplest model
  - $\rightarrow U=0$
  - $\rightarrow t=0$
  - $\rightarrow$ Exact: Bethe

3) Perturbation theory

4) Green's functions
- Photoemission
- Def.
- Matsubara
- ~~Equ. of motion, self energy~~
- Non-interacting case $U=0$
- $A(k,\omega)$ (General)
- $t=0$, U fini $\rightarrow$ Self-energy + example $\cancel{U}$ $V=0$
- Quantum impurity $\rightarrow$ Q.P. ~~Eq. of motion~~ V only.
- ~~$d=\infty$~~

4) Generating functionals
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1) Second quantization:

Creation operators:

(1) $|0\rangle \qquad |r\rangle = \psi^\dagger(r)|0\rangle$

(2) $|r, r'\rangle = \frac{1}{\sqrt{2}}\left(|r\rangle|r'\rangle - |r'\rangle|r\rangle\right) = -|r', r\rangle$

(3) $= \psi^\dagger(r)\psi^\dagger(r')|0\rangle$

(4) $\psi^\dagger(r)\psi^\dagger(r') = -\psi^\dagger(r')\psi(r)$

(5) $\psi^\dagger(r_1)\psi^\dagger(r_2)\psi^\dagger(r_3)|0\rangle = -\psi^\dagger(r_3)\psi^\dagger(r_2)\psi^\dagger(r_1)|0\rangle$

(6) $\psi(r)|0\rangle = 0$.

(7) $\langle r|r'\rangle = \delta(r-r') = \langle 0|\psi(r)\psi^\dagger(r')|0\rangle$

$= \langle 0|\{\psi(r), \psi^\dagger(r')\}|0\rangle$

$\forall$ states

Change of basis

(8) $\cancel{|\alpha\rangle = \sum_r |r\rangle\langle r|\alpha\rangle} \qquad |r\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|r\rangle$

(9) $\cancel{c^\dagger_\alpha = \int d^3r\, \psi^\dagger(r)\langle r|\alpha\rangle} \qquad \psi^\dagger(r) = \sum_\alpha c^\dagger_\alpha \langle\alpha|r\rangle$

~~(10) ψ~~

One-body two-body operators:

(10) $c^\dagger_\alpha c_\alpha \; c^\dagger_\beta |0\rangle = 0$ if $\alpha \neq \beta$

(11) If $\alpha = \beta$:

$$c^\dagger_\alpha c_\alpha c^\dagger_\alpha |0\rangle = c^\dagger_\alpha \left[1 - c^\dagger_\alpha c_\alpha \right] |0\rangle$$

$$= c^\dagger_\alpha$$

= # operator.

(12) If

$$H = \sum_\alpha c^\dagger_\alpha c_\alpha \varepsilon_\alpha \Rightarrow \text{eigenstates: } c^\dagger_1 c^\dagger_2 \dots c^\dagger |0\rangle$$

$$\varepsilon_\alpha = \langle \alpha | H_{\text{first quantized}} | \alpha \rangle$$

(13) $$N = \int d^3r \, \psi^\dagger(r) \psi(r)$$

(14) $$\vec{S} = \int d^3r \sum_{\alpha\beta} \psi^\dagger_\alpha(r) \vec{\sigma}_{\alpha\beta} \frac{\hbar}{2} \psi_\beta(r)$$

(15) $$H = \frac{-\hbar^2}{2m} \sum_\sigma \int d^3r \, \psi^\dagger_\sigma(r) \nabla^2 \psi_\sigma(r)$$

$$+ \frac{1}{2} \sum_{\sigma\sigma'} \int d^3r \, d^3r' \, \psi^\dagger_\sigma(r) \psi^\dagger_{\sigma'}(r') \frac{1}{|r-r'|} \psi_{\sigma'}(r') \psi_\sigma(r)$$

2) Hubbard model

(2.1) $$\psi^\dagger_\sigma(r) = \sum_{ni} c^\dagger_{\sigma ni} \langle ni | r \rangle$$

One band:

(2.2) $$H = -\sum_{ij\sigma} c^\dagger_{i\sigma} t_{ij} c_{j\sigma} + \frac{1}{2} \sum_{\sigma\sigma' ijkl} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} \langle i | \langle j | V | k \rangle | l \rangle c_{l\sigma'} c_{k\sigma}$$

