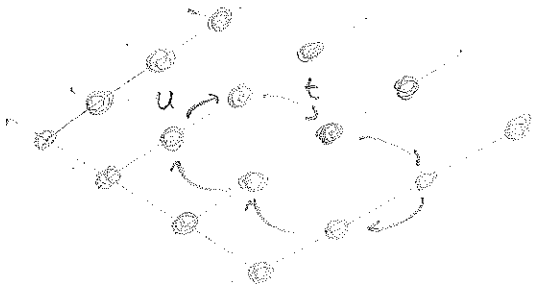
1. Dynamical mean field theory

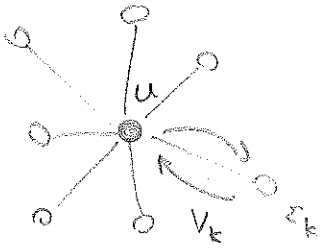
Maps lattice model to a self-consistent solution of a quantum-impurity model.

Hubbard model



$$H_{\text{Hubbard}} = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow})$$

Anderson impurity model



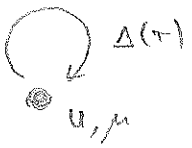
$$H_{\text{AIM}} = \sum_{k,\sigma} \left(V_{k\sigma} c^\dagger_{k\sigma} a_\sigma + \text{h.c.}\right) + \sum_{k,\sigma} \varepsilon_{k\sigma} a^\dagger_{k\sigma} a_{k\sigma} + U n_\uparrow n_\downarrow - \mu (n_\uparrow + n_\downarrow)$$

Bath parameters $\{V_{k\sigma}, \varepsilon_{k\sigma}\}$ (= "mean field") are optimized such that the bath mimics the lattice environment.

Approximation: local (k-independent) lattice self-energy

$$\Sigma_{\text{Hubbard}}(k, i\omega_n) \approx \Sigma_{\text{AIM}}(i\omega_n)$$

Impurity action: integrating out the bath yields



$$S_{\text{AIM}} = \int_0^\beta \int_0^\beta d\tau d\tau' \sum_\sigma c^\dagger_\sigma(\tau)\, \Delta_\sigma(\tau-\tau')\, c_\sigma(\tau') + \int_0^\beta d\tau \left[U n_\uparrow(\tau) n_\downarrow(\tau) - \mu\left(n_\uparrow(\tau) + n_\downarrow(\tau)\right)\right]$$

In this case, the self-consistency fixes the hybridization function

$$\Delta_\sigma(i\omega_n) = \sum_{k,\sigma} \frac{|V_{k\sigma}|^2}{i\omega_n - \varepsilon_{k\sigma}}$$

or equivalently the "Weiss Green's function" $\mathcal{G}^{-1}_{0\sigma}(i\omega_n) = i\omega_n + \mu - \Delta_\sigma(i\omega_n)$

DMFT self-consistency loop :

$G_{loc}(i\omega_n) = \sum_k G_{latt}(k, i\omega_n)$

$\mathcal{G}_0^{-1}(i\omega_n) = G_{loc}^{-1}(i\omega_n) + \Sigma_{imp}(i\omega_n)$ ⟶ DMFT self-consistency ⟶ $\mathcal{G}_0(i\omega_n)$ [$\leftrightarrow \Delta$]

$\mathcal{G}_0(i\omega_n)$ [$\leftrightarrow \Delta$] ⟶ (by impurity solver) ⟶ $G_{imp}(i\omega_n)$, $\Sigma_{imp}(i\omega_n)$

$G_{imp}(i\omega_n)$, $\Sigma_{imp}(i\omega_n)$ ⟵ DMFT approximation: $\Sigma(k, i\omega_n) \approx \Sigma_{imp}(i\omega_n)$

$G_{latt}(k, i\omega_n) = \dfrac{1}{i\omega_n + \mu - \varepsilon_k - \Sigma_{imp}(i\omega_n)}$ ⟵ (k-averaging) ⟵ $G_{loc}(i\omega_n)$

2. Solution of the impurity model (hybridization expansion)

Idea : Expand the partition function $Z = \mathrm{Tr}\left[T e^{-S_{imp}} \right]$ in powers of Δ

View the resulting diagrams as Monte Carlo configurations and generate them stochastically

Measure the contribution of these diagrams to the observables $G(\tau)$, ...

