Impurities in superconductors

Disorder is ubiquitous in materials. Soon after the BCS theory (57'), it was noticed that SC is experimentally insensitive to enormous amounts of physical and chemical impurities!

Ex: . Bismuth ~ amorphous → SC
. Beryllium films
. Disordered alloys with 20-50% of chemical scattering centers but with an almost constant T_c.

However if the impurities which are introduced are magnetic ions SC is progressively destroyed (Matthias 58')

→ Non magnetic impurities seem to have little effects on T_c, transp.

I) Anderson "theorem", (J. Phys. Chem Solids, 11, 28-30, 59')

Actually more a set of arguments: Applies to dirty SCs where elastic scattering (by physical or chemical impurities) is large compared to the SC gap Δ_0. (⇒ non magnetic)

key idea: Time Reversal symmetry is maintained.
Since $\vec{k}$ is not conserved ⇒ forget it.
Pairing will occur between a single particle state and its TR partner

Approach: Start with the disordered single particle Hamiltonian

$$\mathcal{H}_0 = \int d\vec{r} \sum_{\sigma} \Psi_\sigma^\dagger(\vec{r}) \underbrace{\left[\left(-\frac{i\vec{\nabla}}{2m}\right)^2 + V_{dis}(\vec{r})\right]}_{H_0} \Psi_\sigma(\vec{r})$$

TRS is apparent.

Hypothesis : i) non magnetic and elastic scattering disorder
ii) We will assume disorder is not strong enough to localize the system. (Competition between localizat° and SC will be the subject of Mohit's course)

Suppose somebody solves the complicated single-particle pb.

i.e. $H_0 |\alpha\sigma\rangle = \varepsilon_\alpha |\alpha\sigma\rangle$ for both spins $\uparrow$ and $\downarrow$

where $|\alpha\sigma\rangle = \sum_{\vec{k}'} \underbrace{c_{\alpha\vec{k}'}}_{\langle\alpha|\vec{k}\rangle} |\vec{k}\sigma\rangle$ ← plane waves (useless here)

$$H_0\, \phi_{\alpha,\sigma}(\vec{r}) = \varepsilon_\alpha\, \phi_{\alpha,\sigma}(\vec{r})$$

One can always choose $\phi_{\alpha,\sigma}(\vec{r}) \in \mathbb{R}$

$T|\alpha\sigma\rangle$ is the TR partner of $|\alpha\sigma\rangle \Leftrightarrow \phi_{\alpha\uparrow}(\vec{r}) \longrightarrow \phi^*_{\alpha\downarrow}(\vec{r})$ is also an eigenstate of H_0 with energy ε_α

$\phi_{\alpha\uparrow}(\vec{r})$ and $\phi^*_{\alpha\downarrow}(\vec{r})$ form Kramers partners

However $\phi_{\alpha,\uparrow}(\vec{r}) \in \mathbb{R} \Rightarrow \{\phi_{\alpha\uparrow}, \phi_{\alpha\downarrow}\}$ have Kramers degeneracy

Suppose we can write the interaction (resulting from el-phonon interaction) as an effective local attractive interaction

$$H_{el-ph} \simeq -V_0 \int d\vec{r}\; \Psi^\dagger_\uparrow(\vec{r})\Psi^\dagger_\downarrow(\vec{r})\Psi_\downarrow(\vec{r})\Psi_\uparrow(\vec{r})$$

with $V_0 > 0$

we assume the interaction to be constant.

$$H = \sum_\alpha \varepsilon_\alpha \left(c^\dagger_{\alpha\uparrow}c_{\alpha\uparrow} + c^\dagger_{\alpha\downarrow}c_{\alpha\downarrow}\right) - V_0 \int d\vec{r}\; \Psi^\dagger_\uparrow(\vec{r})\Psi^\dagger_\downarrow(\vec{r})\Psi_\downarrow(\vec{r})\Psi_\uparrow(\vec{r})$$

Let us proceed with the BCS mean field approx.

$$H_{el-ph} \simeq -\int d\vec{r} \left(\Delta(\vec{r})\Psi^\dagger_\uparrow(\vec{r})\Psi^\dagger_\downarrow(\vec{r}) + H.c.\right)$$

where $\Delta(\vec{r}) = V_0 \langle \Psi_\downarrow(\vec{r})\Psi_\uparrow(\vec{r})\rangle$