(2.3) $$t_{ij} = \langle i | -\frac{\hbar^2}{2m} \nabla^2 | j \rangle$$

(2.4) $= \quad '' \quad + \frac{1}{2} \sum_{\sigma\sigma'} \sum_i U n_{i\sigma} n_{i\sigma'}$

(2.5) $= \quad '' \quad + \frac{U}{2} \sum_i n_i + U \sum_i n_{i\uparrow} n_{i\downarrow}$

$t = 0 \Rightarrow c^+_{i\sigma} c^+_{j\sigma'} \cdots |0\rangle$

$U = 0 \Rightarrow c^+_{k_1\sigma} c^+_{k_2\sigma'} \cdots |0\rangle$

Otherwise, all mixed up!

Exact: Bethe, $d = \infty$

3) Perturbation theory

(3.1) $K = H - \mu N = H_0 + H_1 - \mu N = K_0 + K_1$

(3.2) $e^{-\beta K} = e^{-\beta K_0} U(\beta)$

(3.3) $\frac{\partial}{\partial \tau} e^{-K\tau} = -K_0 e^{-K_0\tau} U(\tau) + e^{-K_0\tau} \frac{\partial U(\tau)}{\partial \tau}$

(3.4) $(-K_0 - K_1) e^{-K_0\tau} U(\tau)$

(3.5) $\frac{\partial U(\tau)}{\partial \tau} = \left(e^{K_0\tau} K_1 e^{-K_0\tau} \right) U(\tau)$

(3.6) $\frac{\partial U(\tau)}{\partial \tau} = -K_1(\tau) U(\tau)$

(3.7) $U(\beta) - U(0) = -\int_0^\beta K_1(\tau) U(\tau) d\tau$

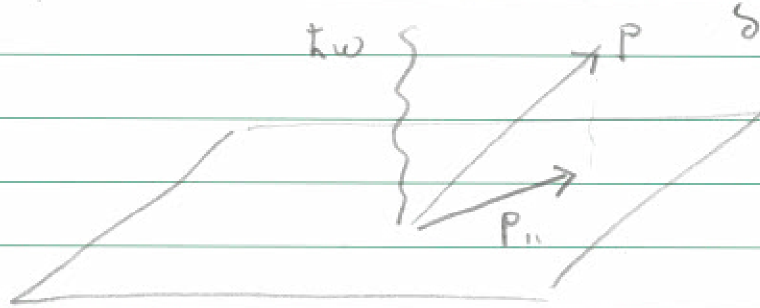
$= -\int_0^\beta d\tau K_1(\tau) - \int_0^\beta d\tau \int_0^\tau d\tau' K_1(\tau) K_1(\tau')$

(3.8) $\boxed{U(\beta) = T_\tau e^{-\int_0^\beta K_1(\tau) d\tau}}$

4) Green's functions

· Photoemission

$$(4.1)\quad \sum_{m\,n} \frac{2\pi}{\hbar} \left| {}_{em}\langle 0| \langle p| \langle m| \sum_{k'} \vec{j}_{k'} \cdot \vec{A}_{-k'} |1\rangle_{em} |0\rangle |n\rangle \right|^2 \frac{e^{-\beta K_n}}{Z} \delta(\hbar\omega + \mu - (E_n - E_m))$$



$$(4.2)\quad j_{k'=0} = \sum_{p\,\sigma} \frac{\vec{p}}{m} c^{+}_{p\sigma} c_{p\sigma} \qquad \hbar = 1$$

$$(4.3)\quad \propto \sum_{n,m}\sum_{\sigma} \int dt\, e^{i(\omega - (K_n - K_m))t} \langle n| c^{+}_{p_{\parallel}\sigma} |m\rangle \langle m| c_{p_{\parallel}\sigma} |n\rangle \frac{e^{-\beta K_n}}{Z}$$

$$(4.4)\quad \propto \sum_{n}\sum_{\sigma} \int dt\, e^{i\omega t} \langle n| c^{+}_{p_{\parallel}\sigma}(0)\, c_{p_{\parallel}\sigma}(t) |n\rangle \frac{e^{-\beta K_n}}{Z}$$

$$(4.5)\quad \propto \sum_{\sigma} \int dt\, e^{i\omega t} \langle c^{+}_{p_{\parallel}}(0)\, c_{p_{\parallel}}(t) \rangle$$

$$(4.6)\quad \propto \boxed{\sum_{m,n} \frac{e^{-\beta K_n}}{Z} \langle n| c^{+}_{p_{\parallel}\sigma} |m\rangle \langle m| c_{p_{\parallel}} |n\rangle\, \delta(\hbar\omega - (K_n - K_m))}$$

