

# 1 Dynamical CPA $\iff$ DMFT

## 1.1 Hubbard Alloy Analogy

Naturally generalizes to to a dynamical, eg. quantum alloy, analogy

The Hubbard Model:

$$\hat{H} = \sum_{i,j;\sigma} [(\epsilon - \epsilon_0)\delta_{i,j} - t_{i,j}] c_{i,\sigma}^\dagger c_{j,\sigma} + \frac{1}{2} U \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} c_{i,-\sigma}^\dagger c_{i,-\sigma}$$

$$\sum_j [(\epsilon - \epsilon_{i,\sigma}^{HF})\delta_{i,l} + t_{i,l}] G_{\sigma,\sigma}^{HF}(l, j; \epsilon) = 0$$

$$\epsilon_{i,\sigma}^{HF} = \epsilon_0 + U\bar{n}_{i,-\sigma}$$

$$n_{i,\sigma} = \xi_i = \begin{matrix} 0 \\ 1 \end{matrix}$$

## 1.2 Hubbard III Approximation=CPA:

$$G_{\sigma,\sigma}(l, j; \epsilon) = \left\langle G_{\sigma,\sigma}^{HF}(l, j; \epsilon; \{n_{i,-\sigma}\}) \right\rangle_{CPA}$$

$$\frac{1}{2}(1 + m)G_{\sigma,\sigma;imp}^{\uparrow}(i, i; \epsilon) + \frac{1}{2}(1 - m)G_{\sigma,\sigma;imp}^{\downarrow}(i, i; \epsilon) = G_{\sigma,\sigma}^c(i, i; \epsilon)$$

$$m = \frac{1}{N} \sum_i^N (\bar{n}_{i,\uparrow} - \bar{n}_{i,\downarrow})$$

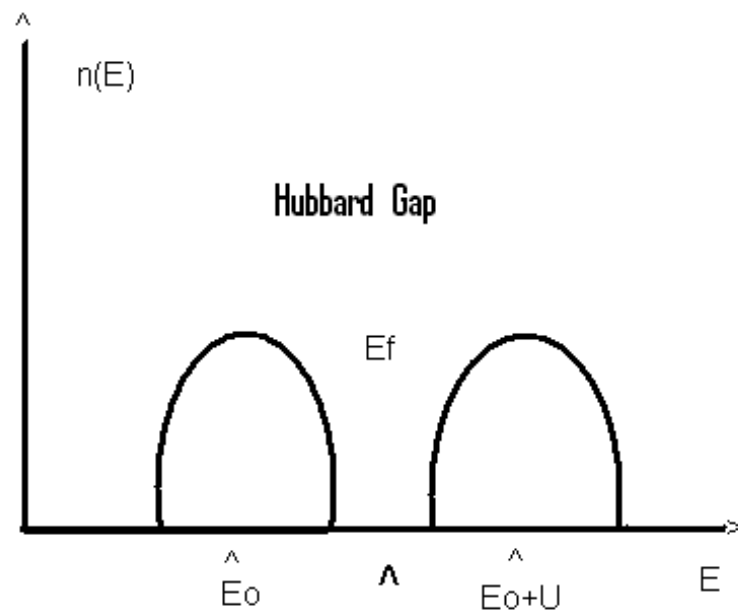
$$\bar{n}_{i,\sigma}(\epsilon) = \frac{1}{\pi} \text{Im} \langle G_{\sigma,\sigma}(i, i; \epsilon) \rangle$$

It may turn out to be the case that

$$\bar{n}_{i,\uparrow}(\epsilon) - \bar{n}_{i,\downarrow}(\epsilon) \neq 0 \text{ this means } \textit{band splitting}.$$

even for  $m=0$  , that is to say  $T \geq T_c$  .and there exist a local moment

$$\mu = \mu_B \int d\epsilon (\bar{n}_{i\uparrow}(\epsilon) - \bar{n}_{i\downarrow}(\epsilon)) \geq 0$$

