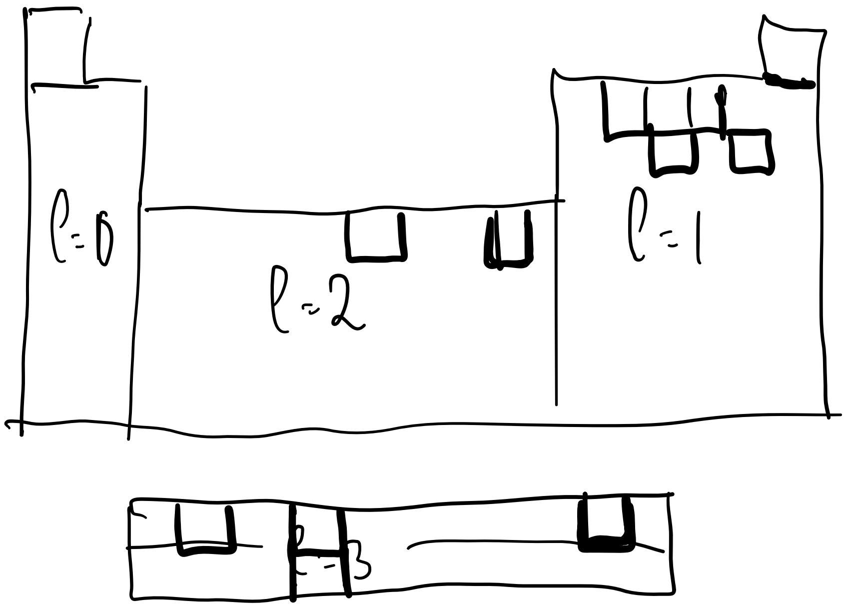
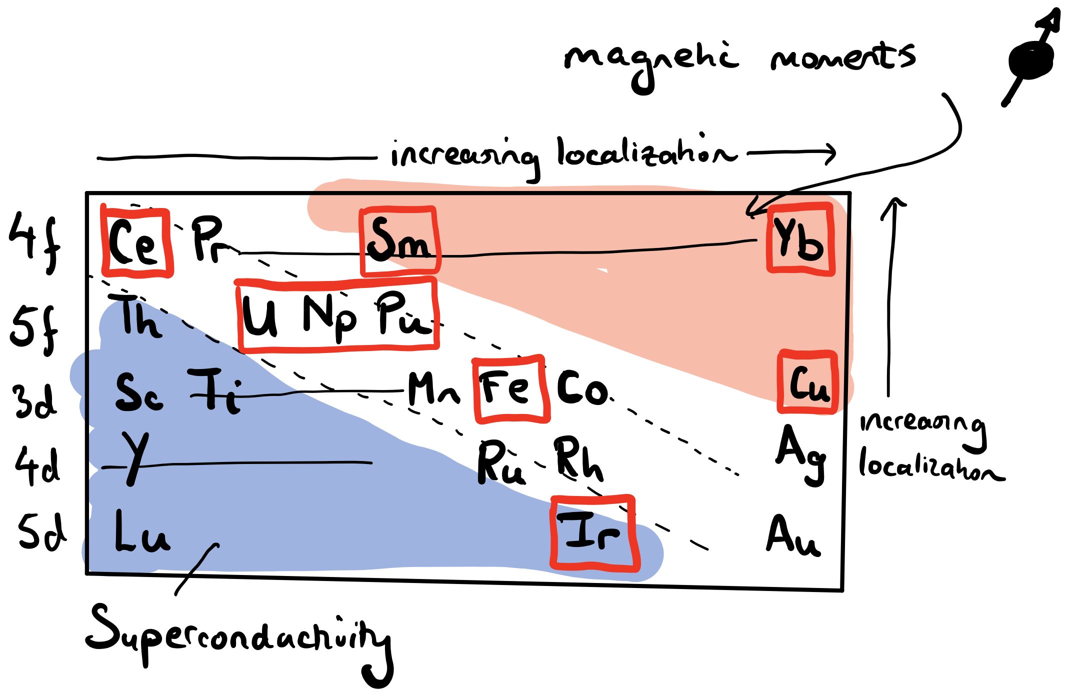
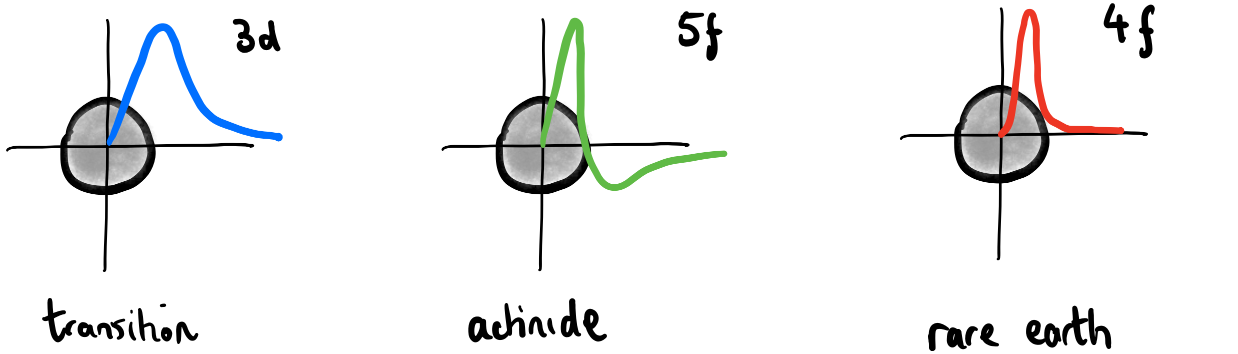
L2 2024 Local Moment Formation Adapted from Ch. 16 IMBP.