Matsubara

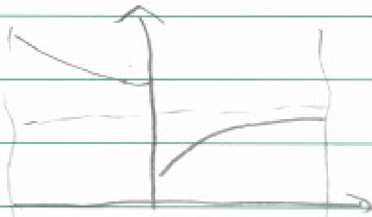
(4.6) $\mathcal{G}_{\alpha\beta}(\tau) = -\langle T_\tau c_\alpha(\tau) c_\beta^+(0)\rangle$

$$= -\theta(\tau)\langle c_\alpha(\tau) c_\beta^+(0)\rangle + \theta(-\tau)\langle c_\beta^+(0) c_\alpha(\tau)\rangle$$

(4.7) $c_\alpha(\tau) = e^{K\tau} c_\alpha e^{-K\tau}$ $\quad \tau-\beta<0$

(4.8) $\mathcal{G}_{\alpha\beta}(\tau-\beta) = -\mathcal{G}_{\alpha\beta}(\tau)$ $\quad Z^{-1}\,\mathrm{Tr}\left[e^{-K\beta} c^+ e^{K(\tau-\beta)} c\, e^{-K(\tau-\beta)}\right]$

$\quad Z^{-1}\,\mathrm{Tr}\left[e^{-\beta K} e^{K\tau} c\, e^{-K\tau} c^+\right]$



$\tau>0$

(4.9) $$\boxed{\mathcal{G}_{\alpha\beta}(\tau) = T\sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau}\,\mathcal{G}_{\alpha\beta}(i\omega_n)}$$

(4.9b) $\omega_n = (2n+1)\pi$

(4.10) $$\boxed{\mathcal{G}_{\alpha\beta}(i\omega_n) = \int_0^\beta d\tau\, \mathcal{G}_{\alpha\beta}(\tau)\, e^{+i\omega_n\tau}}$$

Cas sans interaction:

(4.12) $\dfrac{\partial c_k}{\partial\tau} = [K_0, c_k]$ $\quad K_0 = \sum_p \epsilon_p c_p^+ c_p$

$$= -\epsilon_k c_k \qquad [AB, C] = A\{B,C\} - \{A,C\}B$$

$\quad ABC + ACB - ACB - CAB$

(4.13) $\dfrac{\partial}{\partial\tau}\mathcal{G}_{\alpha\beta}(k,\tau) = -\delta(\tau)\delta_{\alpha\beta} - \epsilon_k\,\mathcal{G}_{\alpha\beta}(k,\tau)$

(4.14) $(-i\omega_n + \epsilon_k)\,\mathcal{G}_{\alpha\beta}(k, i\omega_n) = -\delta_{\alpha\beta}$

(4.15) $\mathcal{G}_{\sigma\sigma}(k, i\omega_n) = \dfrac{1}{i\omega_n - \epsilon_k}$

(4.16) $G^R_{\sigma\sigma}(k, \omega) = \dfrac{1}{\omega + i\eta - \epsilon_k}$

(4.17) $-2\,\mathrm{Im}\, G^R(k, \omega) = 2\pi\, \delta(\omega - \epsilon_k)$

Cas général

(4.18) $\mathcal{G}(k, i\omega_n) = -\int_0^\beta d\tau \, \langle c_k(\tau) c_k^+(0) \rangle \, e^{i\omega_n \tau}$

$$= -\int_0^\beta d\tau \sum_{nm} \frac{e^{i\omega_n\tau}}{Z} e^{-\beta K_n} e^{\tau(K_n - K_m)} \langle n | c_k | m \rangle \langle m | c_k^+ | n \rangle$$