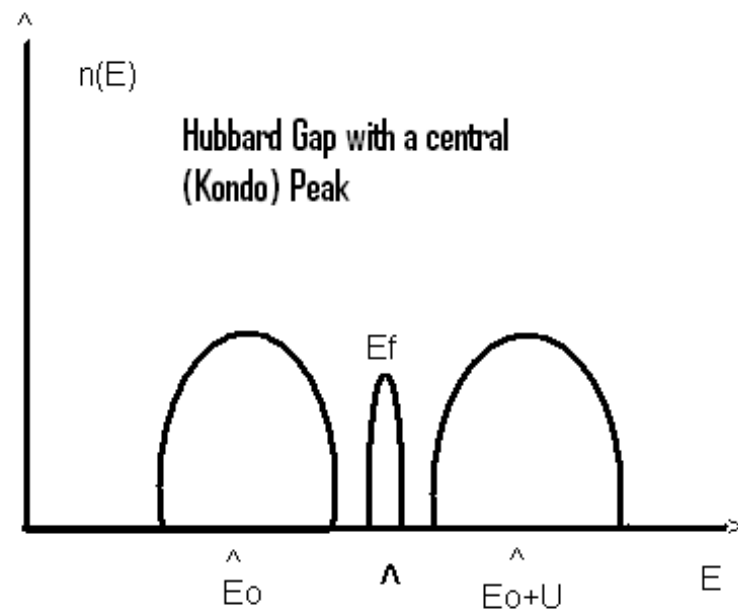


### 1.3 Dynamical CPA=Dynamical Mean Field (DMFT)

(Kakehashi ,Phys.Rev.B 45 7196,**1992** A.Georges and G.Kotliar Phys.Rev.B 45, 6479, (**1992**))

$$\epsilon_{i,\sigma} = \epsilon_0 + U n_{i,-\sigma} \Rightarrow \epsilon_0 + \mathbf{v}_{i,-\sigma}(\tau)$$

$$\underline{G}_{i,i}(\tau, \tau') = \frac{1}{Z} \prod_{i,\sigma} \int D\mathbf{v}_{i,-\sigma}(\tau) \exp\left\{-\frac{1}{U} \sum_{i,\sigma} \int d\tau \mathbf{v}_{i,-\sigma}^2(\tau)\right\} \underline{G}_{i,i}(\tau, \tau'; [\mathbf{v}_{i,-\sigma}(\tau)])$$

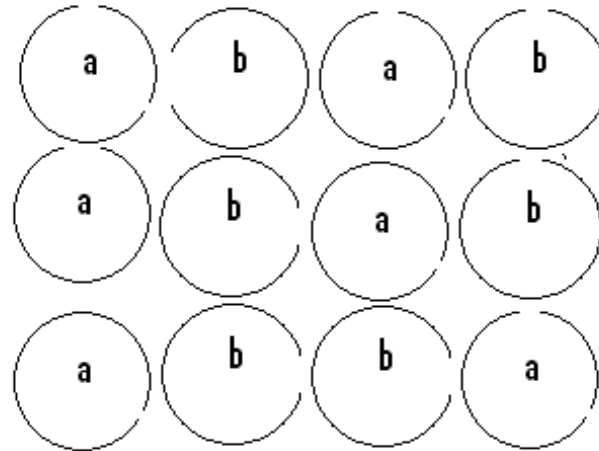


## 2 First principles Alloy analogy

### 2.1 FLUCTUATIONS

in Density Functional theories can be described as follows:

Using Constrained Density Functional Theory force the potential wells at each site to be either  $v_a(\vec{r} - \vec{R}_i)$  or  $v_b(\vec{r} - \vec{R}_i)$  :



**Alloy Analogy Potential Wells**

THEN summ over the sconstraints.

## 2.2 Summing over CONSTRAINTS

In KKR

$$v_a \Rightarrow f_l^a(\epsilon) = \frac{1}{2i} \left( e^{i2\delta_l^a} - 1 \right)$$

$$v_b \Rightarrow f_l^b(\epsilon) = \frac{1}{2i} \left( e^{i2\delta_l^b} - 1 \right)$$

and the summation over STATIC CONSTRAINTS can be done by *KKR-CPA* .

## 2.3 Missing from this discussion:

*Short range Order*

and

*Dynamics*

### **3 Dynamical (quantum) Alloy Analogy**

#### **3.1 Dynamical versus quantum**

description of fluctuations:

$$\text{Dynamics} \Rightarrow \int Dv(\vec{r}, \tau) e^{-S_{eff}[v(\vec{r}, \tau)]}$$

$$\text{Quantum alloy} \Rightarrow \text{Tr}\{e^{-\beta H_{eff}(\hat{S}_x, \hat{S}_y, \hat{S}_z)}\}$$