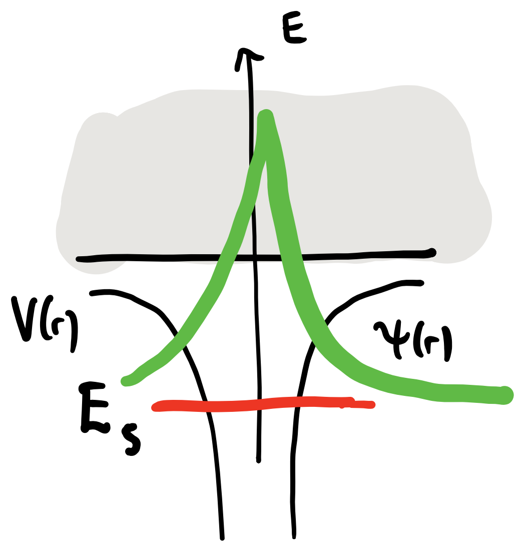


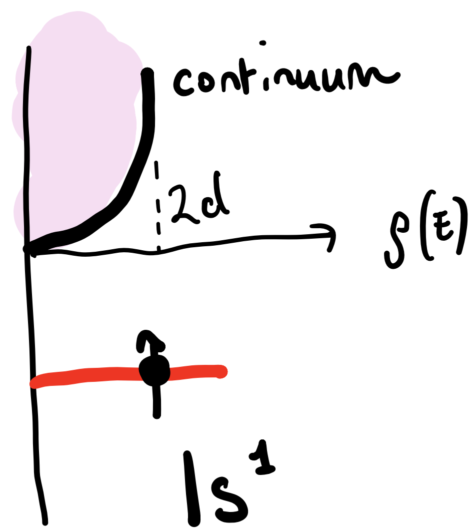
Kmetko-Smith diagram

Degree of localization $5d < 4d < 3d < 5f < 4f$



Interesting physics develops in quantum materials that lie on the brink of magnetism.



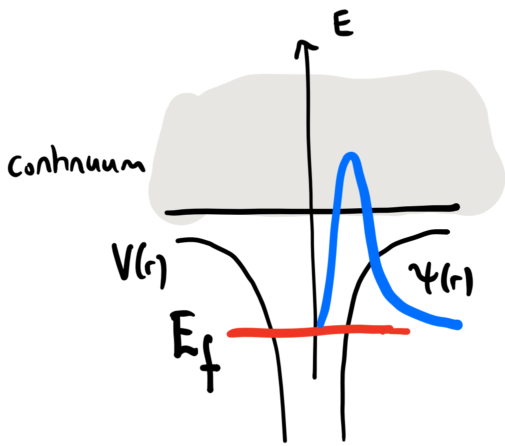


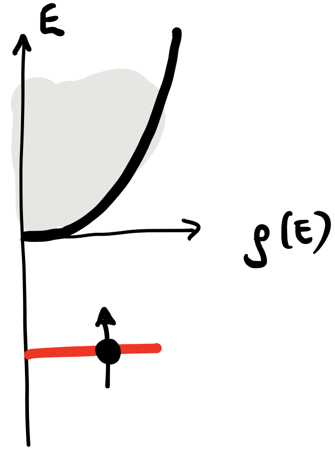
- Fe $3d^6$
- Nd $4f^3$
- Ce $4f^1$
- Yb $4f^{13}$

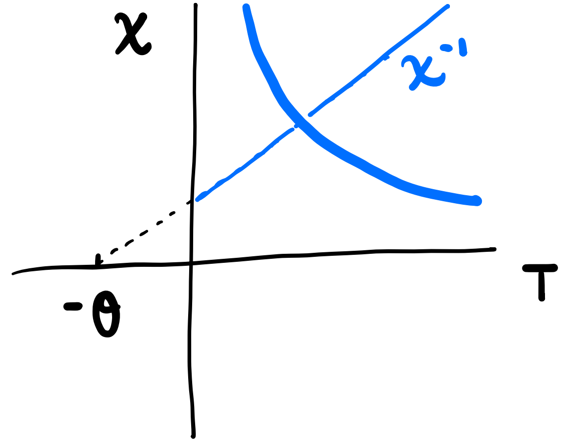
- C_{3000} – TBG
- Quantum Dots

1. LOCAL MOMENTS

In isolation, the localized unpaired electrons in an atom or ion form magnetic moments. Remarkably, these localized magnetic moments can survive inside a metal, providing that the Coulomb interaction between electrons in an unfilled orbital, is sufficiently high.



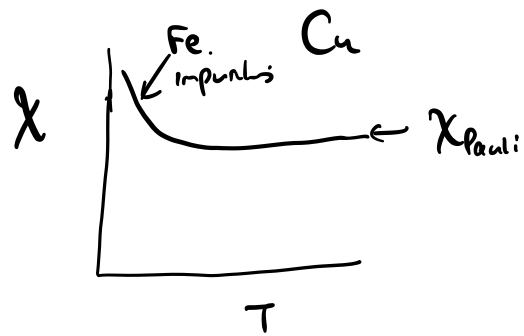




$$\vec{M} = 2\mu_B \vec{S} = \mu_B \vec{\sigma}$$

$\mu_B = (e\hbar/2m)$ = Bohr Magneton

$$\chi(T) = \frac{\partial M}{\partial B} = \frac{\mu_B^2}{T}$$



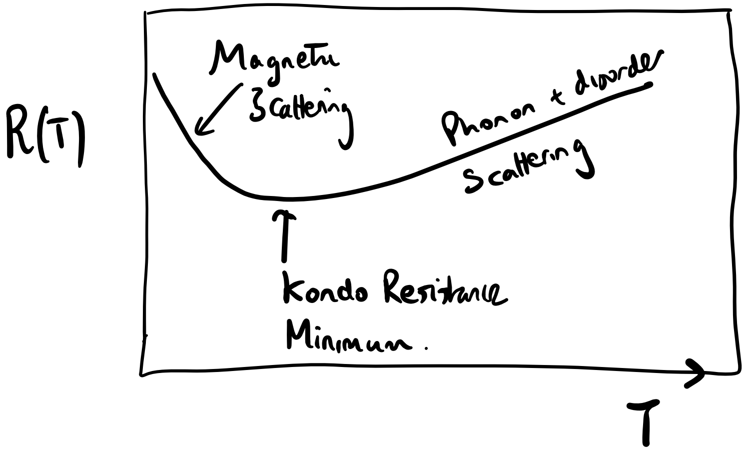
$$M = \mu_B \tanh\left(\frac{\mu_B B}{T}\right)$$

$$\boxed{\chi = \frac{n_i M^2}{3(T+\theta)}}$$

Curie-Weiss Susceptibility

$$M^2 = \frac{(g\mu_B)^2}{3} j(j+1) \qquad g=2;\ j=\tfrac{1}{2}$$

$-\theta$ = Curie Weiss Temperature $= T_{CW}$

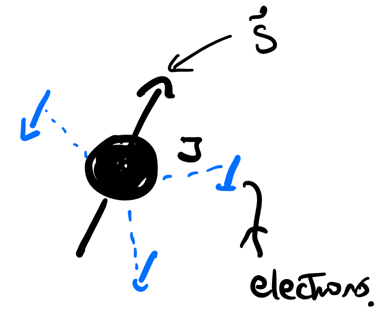


Fe in $Mo_x Nb_{1-x}$ $x > 0.4$ Local moments

How do { moments form ?
moments interact + the surrounding electron sea?