(4.19) $$= -\frac{1}{Z} \sum_{nm} e^{-\beta K_n} \frac{e^{\beta(K_n - K_m)} + 1}{i\omega_n + K_n - K_m} \langle n | c_k | m \rangle \langle m | c_k^+ | n \rangle$$

$$\cancel{= \frac{1}{Z} \sum_{nm} \frac{e^{-\beta K_n} + e^{-\beta K_m}}{i\omega_n + K_n - K_m} \langle \; \rangle \langle \; \rangle}$$

$$= \int \frac{d\omega}{2\pi} \frac{A_{\sigma\sigma}(k, \omega)}{i\omega_n - \omega}$$

N.B. $\cancel{\int \frac{d\omega}{2\pi} A(k, \omega) = 1}$

(4.20) $$\mathcal{G}(k, i\omega_n) = \int \frac{d\omega'}{2\pi} \frac{1}{i\omega_n - \omega'} \sum_{mn} \frac{e^{-\beta K_m}}{Z} \left(1 + e^{+\beta(K_m - K_n)}\right) 2\pi\, \delta(\omega' - (K_m - K_n)) \langle \rangle \langle \rangle$$

(4.21) $$A(k, \omega') = \sum_{mn} \frac{e^{-\beta K_m}}{Z} \left(e^{\beta\omega'} + 1\right) \langle n | c_k | m \rangle \langle m | c_k^+ | n \rangle \, 2\pi\, \delta(\omega' - (K_m - K_n))$$

Constraining field and K.B. functional

(1) $Z[\varphi] = \mathrm{Tr}\left[e^{-\beta K} T_\tau e^{-\psi^\dagger(\bar 1)\varphi(\bar 1,\bar 2)\psi(\bar 2)}\right]$

(2) $-\dfrac{\delta \ln Z}{\delta \varphi(2,1)} = G(1,2) = \dfrac{\delta F}{\delta \varphi}\dfrac{1}{T}$

(3) $\Gamma[G] = F[\varphi[G]] - (\varphi G)_T$

$= F[\varphi[G]] - \mathrm{Tr}\,\varphi G$

↑ contient T

$O(\lambda)$

$= F_0[\varphi_0] - \mathrm{Tr}[\varphi_0 G] + \Delta\Gamma$

$\uparrow$
K_0

(4) $\dfrac{\delta F_0[\varphi_0]}{\delta \varphi_0} = G \Rightarrow \dfrac{\delta \Delta\Gamma}{\delta G} = \varphi_0$ au col

Preuve:

$\dfrac{\delta \Gamma}{\delta G} = -\varphi_0 + \dfrac{\delta \Delta\Gamma}{\delta G} = \varphi = O = G_0^{-1} - G^{-1} - \Sigma$

(5) $\left.\dfrac{\partial \ln Z}{\partial \lambda}\right|_\varphi = \left.\dfrac{\partial \Gamma}{\partial \lambda}\right|_G$ $\quad \varphi = \varphi_0 + \lambda\varphi \ldots$ $\quad S = S_0 + \lambda S \ldots$

$= \left.\dfrac{\partial \Delta\Gamma}{\partial \lambda}\right|_G$

(6) $\Delta\Gamma = \int_0^1 d\lambda \, \langle S_{int} \rangle_{\lambda, \varphi(\lambda, G)}$ $\quad G$

(4.22) $A(k,\omega) = -2\,\mathrm{Im}\,\mathcal{G}(k, i\omega_n \to \omega + i\eta)$

Cross section $\propto A(k,\omega) f(\omega)$

Case $t=0$: (Atomic limit) $K = U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow)$

$$-\langle c_\uparrow(\tau) c^+_\uparrow(0)\rangle = -\frac{1}{Z}\sum_m \langle 0| e^{K\tau} c_\uparrow |m\rangle\langle m| e^{-K\tau} c^+_\uparrow |0\rangle$$

$$= -\frac{1}{Z}\langle 0| \; c_\uparrow e^{-(-\mu)\tau} |\uparrow\rangle\langle\uparrow| c^+_\uparrow |0\rangle$$