For simplicity, consider spinless case : $S_{imp} = \int_0^\beta d\tau\, d\tau'\, c^\dagger(\tau) \Delta(\tau - \tau') c(\tau) - \mu \int_0^\beta d\tau\, n(\tau)$

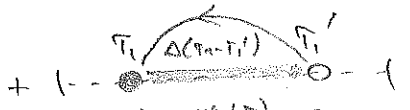
$$Z = \mathrm{Tr}_c \left[T e^{-\int_0^\beta d\tau\, d\tau'\, c^\dagger(\tau)\Delta(\tau-\tau')c(\tau') + \int_0^\beta d\tau\, \mu\, n(\tau)} \right]$$

$$= \sum_n \int_0^\beta d\tau_1 d\tau_1' \cdots \int_0^\beta d\tau_n d\tau_n' \, \frac{(-1)^n}{n!} \, \mathrm{Tr}_c \left[T e^{\int_0^\beta d\tau\, \mu n(\tau)} c^\dagger(\tau_1) c(\tau_1') \cdots c^\dagger(\tau_n) c(\tau_n') \right]$$

$\sum_c$; $\times\ \Delta(\tau_1 - \tau_1') \cdots \Delta(\tau_n - \tau_n')$; w_c

$=$ 

$e^{\beta\mu}$ $\quad O(\Delta^0)$

$+$ 

$\quad O(\Delta^1)$

$+$ 

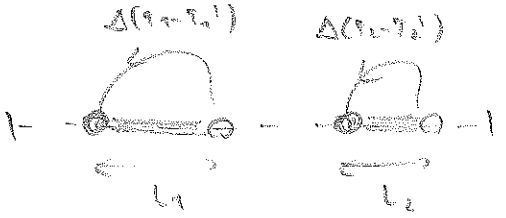
$\quad O(\Delta^2)$

$+ \cdots$ $\qquad \cdots$

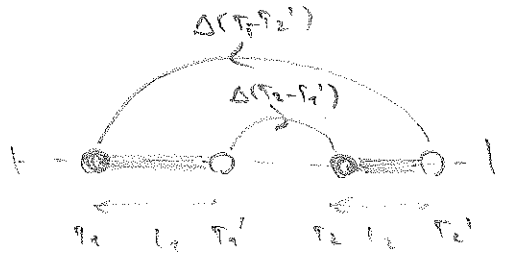
For $n \geq 2$, there are $n!$ diagrams with the same operator sequence

→ weights can be summed up into a determinant !

Example : $n = 2$



$$(-1)^2 e^{\mu(l_1+l_2)} \Delta(\tau_1-\tau_1')\,\Delta(\tau_2-\tau_2')\,(d\tau)^4$$



from time-ordering

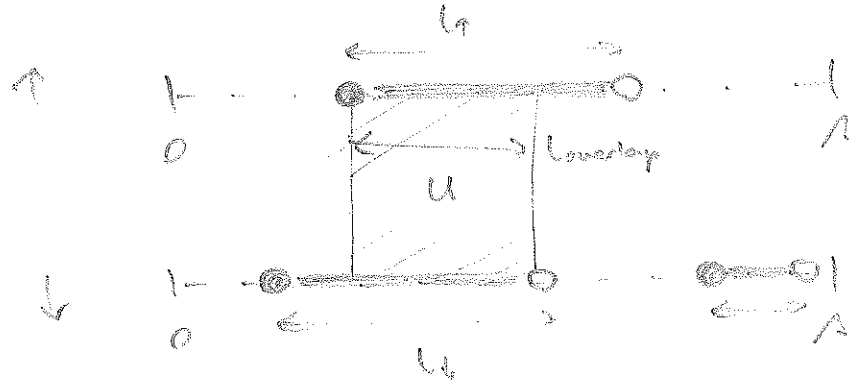
$$\Leftrightarrow (-1)^2(-1)\, e^{\mu(l_1+l_2)} \Delta(\tau_1-\tau_2')\,\Delta(\tau_2-\tau_1')\,(d\tau)^4$$