However $\Psi_\sigma(\vec{r}) = \sum_\alpha \phi_\alpha(\vec{r})\, c_{\alpha\sigma}$

$$\Rightarrow \Delta(\vec{r}) = V_0 \sum_{\alpha,\beta} \phi_\alpha(\vec{r})\, \phi_\beta(\vec{r})\, \langle c_{\alpha\downarrow} c_{\beta\uparrow} \rangle$$

The assumption is that the wave functions remain extended ($k_F l \gg 1$) such that $\Delta(\vec{r})$ averages out

Therefore $\Delta(\vec{r}) \underset{\sim}{\longrightarrow} \Delta \approx \frac{1}{\Omega} \int d\vec{r}\, \Delta(\vec{r})$

$$= \frac{V_0}{\Omega} \int d\vec{r} \sum_{\alpha,\beta} \phi_\alpha(\vec{r})\, \phi_\beta(\vec{r})\, \langle c_{\alpha\downarrow} c_{\beta\uparrow} \rangle$$

However the $\{\phi_\alpha\}$ form an orthonormal basis

$\hookrightarrow \int d\vec{r}\, \phi_\alpha(\vec{r})\, \phi_\beta(\vec{r}) = \delta_{\alpha\beta}$ ($\phi_\alpha(\vec{r}) \in \mathbb{R}$ Kramers deg.)

$$\Delta \approx \frac{V_0}{\Omega} \sum_\alpha \langle c_{\alpha\downarrow} c_{\alpha\uparrow} \rangle$$

Using the same trick for H, one can write the full H as

$$\mathcal{H}_{MF} = \sum_{\alpha,\sigma} \varepsilon_\alpha\, c^\dagger_{\alpha\sigma} c_{\alpha\sigma} - \sum_\alpha \left(\Delta\, c^\dagger_{\alpha\uparrow} c^\dagger_{\alpha\downarrow} + \Delta^* c_{\alpha\downarrow} c_{\alpha\uparrow} \right)$$

$\hookrightarrow E_\alpha = \sqrt{(\varepsilon_\alpha - \mu)^2 + |\Delta|^2}$

after a Bogoliubov transform.

$$\begin{cases} \gamma_{\alpha\uparrow} = u_\alpha c_{\alpha\uparrow} + v_\alpha c^\dagger_{\alpha\downarrow} \\ \gamma^\dagger_{\alpha\downarrow} = v^*_\alpha c_{\alpha\uparrow} + u_\alpha c^\dagger_{\alpha\downarrow} \end{cases}$$

The self-consistent BCS equation reads:

$$\Delta = V_0 \sum_\alpha \frac{\Delta}{\sqrt{(\varepsilon_\alpha - \mu)^2 + |\Delta|^2}} \left(1 - 2 f(E_\alpha)\right)$$

Hyp: If we assume the d.o.s $N(\varepsilon) \sim N(0)$ remains uniform over the whole BZ (at least over a range Λ_D around $\mu \sim \varepsilon_F$)
↳ Debye

$$\Delta \simeq V_0 N(0) \int_{|\varepsilon| < \Lambda_D} d\varepsilon \, \frac{\Delta}{2E(\varepsilon)}$$

we recover the usual BCS gap equation.
→ Gap unaffected ; T_C unaffected (marginally)

Summary of key hypothesis :
- s-wave SC
- TRS to maintain Kramers degeneracy.
- "Weak disorder" to guarantee extended states and self-averaging pairing → $k_F l \gg 1$
  where l elastic mean free path.
- We assume constant $N(\varepsilon) \sim N(0)$ near $\mu \sim \varepsilon_F$
  → disorder that does not affect the D.O.S
  (potential scattering is perfect)

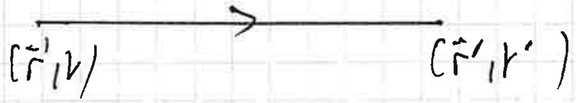
If we break one of those hypothesis, conclusions are to be modified !!!