$$-\frac{e^{\beta\mu}}{Z}\langle\downarrow| e^{(-\mu)\tau} |\downarrow\rangle\langle\downarrow| c_\uparrow e^{-(U-2\mu)\tau} |\uparrow\downarrow\rangle\langle\uparrow\downarrow| c^+_\uparrow |\downarrow\rangle$$

$$= \frac{-1}{Z} e^{\mu\tau} - \frac{1}{Z} e^{-(U-\mu)\tau} e^{\beta\mu}$$

$$\int_0^\beta d\tau\, e^{+i\omega_n\tau}\left(-\frac{1}{Z}\right)\left[e^{\mu\tau} + e^{-(U-\mu)\tau} e^{\beta\mu}\right]$$

$$= -\frac{1}{Z}\left[e^{(i\omega_n+\mu)\tau}\Big|_0^\beta + e^{(i\omega_n - U + \mu)\tau}\Big|_0^\beta e^{\beta\mu}\right]$$

$$= -\frac{1}{Z}\left[\frac{-e^{\beta\mu} - 1}{i\omega_n + \mu} + \frac{-e^{-\beta(U-\mu)} - 1}{i\omega_n + \mu - U} e^{\beta\mu}\right]$$

$\mu = \frac{U}{2}$ $= \frac{1}{2}\frac{1}{i\omega_n + U/2} + \frac{1}{2}\frac{1}{i\omega_n - U/2}$

$$Z = 1 + 2e^{+\beta\mu} + e^{-\beta U + 2\mu\beta} = (1 + e^{\beta\mu}) + e^{\beta\mu}(1 + e^{-\beta U + \mu\beta})$$

$\boxed{\mu = \frac{U}{2}} \Rightarrow$ $Z = 1 + 2e^{\beta\frac{U}{2}} + 1 = 2(1 + e^{\beta U/2})$

$= 2(1 + e^{\beta\mu})$

- Self-energy:

$$A(k,\omega') = \sum_{mn} \frac{e^{-\beta K_m}}{Z} \left(e^{\beta\omega'} + 1\right) \langle n | c_k | m \rangle \langle m | c_k^+ | n \rangle$$

$$2\pi\delta(\omega' - (K_m - K_n))$$

$$\int \frac{d\omega'}{2\pi} A(k,\omega') = \sum_m \langle m | \frac{e^{-\beta K}}{Z} c_k^+ c_k | m \rangle + \sum_n \langle n | \frac{e^{-\beta K}}{Z} c_k c_k^+ | n \rangle$$

$$= \langle \{ c_k^+ , c_k \} \rangle = 1$$

$\Rightarrow$ in general

$$\lim_{i\omega_n \to \infty} G(k, i\omega_n)\, i\omega_n = 1 \Rightarrow G(k, i\omega_n) = \frac{1}{i\omega_n - (\epsilon_k - \mu) - \Sigma(i\omega_n, k)}$$

- Atomic limit

$$\frac{1}{2}\left[\frac{1}{i\omega_n + U/2} + \frac{1}{i\omega_n - \frac{U}{2}}\right] = \frac{1}{i\omega_n - \Sigma + \frac{U}{2}} \quad \mu$$

$$\frac{1}{2} \frac{2 i\omega_n}{(i\omega_n)^2 - \left(\frac{U}{2}\right)^2} = \frac{1}{i\omega_n - \Sigma + \frac{U}{2}}$$

$$\cancel{(i\omega_n)^2} - i\omega_n \left(\Sigma + \frac{U}{2}\right) = \cancel{(i\omega_n)^2} - \left(\frac{U}{2}\right)^2$$

$$\Sigma = \left(\frac{U}{2}\right)^2 \frac{1}{i\omega_n} + \frac{U}{2} \quad \text{singular !}$$

H.F.