## 3.2 Internal Two Level Systemes

External TLS in metals, like an atom tunneling between two equivalent positions in a metallic glass, have been studied for a long time. As was first pointed out by J. Kondo their physics has much in common with magnetic impurities in transition metals, such as Fe in Au. A good review of the theory is by Kondo himself in "Fermi surface Effects" by J. Kondo and Yoshimori (Eds.) (Springer Series in Solid-State Sciences 77, Springer-Verlag 1987). Here I propose to postulate that the local potential  $v(\vec{r} - \vec{R}_i; \eta_i)$  seen by an electron depends not

only on  $\vec{r}$  but also a new ,local, INTERNAL variable  $\eta$  which describes the state of an 'atom' on the site concerned. Such state of the 'site' is described by

$$H_{TLS}\Phi_a(\eta) = \epsilon_a\Phi_a(\eta)$$

$$\Phi_a(\eta) = \langle \eta | \Phi_a \rangle$$

$$\widehat{H}_{TLS} | \Phi_a \rangle = \epsilon_a | \Phi_a \rangle$$

$$\widehat{H}_{TLS} | \Phi_b \rangle = \epsilon_b | \Phi_b \rangle$$

$$| \Phi_a \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, | \Phi_b \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\hat{S}_z = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

$$\hat{H}_{TLS} = \epsilon_a \frac{1}{2} (1 + \hat{S}_z) + \epsilon_b \frac{1}{2} (1 - \hat{S}_z)$$

### 3.3 Classical TLS

$\hat{S}_{z,i}$  commutes with  $\hat{H}_{TLS,i}$  for all sites labeled by  $i$ . Thus the collective state of the internal TLS  $s$  (one TLS for each site) can be defined by assigning an eigen value of  $\hat{S}_{z,i}$ , namely  $M_i = \pm 1$ , to each site. If

$$\widehat{H}_{electrons} = \widehat{H}_0 + \sum_i \widehat{v}_{a,i} \frac{1}{2} (1 + \widehat{S}_{z,i}) + \widehat{v}_{b,i} \frac{1}{2} (1 - \widehat{S}_{z,i})$$

an energy eigen state of the combined , electrons+ TLSs sytem,  $| n \rangle$ , is defined by

$$\left( \widehat{H}_{electrons} + \sum_i \widehat{H}_{TLS,i} \right) | n \rangle = E_n(\{M_i\}) | n \rangle$$

and the partition function  $Z$  is

$$\begin{aligned} Z &= \text{tr} \left\{ e^{-\beta(H_{electrons} + \sum_i \widehat{H}_{TLS,i})} \right\} \\ &= \sum_{\{M_i\}} \sum_n e^{-E_n(\{M_i\})} = Z_{TLS} \langle Z(\{M_i\}) \rangle \end{aligned}$$

where

$$Z_{TLS} = \sum_{\{M_i\}} e^{-\beta \sum_i \left( \epsilon_a \frac{1}{2}(1+M_i) + \epsilon_b \frac{1}{2}(1-M_i) \right)}$$

and  $\langle O(\{M_i\}) \rangle$  is the average of  $O(\{M_i\})$  over the configurations  $\{M_i\}$  with the weight

$$P_{TLS}(\{M_i\}) = \frac{1}{Z_{TLS}} e^{-\beta \sum_i \left( \epsilon_a \frac{1}{2}(1+M_i) + \epsilon_b \frac{1}{2}(1-M_i) \right)}$$

Evidently this is the usual, classical, alloy picture. When  $\epsilon_a = \epsilon_b$  all configurations have equal weight. Interestingly, it is also the beginning of the 'augmented space formalism' of Mookerjee.

### 3.4 Quantum TLS

To 'quantize' the above (Ising) spin system we introduce, as well as  $\hat{S}_z$ , the other components,  $\hat{S}_x$  and  $\hat{S}_y$ , of the spin (1/2) operator  $\vec{S}$ .

$$\hat{S}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{S}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Equivalent but more useful in the present context are  $\hat{S}_z, S^+, S^-$  where

$$S^\pm = \hat{S}_x \pm i\hat{S}_y$$

$$S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, S^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Evidently, at each site  $i$

$$S_i^+ |a, i\rangle = 0, S_i^- |a, i\rangle = |b, i\rangle$$

$$S_i^+ |b, i\rangle = |a, i\rangle, S_i^- |b, i\rangle = 0$$

The collective state of the TLSs is

$$|\{M_i\}\rangle = |M_1, M_2, \dots, M_i, \dots\rangle = \prod_i |M_i\rangle$$

Thus the full Hamiltonian is

$$\widehat{H} = \widehat{H}_0 + \widehat{H}_{TLS} + \widehat{V}_a + \widehat{V}_b + \widehat{V}_+ + \widehat{V}_-$$

$$\widehat{V} = \sum_i \widehat{v}_i$$

$$\widehat{v}_{a,i} = \int d^3\psi_s^\dagger(\widehat{r}) \frac{1}{2} (\widehat{1} + \widehat{S}_{z,i}) v_{s,s'}^{a,a}(\widehat{r} - \widehat{R}_i) \Psi_{s'}(\widehat{r})$$