Philip W. Anderson : model for local moment formation 1961
driven by Coulomb interaction'

$$H_I = J \vec{\sigma}(0) . \vec{S}$$



Jun Kondo : $\frac{1}{\tau} \propto \rho \left[J + 2(J^2 \rho) \ln \frac{D}{T} \right]^2$

Grows as $T \to 0$

For $T \lesssim T_K$, $2 J \rho \ln \frac{D}{T_K} \sim 1$ $T_K \sim D \exp\left[\frac{-1}{2 J \rho} \right]$

the second order term exceeds the first order term.

J grows to

2. Anderson Model

$$\boxed{H = \overbrace{\sum \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{\vec{k}\sigma} \left[V c^\dagger_{k\sigma} f_\sigma + V^* f^\dagger_\sigma c_{k\sigma} \right]}^{H_{\text{resonance}}} + \underbrace{E_f n_f + U n_{f\uparrow} n_{f\downarrow}}_{H_{\text{Atomic}}}}$$

$$V \sum_\sigma \psi^\dagger_\sigma(0) f_\sigma + \text{H.C}$$

$$\Big\downarrow \text{R.G}$$

$$\boxed{H_K = \sum \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \, \vec{\sigma}(0) \cdot \vec{S}}$$

$$\vec{\sigma}(0) = \psi^\dagger_\alpha(0) \, \vec{\sigma}_{\alpha\beta} \, \psi(0)$$

$$\psi_\sigma(\vec{x}) = \frac{1}{\sqrt{V}} \sum e^{i\vec{k}\cdot\vec{x}} c_k$$

$\langle \vec{x} |$ $\qquad$ $\langle x | k \rangle \langle k |$

$\downarrow$

"$V=1$"

2. Anderson Model

$$\boxed{H = \overbrace{\sum \epsilon_k c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \sum_{\vec{k}\sigma}\left[V c^\dagger_{k\sigma} f_\sigma + V^* f^\dagger_\sigma c_{k\sigma}\right]}^{H_{\text{resonance}}} + \underbrace{E_f n_f + U n_{f\uparrow} n_{f\downarrow}}_{H_{\text{Atomic}}}}$$

$$U = \frac{e^2}{4\pi\epsilon_0}\int_{r,r'} \frac{1}{|r-r'|}\rho_f(r)\rho_f(r')$$

$$\rho_f(r) = |\psi_f(r)|^2$$

$$\int_r \equiv \int d^3 r$$

$$f^\dagger_\sigma = \int_r \hat{\psi}^\dagger_\sigma(r)\,\psi_f(\vec{r})$$

$$|f\sigma\rangle = \int_r |\vec{r}\sigma\rangle \underbrace{\langle \vec{r}|f\rangle}_{\psi_f(\vec{r})}$$

$V(k)$

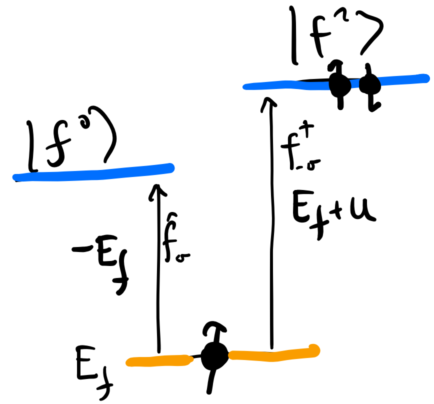
2.1 Atomic Limit

$$H_{atomic} = E_f \hat{n}_f + U \hat{n}_{f\uparrow} \hat{n}_{f\downarrow}$$

$|f^2\rangle \qquad E(f^2) = 2E_f + U$

$|f^0\rangle \qquad E(f^0) = 0$

non magnetic



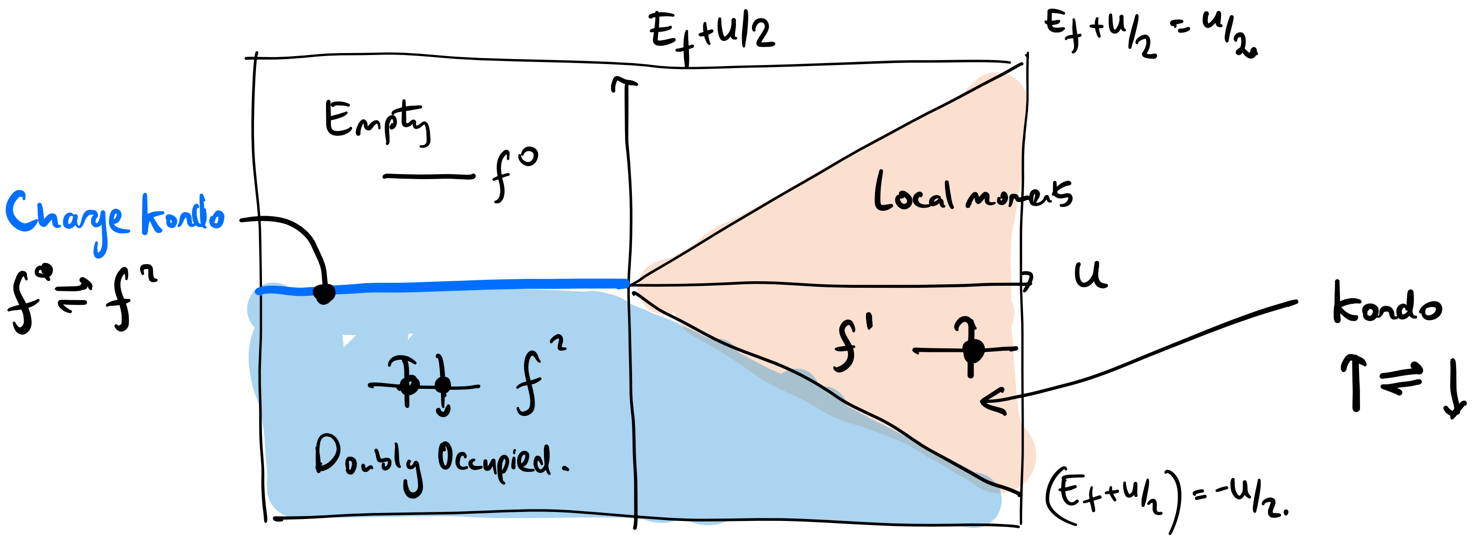
$|f^1\uparrow\rangle, \ |f^1\downarrow\rangle \qquad E(f^1) = E_f$