$$= (-1)^2 e^{\mu(l_1+l_2)} \det \begin{pmatrix} \Delta(\tau_1-\tau_1') & \Delta(\tau_1-\tau_2') \\ \Delta(\tau_2-\tau_1') & \Delta(\tau_2-\tau_2') \end{pmatrix} (d\tau)^4$$

$\Rightarrow$ becomes the sum over all segment configurations with weight

$$w_c \sim e^{\mu l_{segments}} \det[\Delta]$$

Anderson impurity model : one segment configuration and hybridization matrix determinant for spin up and spin down ; interaction contribution from segment overlaps

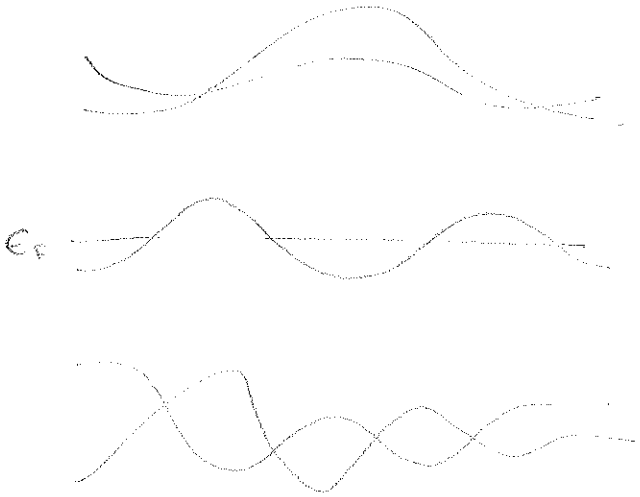


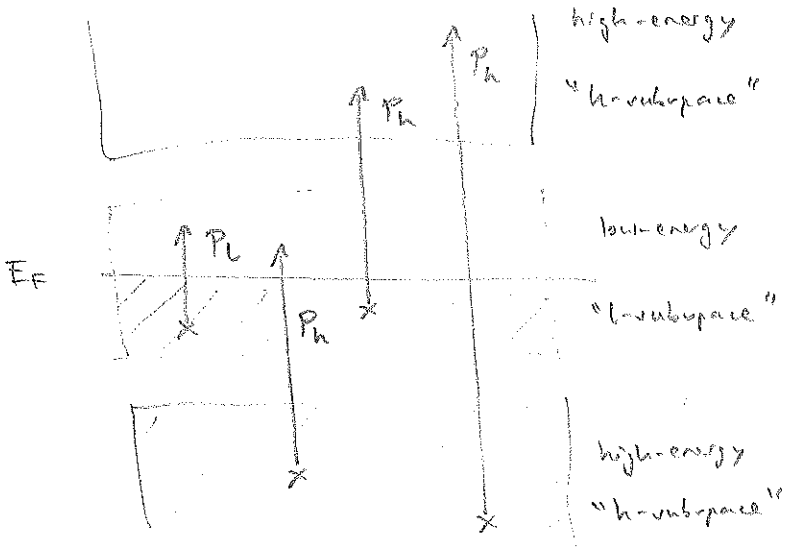
$$w_c \sim e^{\mu(l_\uparrow+l_\downarrow) - U\, l_{overlap}} \det[\Delta_\uparrow] \det[\Delta_\downarrow]$$

3. Dynamical screening

Calculation of the "Hubbard U" for a low-energy effective model[1]:

Consider a narrow (d-) band near the Fermi level, which is separated from other (s-, p-, ...) bands:





Separate the total polarization of the system into a contribution from the low-energy subspace (P_l) and the rest (P_h):

$$P = P_l + P_h$$

The fully screened interaction W is related to the bare interaction v and the total polarization P by

$$W = v + vPW \quad \text{or} \quad W = [1 - vP]^{-1} v$$

Because the polarization effects within the low-energy subspace (P_l) are captured by the DMFT solution, we use only P_h in the definition of the interaction parameters:

$$W_h = [1 - vP_h]^{-1} v \qquad (\Rightarrow W = [1 - W_h P_l]^{-1} W_h \text{, i.e. if } W_h \text{ is further screened by } P_l \text{ we get } W)$$

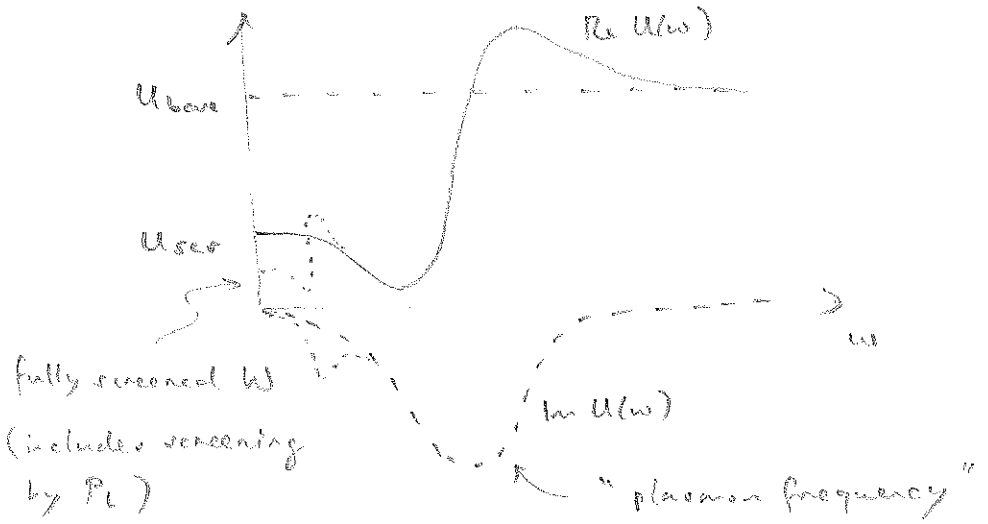
The "Hubbard U" is given by the matrix elements of $W_h(r, r', \omega)$ in a basis of localized Wannier orbitals $\{\varphi_R(r)\}$

$$U(\omega) = \iint dr\, dr' \, |\varphi_i(r)|^2 \, W_h(r, r', \omega) \, |\varphi_i(r')|^2$$

Comments:

- The polarization $P_h(r,r';\omega)$ is frequency dependent, and hence also $W_h(r,r';\omega)$

  → The proper notion of the "Hubbard U" in a low-energy effective theory is a frequency-dependent object, which ranges from the bare Coulomb interaction U_{bare} (≈ 20 eV) at high ω to a screened value U_{scr} (≈ 3–4 eV) at $\omega = 0$:



- $W_h = [1 - vP_h]^{-1}v$ is exact, in practice one however evaluates P_h in the random phase approximation (→ cRPA method)

- Since P_h does not contain low-energy polarization P_t responsible for metallic screening, $U(\omega)$ becomes long-ranged (→ Hubbard model description becomes problematic)

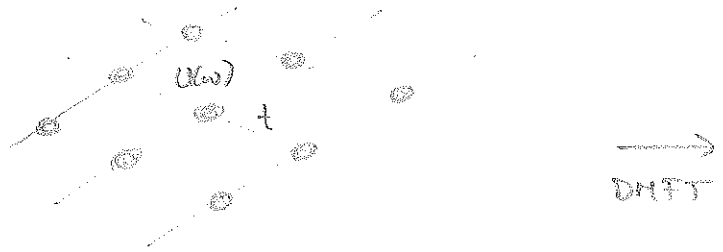
- Justification for the use of RPA: only P_h enters the calculation of W_h, and the high-energy (e_-, p_-) bands are typically weakly correlated extended states.