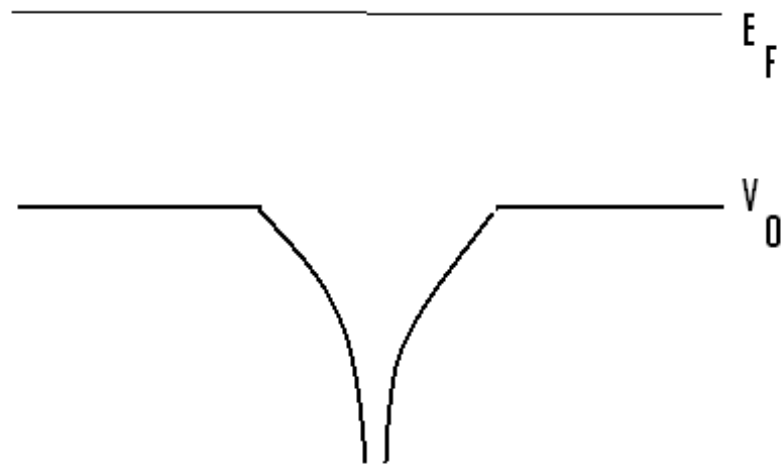
$$\widehat{v}_{b,i} = \int d^3\psi_s^\dagger(\widehat{r}) \frac{1}{2} (\widehat{1} - \widehat{S}_{z,i}) v_{s,s'}^{b,b}(\widehat{r} - \widehat{R}_i) \Psi_{s'}(\widehat{r})$$

$$\hat{v}_{+,i} == \int d^3\psi_s^\dagger(\hat{r}) \frac{1}{2} S_+ v_{s,s'}^{a,b}(\hat{r} - \hat{R}_i) \psi_{s'}(\hat{r})$$

$$\hat{v}_{-,i} == \int d^3\psi_s^\dagger(\hat{r}) \frac{1}{2} S_- v_{s,s'}^{b,a}(\hat{r} - \hat{R}_i) \psi_{s'}(\hat{r})$$

### 3.5 Many-Particle Single Scatterer Theory

A single (muffin-tin type) potential well scatters a degenerate system of non-interacting electrons:



Scattering of a degenerate electron system from a potential well

The usual one-particle t-matrix  $t_{\vec{k}', \vec{k}}(\epsilon)$  generalizes to

$$T_{\vec{k}'s'; \vec{k},s}(E) = \langle \Psi_{\vec{k}',s'} | \hat{T}(E) | \Psi_{\vec{k},s} \rangle$$

where

$$\hat{T}(E) = \hat{V} + \hat{V} \hat{G}_0(E) \hat{T}(E)$$

$$\hat{G}_0(E) = \frac{1}{E - \hat{H}_0}$$

$$\hat{H}_0 = \sum_{\vec{k},s} \epsilon_{\vec{k},s} c_{\vec{k},s}^\dagger c_{\vec{k},s}$$

$$|\Psi_{\vec{k},s}\rangle = c_{\vec{k},s}^\dagger |\Psi_0\rangle$$

$$\hat{V} = \sum_{\vec{k}',s',\vec{k},s} v_{\vec{k}',s';\vec{k},s}^I \hat{S}_I c_{\vec{k}',s'}^\dagger c_{\vec{k},s}$$

$$I = z, \pm$$

Clearly, for  $v_{\vec{k}',s';\vec{k},s}^z \neq 0$  but  $v_{\vec{k}',s';\vec{k},s}^\pm = 0$  we recover the usual KKR-CPA.

$$v_{\vec{k}',s';\vec{k},s}^\pm \neq 0$$

$$\text{Quantum Alloy} \implies \langle M \pm 1 | \hat{S}_\pm | M \rangle \neq 0$$

$$\epsilon_{M\pm 1} - \epsilon_M \neq 0$$

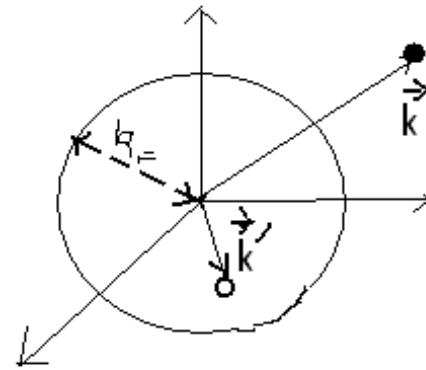
$$\implies \text{Dynamics}$$

Perturbation theory::

$$\hat{T}(E) = \hat{V} + \hat{V} \frac{1}{E - \hat{H}_0} \hat{V} + \hat{V} \frac{1}{E - \hat{H}_0} \hat{V} \frac{1}{E - \hat{H}_0} \hat{V} \dots$$