Adding $\quad E(f^2) - E(f^1) = U + E_f$

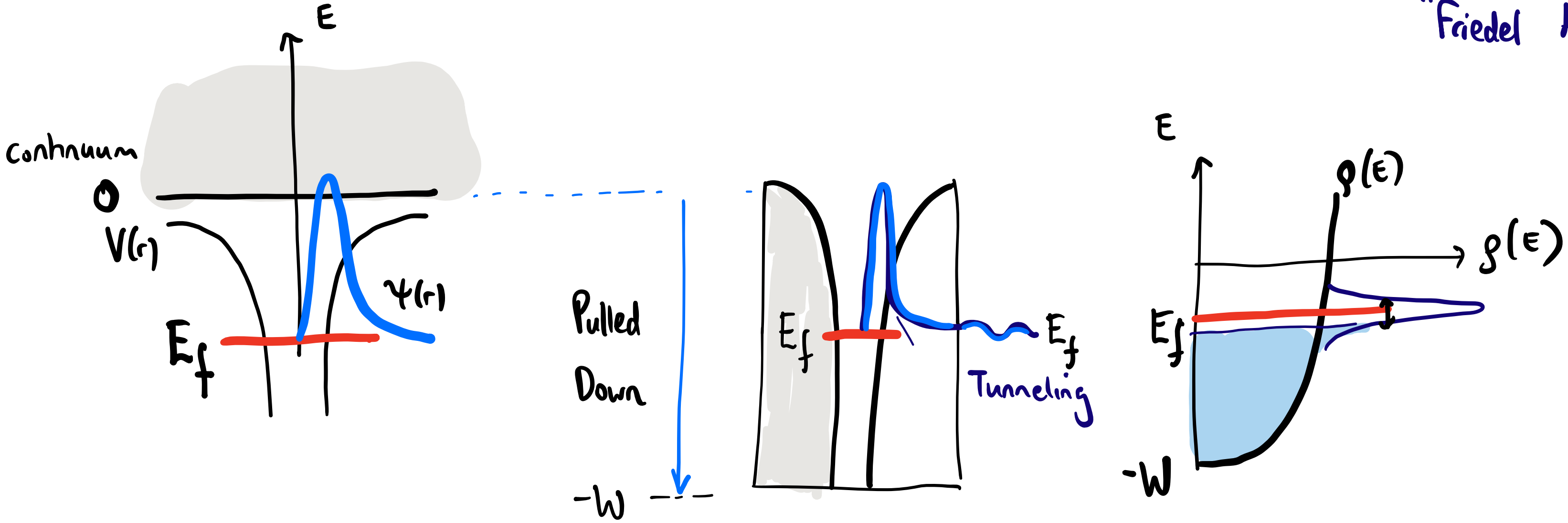
Subtracting $\quad E(f^0) - E(f^1) = -E_f$

$$\Delta E = \frac{U}{2} \pm \left(E_f + \frac{U}{2}\right)$$

Local moment is stable if $\boxed{U/2 > |E_f + U/2|}$



"Friedel Anderson Resonance"



$$\Delta = \pi \sum_{\vec{k}} |V|^2 \delta(\epsilon_k - E_f)$$ = Full width @ half maximum.

= Resonant level Width.

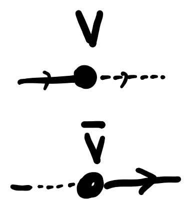
$$\Delta(\epsilon) = \pi \sum_{k} |V|^2 \delta(\epsilon_k - \epsilon)$$

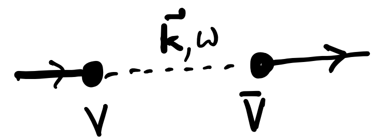
"Integrating out conduction electrons"

$$\frac{1}{\omega - E_f} = G_f^{(0)}$$

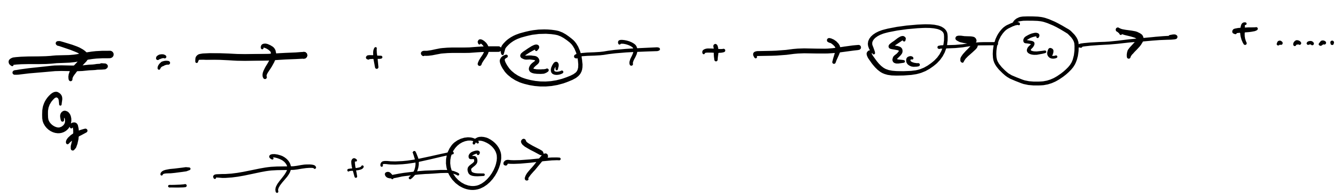
$$H = \sum \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \underbrace{\sum_{k\sigma} \left[V c^\dagger_{k\sigma} f_\sigma + V^* f^\dagger_\sigma c_{k\sigma} \right]}_{\text{Treat as perturbation}} + E_f n_f$$

$$\frac{1}{\omega - \epsilon_{\vec{k}}}$$



$\Sigma_c(\omega) =$ 

$$= \sum_k \frac{\bar{V} V}{\omega - \epsilon_{\vec{k}}} \equiv$$



$$\boxed{G_f(\omega) = \frac{1}{\omega - E_f - \Sigma^\circ(\omega)} = \frac{1}{\omega - E_f - \sum_k \frac{|V|^2}{\omega - \epsilon_k}}}$$

$$\Sigma^0(\omega - i\delta) \int \frac{d\epsilon}{\pi}\,\rho(\epsilon)\,\frac{\pi V^2}{\omega-\epsilon} = \int\frac{d\epsilon}{\pi}\,\frac{\Delta(\epsilon)}{\omega-\epsilon-i\delta} \approx +i\Delta(\omega)$$

$$\sum_k \to \int d\epsilon\, \rho(\epsilon)$$

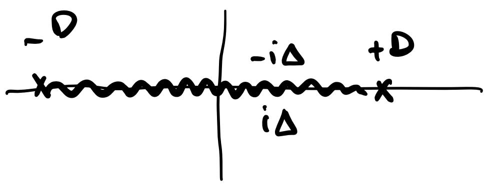
$$\Sigma_c(\omega-i\delta) = \Sigma_c' + i\Sigma_c''$$

$$\Sigma_c'' = \mathrm{Im}\,\Sigma_c(\omega-i\delta) = \mathrm{Im}\int \frac{d\epsilon}{\pi}\,\frac{\Delta(\epsilon)}{\omega-\epsilon-i\delta} = \Delta(\epsilon)$$