  However: recent systematic tests of cRPA show that the approximation yields bad results if the screening bands are close to E_F

4. DMFT calculations with $U(\omega)$

Hubbard model with $U(\omega)$
↓
local coupling to bosonic modes with energy ω

Anderson impurity model with retarded interaction



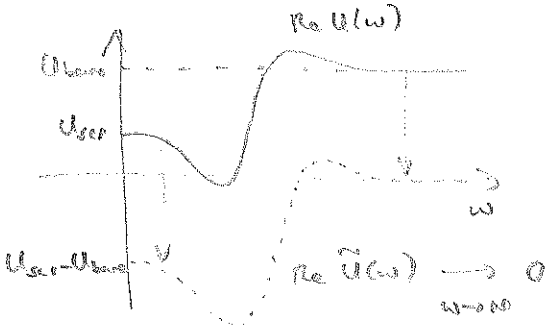
$$S_{imp} = \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' \, c^\dagger_\sigma(\tau) \Delta_\sigma(\tau-\tau') c_\sigma(\tau') + \int_0^\beta d\tau \, \mu \, (n_\uparrow(\tau) + n_\downarrow(\tau)) + \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \, N_{\sigma\sigma'}(\tau) \, U(\tau-\tau') \, N_{\sigma'\sigma}(\tau')$$

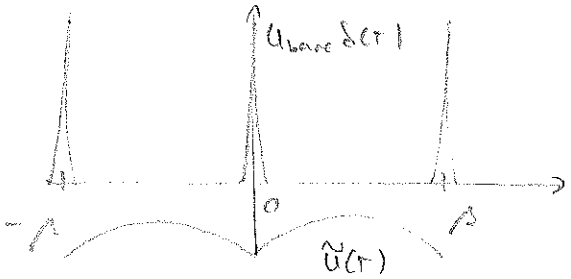
$$U(\omega) = U_{bare} + \tilde{U}(\omega)$$

$$U(\tau) = U_{bare}\,\delta(\tau) + \tilde{U}(\tau)$$

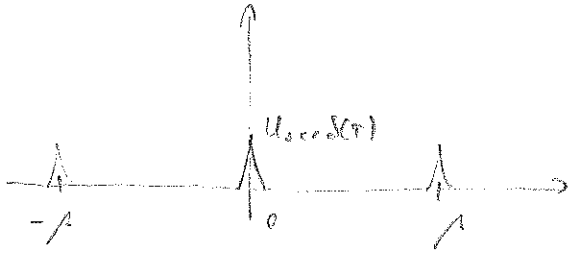
repulsive bare Coulomb interaction

attractive retarded interaction (screening effect)





This should be compared to the static approximation $U(\omega) \approx U_{scr} = U(\omega = 0)$



Spectral representation: $\tilde{U}(\tau) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \, \mathrm{Im}\,\tilde{U}(\omega) \frac{e^{-\omega\tau}}{e^{-\omega\beta} - 1} = \frac{1}{\pi} \int_0^\infty d\omega \, \mathrm{Im}\,\tilde{U}(\omega) \frac{\cosh(\omega(\tau - \beta/2))}{\sinh[\omega\beta/2]}$