### 3.5.1 Particles and holes

$$\begin{aligned} C_{\vec{k}}^\dagger &= \alpha_{\vec{k}}^\dagger \quad \text{for } |\vec{k}| > k_F \\ C_{\vec{k}}^\dagger &= \beta_{-\vec{k}} \quad \text{for } |\vec{k}| < k_F \\ C_{\vec{k}} &= \alpha_{\vec{k}} \quad \text{for } |\vec{k}| > k_F \\ C_{\vec{k}} &= \beta_{-\vec{k}}^\dagger \quad \text{for } |\vec{k}| < k_F \end{aligned}$$



$$E_{\vec{k}} > E_F$$

$$E_{\vec{k}'} < E_F$$

Particles

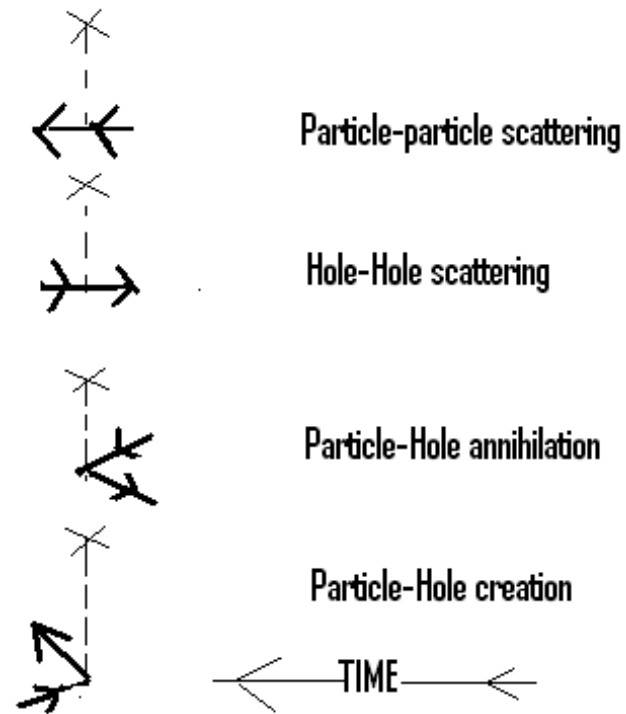
Holes

$$\begin{aligned}
\widehat{H}_0 - \mu \widehat{N} &= \sum_{\vec{k}} \epsilon_{\vec{k}} C_{\vec{k}}^\dagger C_{\vec{k}} - \mu \sum_{\vec{k}} C_{\vec{k}}^\dagger C_{\vec{k}} = \sum_{\vec{k} \cdot > k_F} \epsilon_{\vec{k}} \alpha_{\vec{k}}^\dagger \alpha_{\vec{k}} \\
+ \sum_{\vec{k} \cdot < k_F} \epsilon_{\vec{k}} \beta_{\vec{k}} \beta_{\vec{k}}^\dagger &- \mu \sum_{\vec{k} \cdot > k_F} \alpha_{\vec{k}}^\dagger \alpha_{\vec{k}} - \mu \sum_{\vec{k} \cdot < k_F} \epsilon_{\vec{k}} \beta_{\vec{k}} \beta_{\vec{k}}^\dagger
\end{aligned}$$

$$\begin{aligned}
&= \sum_{\vec{k} < k_F} (\epsilon_{\vec{k}} - \mu) + \sum_{\vec{k} \cdot > k_F} (\epsilon_{\vec{k}} - \mu) \alpha_{\vec{k}}^\dagger \alpha_{\vec{k}} + \\
&\quad \sum_{\vec{k} \cdot < k_F} (\mu - \epsilon_{\vec{k}}) \beta_{\vec{k}}^\dagger \beta_{\vec{k}}
\end{aligned}$$

$$\widehat{V} = \sum (v_{\vec{k}', \vec{k}} \alpha_{\vec{k}}^\dagger \alpha_{\vec{k}} + v_{\vec{k}', \vec{k}} \alpha_{\vec{k}}^\dagger \beta_{-\vec{k}}^\dagger + \beta_{-\vec{k}} \alpha_{\vec{k}} + v_{\vec{k}', \vec{k}} \beta_{-\vec{k}} \beta_{-\vec{k}}^\dagger)$$