Consider case when $\Delta(\epsilon) = \Delta$ is constant

$$\Sigma(z) = \frac{\Delta}{\pi}\int_{-D}^{D}\frac{d\epsilon}{z-\epsilon} = \frac{\Delta}{\pi}\ln\left[\frac{z+D}{z-D}\right]$$

$$\Sigma(\omega-i\delta) = \frac{\Delta}{\pi}\ln\left[\frac{\omega-i\delta+D}{\omega-i\delta-D}\right] = \frac{\Delta}{\pi}\overbrace{\ln\left|\frac{\omega+D}{\omega-D}\right|}^{O(\omega/D)} + i\Delta$$



$$\ln[-x-i\delta] = \ln(|x|e^{-i\pi}) = -i\pi + \ln|x|$$

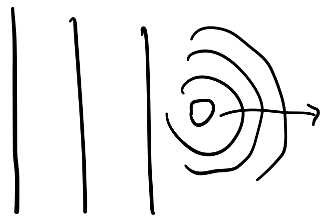
$$\Sigma(\omega+i\omega') = -i\Delta\,\mathrm{sgn}\,\omega' + O\left(\frac{\omega}{D}\right)$$

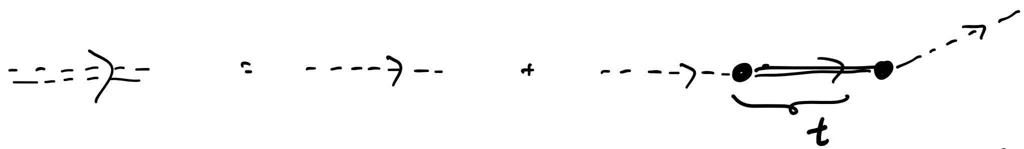
We can approximate Σ by its imaginary part

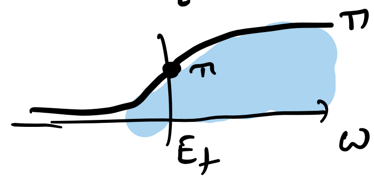
REMARKS ABOUT $\mathcal{G}$ AND PHASESHIFT

$$G_f(\omega - i\eta) = \frac{1}{\omega - (E_f + i\Delta)}$$ Advanced G.f

$$A_f(\omega) = \frac{1}{\pi} \operatorname{Im} G_f(\omega - i\eta) = \frac{\Delta}{(\omega - E_f)^2 + \Delta^2}$$ Resonant level.







$$\boxed{\mathcal{G}^{-1}(\omega - i\eta) = |\mathcal{G}^{-1}| e^{i\delta}}$$

$$\delta = \tan^{-1}\left(\frac{\Delta}{E_f - \omega}\right)$$

$$\left(\frac{e^{-ikr}}{r} - \frac{e^{ikr} e^{2i\delta}}{r}\right)$$

$$= \frac{e^{i\delta}}{r} 2i \sin(kr - \delta)$$

$$\propto \sin(kr - \delta)$$

$$\boxed{\begin{aligned} t(\omega) &= V^2 G_f(\omega + i\eta) \sim e^{i\delta} \sin\delta \\ S &= 1 - 2\pi i \rho\, t(\omega + \eta) \\ &= e^{2i\delta} \end{aligned}}$$

$$\Rightarrow \quad t = \left(\frac{S - 1}{-2\pi i \rho}\right) = -\frac{(e^{2i\delta} - 1)}{2\pi i \rho}$$

$$= -\frac{e^{i\delta} \sin\delta}{\pi\rho}$$

$$\boxed{S = 1 - \frac{2\pi i \rho V^2}{\omega - E + i\Delta} = \frac{\omega - E - i\Delta}{\omega - E + i\Delta} = \frac{\mathcal{G}^{-1}(\omega - i\delta)}{\mathcal{G}^{-1}(\omega + i\delta)}}$$

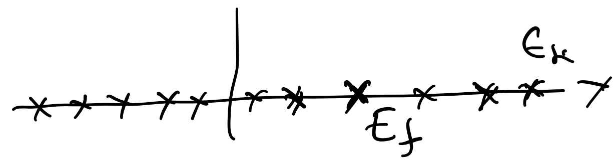
$$V^2 G_f = \frac{1}{\pi\rho} \frac{\Delta}{(\omega - E_f) + i\Delta} = \frac{1}{\pi\rho} \frac{1}{i + \left(\frac{\omega - E_f}{\Delta}\right)}$$

$$= \frac{-1}{\pi\rho} \frac{1}{\left[\left(\frac{E_f - \omega}{\Delta}\right) - i\right]}$$

$$= -\frac{\sin\delta}{\pi\rho(\cos\delta - i\sin\delta)}$$

$$= -\frac{1}{\pi\rho(\cot\delta - i)}$$

$$0 = \mathrm{Det}\left[\begin{pmatrix} \omega - E_f & -V^* \\ V & \omega - \epsilon_k \end{pmatrix}\right] = \mathrm{Det}\begin{pmatrix} \omega - E - \sum \frac{V^* V}{\omega - \epsilon_k} & 0 \\ V & \omega - \epsilon_k \end{pmatrix}$$



$$\underbrace{(\partial_\tau + H)} = (H - i\omega_n) = -\mathcal{G}^{-1}$$

$$\mathrm{Det}\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \mathrm{Det}\left(\begin{bmatrix} 1 & -BD^{-1} \\ 0 & 1 \end{bmatrix}\begin{bmatrix} A & B \\ C & D \end{bmatrix}\right) = \mathrm{Det}\begin{pmatrix} A - BD^{-1}C & 0 \\ C & D \end{pmatrix}$$

$$= \mathrm{Det}(A - BD^{-1}C)\, \mathrm{Det}(D)$$

$$\int \mathcal{D}[\bar\alpha, \alpha] \int \mathcal{D}[\bar\beta, \beta] \exp\left[(\bar\alpha, \bar\beta)\begin{pmatrix} A & B \\ C & D \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}\right] = \int \mathcal{D}[\bar\alpha, \alpha]\, e^{\bar\alpha A \alpha} \times \underbrace{\int \mathcal{D}[\bar\beta, \beta]\, e^{[\bar\beta D \beta + \bar{J}\beta + \bar\beta j]}}$$

$$\bar{J} = \bar\alpha B \quad j = C\alpha$$

$$\mathrm{Det}(D) \times \exp[-\bar\alpha B D^{-1} C \alpha]$$

$$= \int \mathcal{D}[\bar\alpha, \alpha]\, e^{\bar\alpha (A - BD^{-1}C)\alpha} \det D$$