- Weak interaction

$$A(k,\omega) = -2\,\mathrm{Im}\left[\frac{1}{\omega + i\eta - (\epsilon_k - \mu) - \Sigma}\right]$$

Z^{-1}

$$G^{-1} = \omega\left[1 - \frac{\partial \Sigma'}{\partial \omega}\right] + i\eta - (\epsilon_k - \mu) - i\Sigma''(k,\omega)$$

$$-2\,\mathrm{Im}\,\frac{1}{a-ib} = -2\,\mathrm{Im}\left[\frac{ib}{a^2+b^2}\right] = \frac{-2b}{a^2+b^2}$$

F. L.

$$A(k,\omega) = \frac{-2\Sigma''}{\left[Z^{-1}\omega - (\epsilon_k-\mu)\right]^2 + \left(\Sigma''\right)^2}$$

$$= \frac{Z\,(-2Z\Sigma'')}{\left[\omega - Z(\epsilon_k-\mu)\right]^2 + (Z\Sigma'')^2} + \underline{\underline{\mathrm{Inc.}}}$$

$\frac{\partial \Sigma}{\partial k}$ pour renormalisation de m.

$$\boxed{A = \frac{-2\Gamma}{(\omega - \tilde{\epsilon}_k)^2 + \Gamma^2}}$$

Anderson impurity

$$H = H_f + H_c + H_{fc} - \mu N$$

$$H_f = \sum_\sigma \epsilon f^\dagger_{i\sigma} f_{i\sigma} + U \left(f^\dagger_{i\uparrow} f_{i\uparrow}\right)\left(f^\dagger_{i\downarrow} f_{i\downarrow}\right)$$

$$H_c = \sum_\sigma \sum_k \epsilon_k c^\dagger_{k\sigma} c_{k\sigma}$$

$$H_{fc} = \sum_\sigma \sum_k \left(V_{ik}\, c^\dagger_{k\sigma} f_{i\sigma} + V^*_{ki}\, f^\dagger_{i\sigma} c_{k\sigma} \right)$$

$$c^+ f c - c c^+ f = -(c^+ c + c c^+) f$$

Go back to Hubbard: $\Rightarrow$ fluct. in imag. time

$$\begin{cases} \dfrac{\partial c_{k\sigma}}{\partial \tau} = [H, c_{k\sigma}] = -(\epsilon_k - \mu) c_{k\sigma} - V_{ik} f_{i\sigma} \\[2ex] \dfrac{\partial f_{i\sigma}}{\partial \tau} = -(\epsilon - \mu) f_{i\sigma} - U f^\dagger_{i-\sigma} f_{i-\sigma} f_{i\sigma} - \sum_k V^*_{ik} c_{k\sigma} \end{cases}$$

$$\frac{\partial \mathcal{G}_{ff}(\tau)}{\partial \tau} = -\delta(\tau) - (\epsilon - \mu)\mathcal{G}_{ff} + U \underbrace{\langle T_\tau f^\dagger_{i-\sigma}(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f^\dagger_{i\sigma} \rangle}_{\Sigma \mathcal{G}}$$

$$- \sum_k V^*_{ik}\, \mathcal{G}_{cf}(k, i; \tau)$$

$$\mathcal{G}_{cf}(k, i; \tau) = -\langle T_\tau c_{k\sigma}(\tau) f^\dagger_{i\sigma} \rangle$$

$$\frac{\partial \mathcal{G}_{cf}(k,i;\tau)}{\partial \tau} = -(\epsilon_k - \mu)\mathcal{G}_{cf}(k,i;\tau) - V_{ik}\mathcal{G}_{ff}(\tau)$$

$$\Rightarrow \boxed{\mathcal{G}_{cf}(k, i; ik_n) = \frac{+1}{ik_n - (\epsilon_k - \mu)} V_{ik}\, \mathcal{G}_{ff}(\tau)}$$

$$\left[ik_n - (\epsilon-\mu) - \sum_k V_{ik}^* \frac{1}{ik_n-(\epsilon_k-\mu)} V_{ik}\right] \mathcal{G}_{ff}(ik_n)$$

$$= 1 - U\int_0^\beta d\tau\, e^{ik_n\tau} \underbrace{\langle T_\tau f^\dagger_{i-\sigma}(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f^\dagger_{i\sigma}\rangle}_{\Sigma(ik_n)\mathcal{G}_{ff}(ik_n)}$$

$$\mathcal{G}^{0\,-1}_{ff} = ik_n - (\epsilon-\mu) - \Delta(ik_n)$$

$$\Delta(ik_n) = \sum_k V^*_{ik}\frac{1}{ik_n-(\epsilon_k-\mu)}V_{ik}$$

Hybridization fuction