# Diagrammatically



### 3.5.2 Scattering from a static potential $v_{\vec{k}', \vec{k}}$ :

For spinless 'particle-particle' scattering

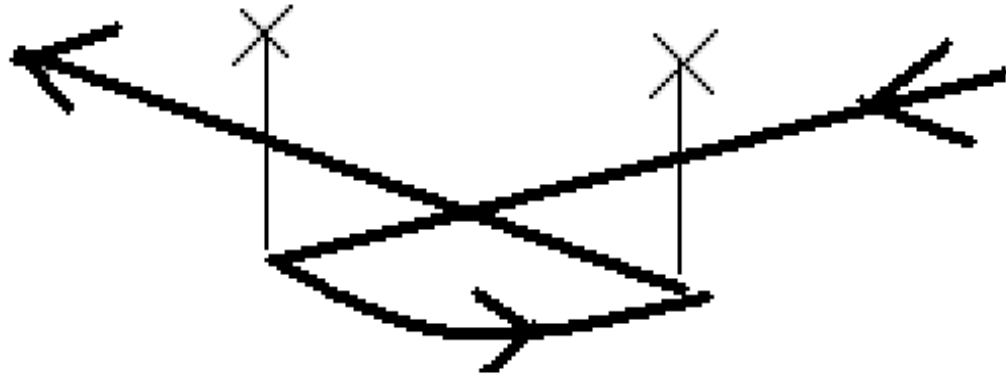
$$|\Psi_{\vec{k}}\rangle = \alpha_{\vec{k}}^\dagger |\Psi_0\rangle$$

$$T_{\vec{k}', \vec{k}}^{(1)}(\epsilon_{\vec{k}}) = \begin{array}{c} \times \\ | \\ \hline \leftarrow \quad \rightarrow \end{array} = v_{\vec{k}', \vec{k}}$$



$$T_{\vec{k}', \vec{k}}^{2a}(\epsilon_{\vec{k}}) =$$

$$= \sum_{\vec{k}''} v_{\vec{k}', \vec{k}''} \frac{1 - f_{\vec{k}''}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}''}} v_{\vec{k}'', \vec{k}}$$



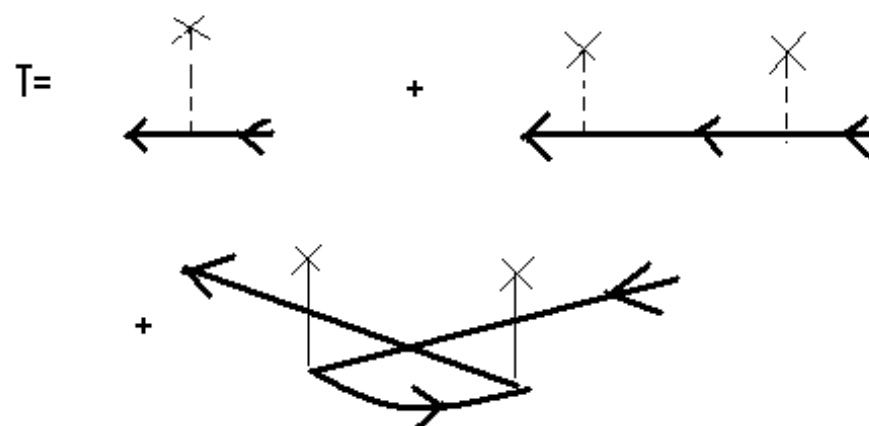
$$T_{\vec{k}', \vec{k}}^{2b)}(\epsilon_{\vec{k}}) = - \sum_{\vec{k}''} v_{\vec{k}'', \vec{k}} \frac{f_{\vec{k}''}}{-\epsilon_{\vec{k}'} + \epsilon_{\vec{k}''}} v_{\vec{k}', \vec{k}''}$$

$$T_{\vec{k}', \vec{k}}^{2a)}(\epsilon_{\vec{k}}) + T_{\vec{k}', \vec{k}}^{2b)}(\epsilon_{\vec{k}}) =$$

$$\begin{aligned}
& v_{\vec{k}', \vec{k}} + \int d^3 k'' v_{\vec{k}', \vec{k}''} \frac{1}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}''}} v_{\vec{k}'', \vec{k}} \\
& + \left[ - \int d^3 k'' \left( v_{\vec{k}', \vec{k}''} v_{\vec{k}'', \vec{k}} - v_{\vec{k}'', \vec{k}} v_{\vec{k}', \vec{k}''} \right) f_{\vec{k}''} \right] \implies 0
\end{aligned}$$

This happens to all orders and hence  $T_{\vec{k}', \vec{k}}(\epsilon_{\vec{k}})$  is given by the conventional Born series for one particle scattering. If the target can change its state and therefore, in general, its energy the scattering electron will be knocked off the energy shell. Namely, electron hole pairs will be created resulting in the famous Kondo divergences.