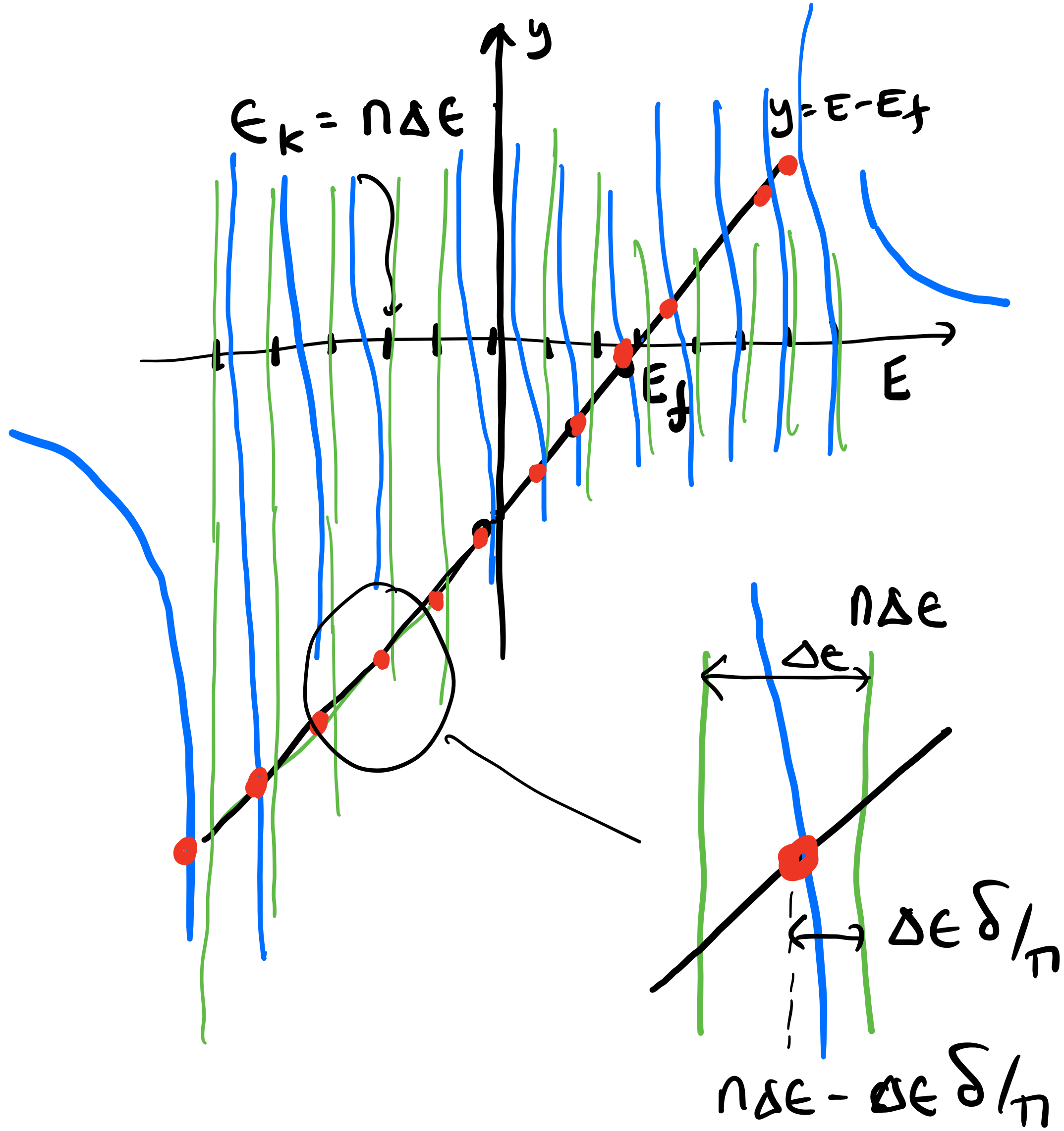
Relationship of phase shift with energy levels

$$G(\omega) = \frac{1}{\omega - E_f - \sum \frac{V^2}{\omega - \epsilon_K}}$$

Poles at $G^{-1}(E) = 0$

$$E - E_f = \sum \frac{V^2}{E - E_K}$$

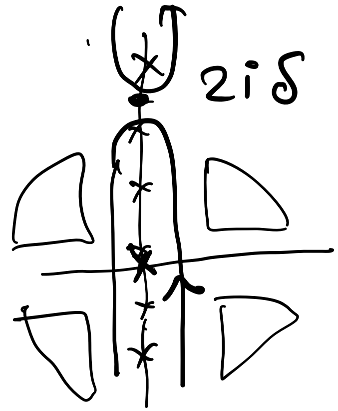
$$\bar{E} = m\Delta\epsilon - \frac{\delta(E)}{\pi}\Delta\epsilon$$



$$E - E_f = \frac{V^2}{\Delta\epsilon} \sum_n \frac{1}{(m-n) - \delta/\pi}$$

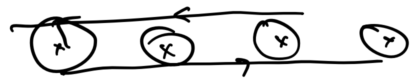
$$= \frac{V^2}{\Delta\epsilon} \sum_{n=-\infty}^{\infty} \frac{1}{(n - \delta/\pi)} = -\frac{V^2}{\Delta\epsilon}(\cot\delta)$$

$$\sum \frac{1}{(n-\delta/\pi)} = \mathrm{Re} \oint \frac{dz}{2\pi i}\, n(z)\, \frac{e^{z0^+}}{\frac{z}{2\pi i} - \delta/\pi}$$