Segment configuration – interaction contribution

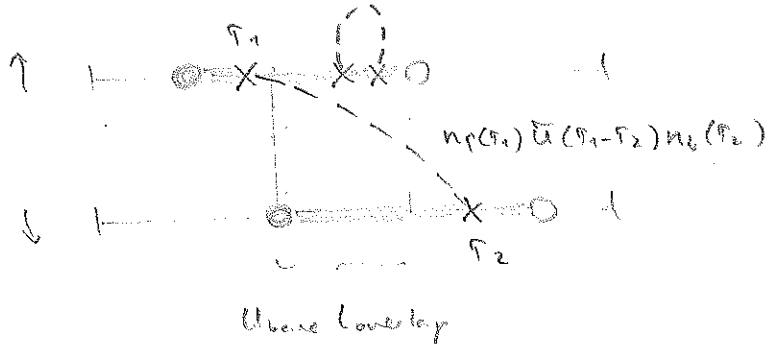
$$\frac{1}{2}\int d\tau\, d\tau'\, N_{tot}(\tau)\, U(\tau-\tau')\, N_{tot}(\tau') \qquad N_{tot} = n_1 + n_2$$

$$U_{bare}\,\delta(\tau-\tau') + \tilde{U}(\tau-\tau')$$

$$= U_{bare}\int d\tau\, n_1(\tau) n_2(\tau) + \frac{U_{bare}}{2}\int d\tau\,(n_1(\tau)+n_2(\tau)) + \int d\tau\, d\tau'\, n_1(\tau)\,\tilde{U}(\tau-\tau')\,n_2(\tau')$$

U_{bare} overlap — shift of μ

$$+ \sum_\sigma \frac{1}{2}\int d\tau\, d\tau'\, n_\sigma(\tau)\,\tilde{U}(\tau-\tau')\,n_\sigma(\tau')$$



Retarded contribution: let k_i denote segment i (irrespective of spin)

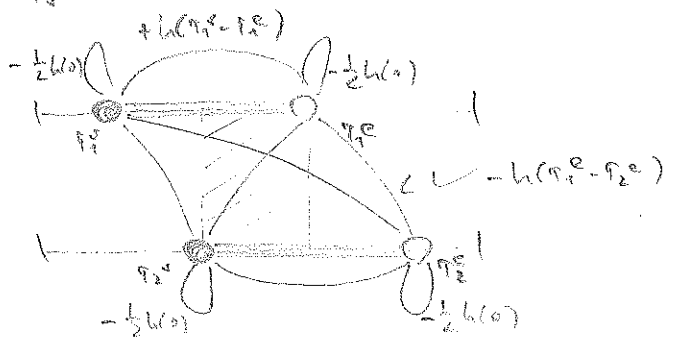
$$\sum_{k_1 \neq k_2}\int_{k_1} dr_1 \int_{k_2} dr_2\, \tilde{U}(r_1-r_2) + \frac{1}{2}\sum_k \int_k dr_1 \int_k dr_2\, \tilde{U}(r_1-r_2)$$

inter-segment contribution (both spins) — intra-segment contribution (both spins)

Let $h(\tau)$ be a bosonic function, symmetric around $\tau = \beta/2$, which satisfies $h''(\tau) = \tilde{U}(\tau)$ — determines integration constants

$$\int_{r_1^s}^{r_1^e} dr_1 \int_{r_2^s}^{r_2^e} dr_2\, \tilde{U}(r_1-r_2) = -h(r_1^e - r_2^e) + h(r_1^e - r_2^s) + h(r_1^s - r_2^e) - h(r_1^s - r_2^s)$$

$$\frac{1}{2}\int_{r_c}^{r_e} dr_1 \int_{r_c}^{r_e} dr_2\, \tilde{U}(r_1-r_2) = \frac{1}{2}\left[-2h(0) + \underbrace{h(r_e-r_c)+h(r_c-r_e)}_{2h(r_e-r_c),\ h \text{ even}}\right] = h(r_e-r_c) - \tfrac{1}{2}h(0) - \tfrac{1}{2}h(0)$$