$$T = V + VGT$$



Feynman Diagram for Kondo Scattering

### 3.5.3 The break down of the Born perturbation series

$$T_{\vec{k}' M', \vec{k} M}^{(1)}(E) = \sum_I V_{\vec{k}', \vec{k}}^I S_{M', M}^I$$

$$\begin{aligned} \hat{T}_{\vec{k}' M', \vec{k} M}^{(2)}(\epsilon_{\vec{k}}) = & \sum_{I, J} \sum_{M''} \sum_{\vec{k}''} V_{\vec{k}', \vec{k}''}^I S_{M', M''}^I V_{\vec{k}'', \vec{k}}^J S_{M'', M}^J \frac{1 - f_{\vec{k}''}}{\epsilon_{\vec{k}'} - \epsilon_{\vec{k}''}} \\ & - V_{\vec{k}'', \vec{k}}^I S_{M', M''}^I V_{\vec{k}', \vec{k}''}^J S_{M'', M}^J \frac{f_{\vec{k}''}}{-\epsilon_{\vec{k}} + \epsilon_{\vec{k}''}} \end{aligned}$$

If, for a noncommutative model, (non spherically symmetric potentials)

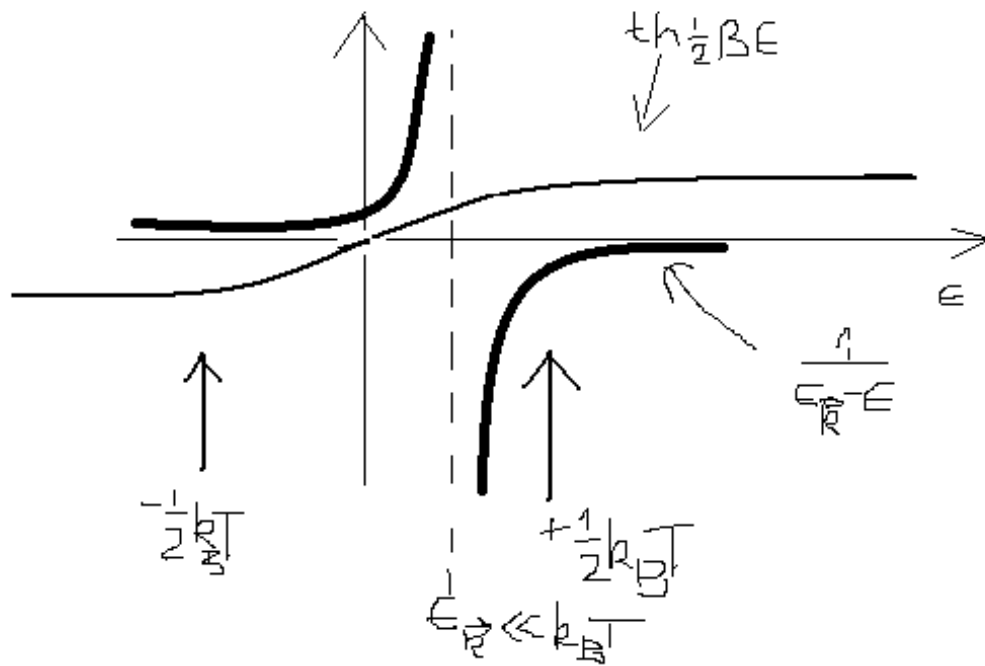
$$V_{\vec{k}', \vec{k}}^I = \sum_{L', L} V_{L', L}^I(k', k) Y_{L'}(\hat{k}') Y_L(\hat{k})$$

Take the simplest case  $L=0$  and  $1$ . Then the quantities  $V_{L', L}^I$  are  $2 \times 2$  matrices and can be parametrized as

$$V_{L', L}^I = \sigma_{L', L}^I V^I$$

Then, for  $\epsilon_{\vec{k}'} = \epsilon_{\vec{k}''} = \epsilon_F$  and

$$\sum_{\vec{k}''} \left( \frac{P}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}''}} \right) (1 - 2f_{\vec{k}''}) = n(\epsilon_F) \int_{-D}^D d\epsilon \frac{P}{\epsilon_{\vec{k}} - \epsilon} \text{th} \left( \frac{1}{2} \beta \epsilon \right)$$



For  $\epsilon \rightarrow \ll k_B T$

$$\approx 2 \ln \frac{k_B T}{D}$$

For  $\epsilon_{\vec{k}} \gg k_B T$

$$\approx 2 \ln \frac{\epsilon_{\vec{k}}}{D}$$

Finally

$$\delta \hat{T}_{\vec{k}'M'; \vec{k}, M}^{(2)}(\epsilon_{\vec{k}}) \approx \sum_{I, J, M''} (V_{L', L''}^I V_{L'', L}^J - V_{L'', L}^I V_{L', L''}^J) (S_{M', M''}^I S_{M'', M}^J) \frac{k_F}{4\pi} \ln \left( \frac{D}{\epsilon_{\vec{k}}, k_B T} \right)$$