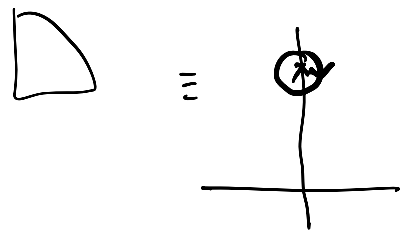


$$= \mathrm{Re} \oint dz\, n(z)\, \frac{e^{z0^+}}{z - 2i\delta}$$

$$\frac{1}{e^z - 1} - \frac{1}{2} \qquad z = 2\pi i n$$



$$\frac{1}{e^{z/2\pi i} - 1} \qquad z = n$$



$$\frac{e^{z/2} + e^{-z/2}}{e^{z/2} - e^{-z/2}}$$

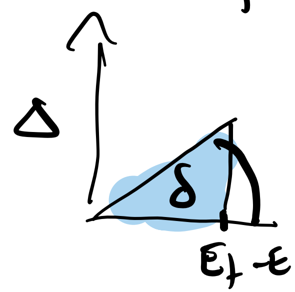
$$= -2\pi i \left(n(2i\delta) - \tfrac{1}{2} \right)$$

$$= -2\pi i \frac{1}{e^{2i\delta} - 1} = -\pi e^{-i\delta} \frac{2i}{e^{i\delta} - e^{-i\delta}} \Rightarrow -\pi \cot\delta$$

$$E - E_f = -\pi V^2 \rho \cot \delta$$

$$\delta = \cot^{-1}\left(\frac{E_f - E}{\Delta}\right) = \tan^{-1}\left(\frac{\Delta}{E_f - E}\right)$$

$$E_f + i\Delta - E = \left|E_f + i\Delta - E\right| e^{i\delta}$$



$$\cot \delta_f(\omega) = \frac{E_f - \omega}{\Delta} \Rightarrow \tan\delta = \left(\frac{\Delta}{E_f - \omega}\right) \qquad \delta = \mathrm{Im} \ln\left(E_f + i\Delta\right)$$

$$E_f + i\Delta = \sqrt{E_f^2 + \Delta^2}\, e^{i\delta}$$

$$\langle n_f \rangle = 2\int_{-\infty}^{0} \frac{d\omega}{\pi} A_f(\omega) = 2\,\mathrm{Im}\int_{-D}^{0} \frac{d\omega}{\pi} \frac{1}{\omega - E_f - i\Delta} = \frac{2}{\pi}\mathrm{Im}\ln\left[\frac{+E_f + i\Delta}{+D}\right]$$

$$= \frac{2}{\pi}\delta_f(\omega=0) = \sum \frac{\delta_\sigma}{\pi} \qquad \text{"Friedel sum rule"}$$

$$\boxed{f_\sigma(\tau) = \frac{1}{\sqrt{\beta}}\sum_n f_{\sigma n} e^{-i\omega_n \tau}}$$

$$S_F^0 = \sum_{\sigma, n} \bar{f}_{\sigma n}\left[-G_f^{-1}(i\omega_n)\right] f_{\sigma n} = \sum \bar{f}_{\sigma n}\Big[E_f \underbrace{- i\Delta\,\mathrm{sgn}(\omega_n)}_{\Sigma(i\omega_n)} - i\omega_n\Big] f_{\sigma n}$$

$$= \int d\tau\, d\tau'\, \bar{f}_\sigma(\tau)\left[-\mathcal{G}^{-1}(\tau,\tau')\right] f_\sigma(\tau')$$

$$S_F = S_F^0 + U\int d\tau\, n_{f\uparrow} n_{f\downarrow}$$

$$\boxed{U n_\uparrow n_\downarrow \rightarrow U n_\uparrow \langle n_\downarrow\rangle + U n_\downarrow \langle n_\uparrow\rangle - U\langle n_\uparrow\rangle\langle n_\downarrow\rangle}$$

$$\rightarrow S_F^0 + \int\left[\phi_\uparrow n_\uparrow + \phi_\downarrow n_\downarrow - \frac{\phi_\uparrow\phi_\downarrow}{U}\right] d\tau.$$

$$-G_{f\sigma}^{-1} = \left[E_f + \phi_\sigma - i\Delta\,\mathrm{sgn}(\omega_n) - i\omega_n\right] \qquad \phi_\sigma = U\langle n_{f-\sigma}\rangle$$

$(\sin\delta)$

$$\frac{\delta S_F}{\delta\phi_\sigma} = \langle n_\sigma\rangle - \frac{\phi_{-\sigma}}{U}.$$

$$\langle n_\sigma\rangle = \delta_\sigma/\pi = \frac{1}{\pi}\tan^{-1}\left[\frac{\Delta}{E_f+\phi_\sigma}\right] = \frac{\phi_{-\sigma}}{U}.$$

$\phi_\sigma = \lambda - \sigma h$

$h = UM/2$

$\lambda = Un_f/2.$

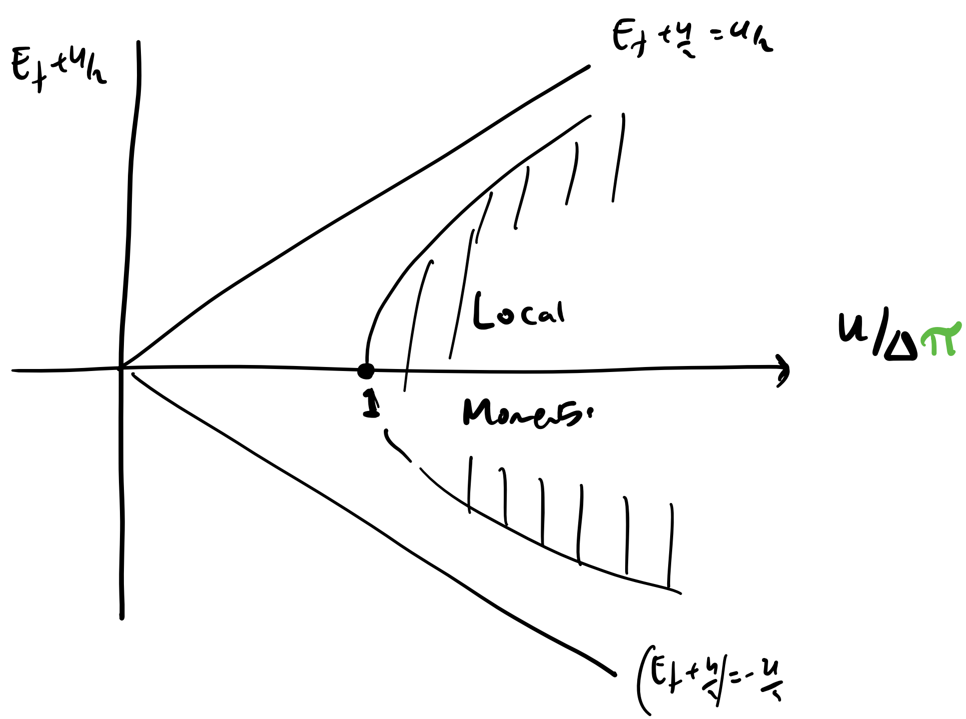
$$n_{f\uparrow} = n_{f\downarrow} = n_f/2 = \frac{1}{\pi}\tan^{-1}\frac{\Delta}{E_f + \frac{Un_f}{2}}$$

$$\frac{1}{\pi}\tan^{-1}\frac{\Delta}{E_f+\frac{Un_f}{2}\mp h} = \frac{n_f}{2}\pm\frac{h}{U}$$

$$\frac{\pm h}{\Delta\pi\left(1+\left(\frac{E_f+Un_f/2}{\Delta}\right)^2\right)} = \frac{\pm h}{U}$$