Hence, we can express the retarded interaction energy (for n creation and n annihilation operators) as

$$-n\,h(0) - \sum_{i>j} s_i s_j\, h(\tau_i - \tau_j) \qquad s_i = \begin{cases} +1 & \text{if operator } i \text{ is } c^\dagger \\ -1 & \text{if operator } i \text{ is } c \end{cases}$$

$$= -\sum_{i>j} s_i s_j \left[h(\tau_i - \tau_j) - h(0) \right]$$

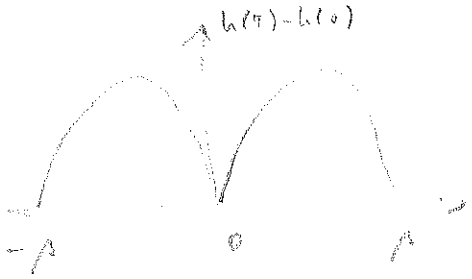
↳ because of $s_i s_j$ cancellations, there is only an intra-segment contribution $-h(0)$

Since $h''(\tau) = \tilde{U}(\tau) = \frac{1}{\pi}\int_0^\infty d\omega\, \mathrm{Im}\,\tilde{U}(\omega)\, \frac{\cosh[\omega(\tau - \beta/2)]}{\sinh[\omega\beta/2]}$ we find

$$h(\tau) - h(0) = \frac{1}{\pi}\int_0^\infty d\omega\, \frac{\mathrm{Im}\,\tilde{U}(\omega)}{\omega^2}\, \frac{\cosh[\omega(\tau - \beta/2)] - \cosh[\omega\beta/2]}{\sinh[\omega\beta/2]} \qquad 0 \le \tau \le \beta$$

(and even for $-\beta \le \tau \le 0$)

Note that this function has a slope discontinuity at $\tau = 0$:



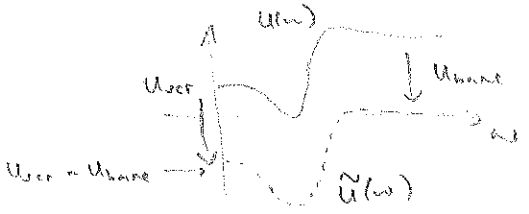
→ 1st derivative has a jump, and 2nd derivative a δ-function at $\tau = 0$, with weight

$$2h'(0_+) = 2\,\underbrace{\frac{1}{\pi}\int_0^\infty d\omega\, \frac{\mathrm{Im}\,\tilde{U}(\omega)}{\omega}}_{\mathrm{Re}\,\tilde{U}(\omega=0)} (-1)$$

transverse-kronig

So, if we use this $h(\tau)$, we have to subtract an instantaneous interaction

$$-\mathrm{Re}\,\tilde{U}(\omega=0)\,\delta(\tau) = -\left[U_{\mathrm{scr}} - U_{\mathrm{bare}}\right]\delta(\tau)$$



The total instantaneous interaction is thus $\left[U_{\mathrm{bare}} + \mathrm{Re}\,\tilde{U}(\omega=0)\right]\delta(\tau)$

$= U_{\mathrm{scr}}\,\delta(\tau)$

In conclusion, the local contribution to the weight of a segment configuration is

$$w_{loc} = \exp\left[-U_{user}\, l_{overlap} + \left(\mu - \frac{U_{user}}{2}\right) l_{segments} + \sum_{i>j} s_i s_j \left[h(\tau_i - \tau_j) - h(0)\right]\right]$$

with $h(\tau) - h(0) = \frac{1}{\pi} \int_0^\infty d\omega \, \frac{\mathrm{Im}\,\tilde{\Delta}(\omega)}{\omega^2} \, \frac{\cosh\left[\omega\left(\tau - \frac{\beta}{2}\right)\right] - \cosh\left[\omega \frac{\beta}{2}\right]}{\sinh\left[\omega \frac{\beta}{2}\right]}$

The MC sampling proceeds as before, except

- $U \to U_{user}$ in overlap contribution
- $\mu \to \mu - \frac{U_{user}}{2}$ in μ contribution
- For inserted/removed segment, have to compute the non-local interaction with all operators :