**Evidently the perturbation series diverges.** A way to sum up such logarithmically divergent series is to use scaling arguments as follows

### 3.6 Poorman Scaling:

$$T(\epsilon; V_1 + \delta V_1, V_2 + \delta V_2, V_3 + \delta V_3; D + \delta D) = 0$$

**In the case of magnetic impurities**

$$T_{\vec{k}', \vec{k}}(z) = [J_{\perp}(S^{+}\sigma^{-} + S^{-}\sigma^{+}) + J_{\parallel}S^{z}\sigma^{z}] - [J_{\parallel}J_{\perp}(S^{+}\sigma^{-} + S^{-}\sigma^{+}) + J_{\parallel}^2S^{z}\sigma^{z}]n(\epsilon_F)\ln\frac{z}{D} + \dots$$

$$\delta J_{\perp} = -J_{\perp}J_{\parallel}n(\epsilon_f)\delta\ln\frac{z}{D} = -J_{\perp}J_{\parallel}N(\epsilon_F)\delta\ln\frac{\delta D}{D}$$

$$\delta J_{\parallel} = -J_{\parallel}^2N(\epsilon_F)\delta\ln\frac{z}{D} = -J_{\parallel}^2N(\epsilon_F)\delta\ln\frac{\delta D}{D}$$

$$\frac{\partial J_{\perp}}{\partial \ln D} = -nJ_{\parallel}J_{\perp} \quad , \quad \frac{\partial J_{\parallel}}{\partial \ln D} = -nJ_{\parallel}^2$$

For  $J_{\parallel} = J_{\perp} = -J$  ( $J > 0$ )

$$\frac{dJ}{dD} = n \frac{J^2}{D}$$

$$\int_{J_0}^J dJ' \frac{1}{J'^2} = n \int_{D_0}^D \frac{dD}{D}$$

$$-\frac{1}{J} + \frac{1}{J_0} = n \ln \frac{D}{D_0}$$

$$J = \frac{nJ_0}{1 - nJ_0 \ln \frac{D}{D_0}}$$

$$k_B T_K = D_0 e^{-\frac{1}{nJ_0}}$$

$$k_B T_K = D e^{-\frac{1}{nJ}}$$

**So  $k_B T_K$  is a scale invariant low energy scale**

**As the temperature is lowered**

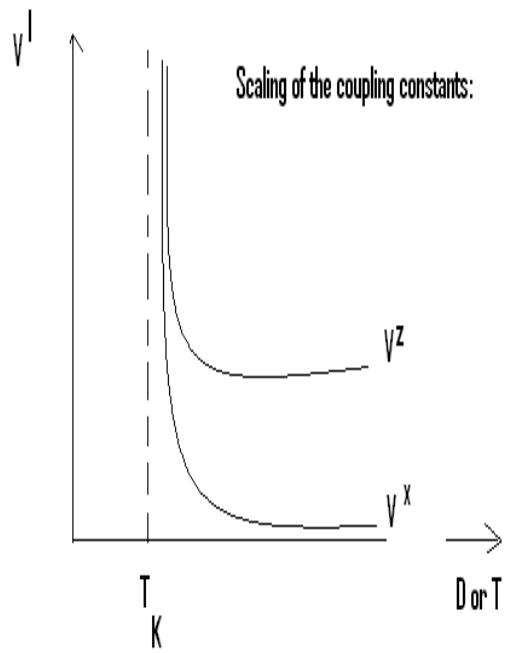
$$nJ(T) = \frac{1}{\ln \frac{T}{T_K}}$$

**For the internal TLS**, following Zawadowski and Vladar , '92he we find that Scattering Aplitude scales to the strong couplig regime:

$$\begin{aligned} \frac{dV^x}{dx} &= -4V^yV^z \\ \frac{dV^y}{dx} &= -4V^zV^x \\ \frac{dV^z}{dx} &= -4V^xV^y \end{aligned}$$

where  $x = \ln \frac{D}{D_0}$

$$k_B T_K = D_0 \left( \frac{V_0^x}{4V_0^z} \right)^{\frac{1}{4V_0^z}}$$



**4 The challenge is to find a material specific, quantitative theory of the low energy scale**

$$k_B T_K = (?) e^{-\frac{1}{n((\epsilon_F)J)}}$$