$\cot^2$

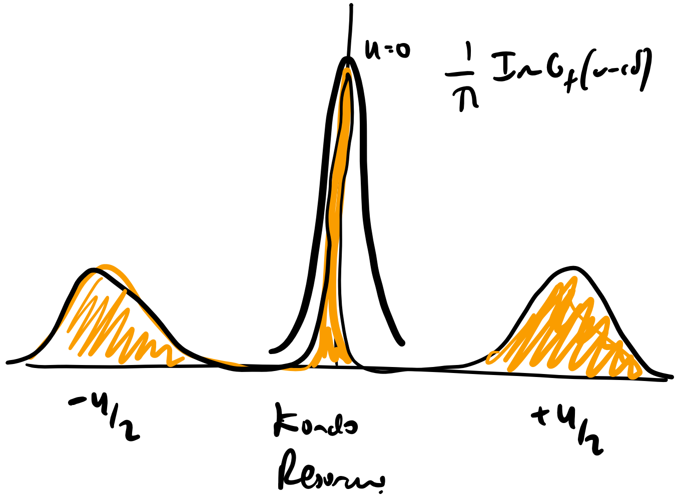
$$= \pm\frac{1}{\pi\Delta}\sin^2\delta_f$$



$$\frac{U}{\pi\Delta}\sin^2\delta_f = 1$$

$$\frac{U}{\pi\Delta} = \frac{1}{\sin^2\delta_f};$$

$$\left(E_f + \frac{U\delta}{\pi}\right)/\Delta = \cot\delta$$



$$\frac{1}{\pi}\,\mathrm{Im}\,G_f(\omega - i\delta) = \left(\frac{\sin^2\delta}{\pi\Delta}\right)$$ Adiabatic Inv

$$\Delta \cot\delta = E_f + \frac{U\delta}{\pi}$$

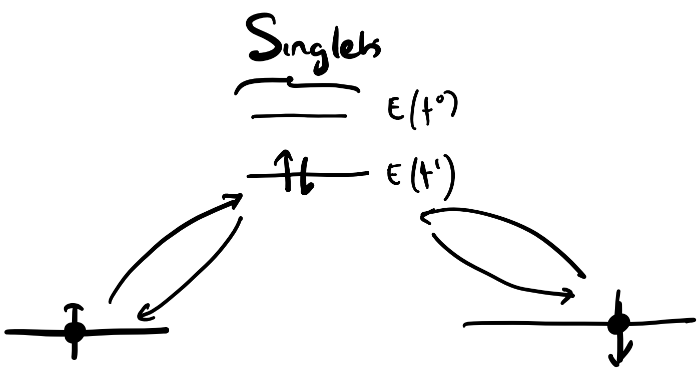
$$\Delta\cot\delta - \frac{U\delta}{\pi} = E_f$$

$$\frac{\pi\Delta}{2\sin^2\delta} + \Delta\cot\delta - \frac{\delta}{\pi}\frac{\Delta\pi}{\sin^2\delta} = E_f + U/2$$

$$E_f + U/2 = \Delta\cot\delta + \frac{\Delta\pi}{\sin^2\delta}\left(\frac{1}{2} - \frac{\delta}{\pi}\right)$$

$$\mathrm{Im}\,G_f(\omega=0) = \mathrm{Im}\,\frac{1}{-E_f - i\Delta}$$

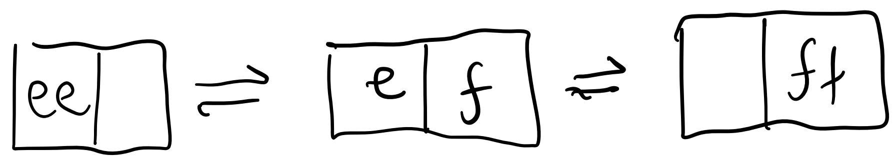
$$E_f + i\Delta = e^{i\delta}\sqrt{\Delta^2 + E_f^2} \qquad = \left(\frac{\sin^2\delta}{\Delta}\right)$$



Virtual Charge fluctuation

$$e_\uparrow + f^1_\downarrow \rightleftharpoons f^2 \rightleftharpoons e_\downarrow + f^1_\uparrow \qquad \Delta E_I = U + E_f$$

$$\underbrace{e_\uparrow + f^1_\downarrow}_{\text{singlet}} \rightleftharpoons \underbrace{e_\uparrow + e_\downarrow}_{\text{singlet}} \rightleftharpoons e_\downarrow + f^1_\uparrow \qquad \Delta E_{II} = -E_f$$



$c^\dagger_\uparrow c^\dagger_\downarrow$ $\quad$ $(c^\dagger_\uparrow f^\dagger_\downarrow + c^\dagger_\downarrow f^\dagger_\uparrow)/\sqrt{2}$ $\quad$ $f^\dagger_\uparrow f^\dagger_\downarrow$

$$\Delta E = -2J \sim -2V^2\left[\frac{1}{\Delta E_I} + \frac{1}{\Delta E_{II}}\right] = -2V^2\left[\frac{1}{-E_f} + \frac{1}{E_f+U}\right]$$

P_{singlet}

$$= \tfrac{1}{4} \text{ trpl}$$

$$(S_1+S_2)^2 = 0 \Big\{ {2 \atop 0}$$

$$\frac{3}{2} + 2S_1 \cdot S_2 = 0 \qquad S_1 \cdot S_2 = -\tfrac{3}{4} \text{ s,l}$$

$$\left[-(S_1 \cdot S_2) + \tfrac{1}{4}\right] P$$

$$-\left(\tfrac{1}{4} - \frac{\vec{S}\cdot\vec{\sigma}}{2}\right]\left(-2J\right) \equiv J\,\vec{S}\cdot\vec{\sigma}$$

$$\boxed{H = \sum \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + J\,\vec{S}\cdot\vec{\sigma}(0)}$$