Ex : • magnetic impurities or magnetic field (still SC can accomodate it)
- Non s-wave SC → less resilient toward disorder
  ↳ (May explain why s-wave seems more spread ?)
- Strong disorder → Randeria's talk.
- non-interacting Anderson impurity model

II) The impurity point of view (T-matrix formalism)

2.1) Metallic case

Bare propagator: $g_0(\vec r',t';\vec r,t)$ → electron prop. from $(\vec r,t)\to(\vec r',t')$



sol. of $\left[i\hbar\frac{\partial}{\partial t} - H_0(\vec r)\right] g_0(\vec r,t;\vec r',t') = \hbar\,\delta(\vec r-\vec r')\,\delta(t-t')$

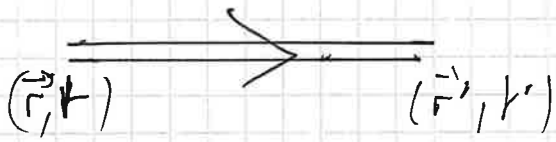
For translat° invariant and time-independent H_0, $g_0 \equiv g_0(\vec r-\vec r';t-t')$

for $t>t'$: $|\Psi_0(\vec r,t)\rangle = \int dt'\, g_0(\vec r,t;\vec r',t')\,|\Psi_0(\vec r',t')\rangle$

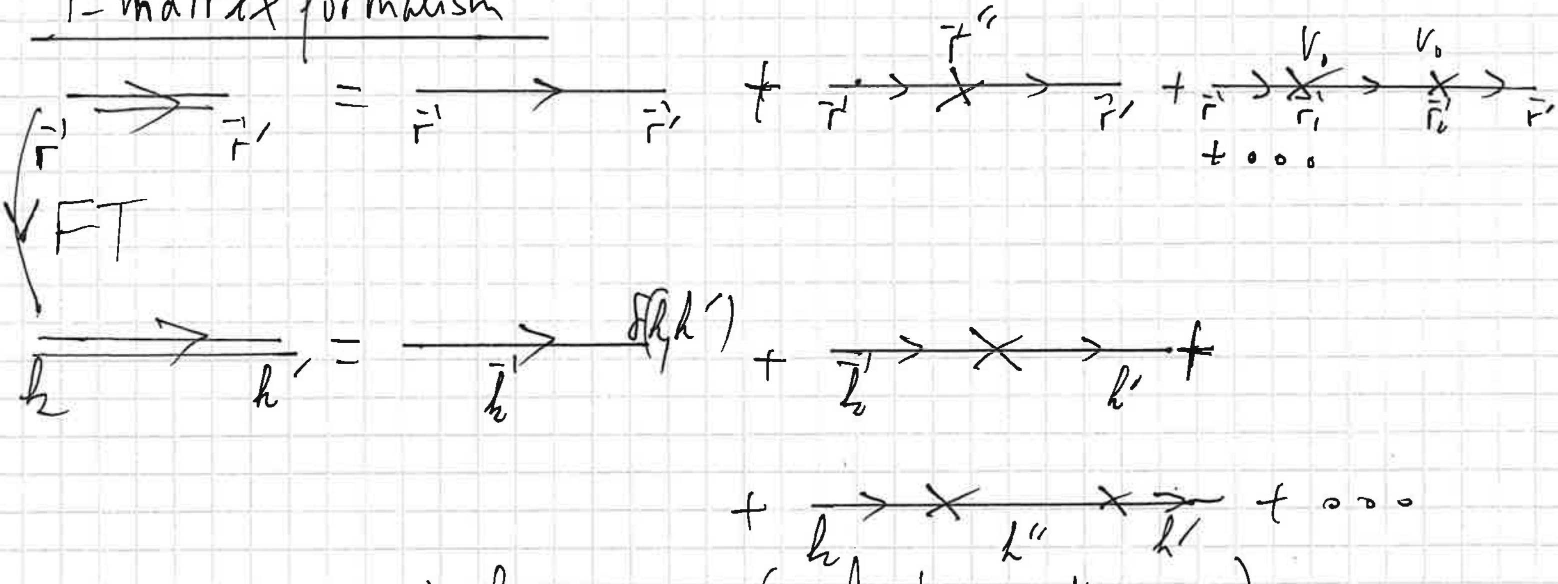
$\Leftrightarrow\ g_0(\vec r,t;\vec r',t') = -i\theta(t-t')\,\langle\vec r|\,e^{-\frac{iH_0(t-t')}{\hbar}}\,|\vec r'\rangle$

Impurity: $V(\vec r-\vec r_0) = V_0\,\delta(\vec r-\vec r_0) \xrightarrow{FT} V_{kk'} = V_0\,\delta_{kk'}$

Propagator (exact): $g(\vec r',t';\vec r,t)$



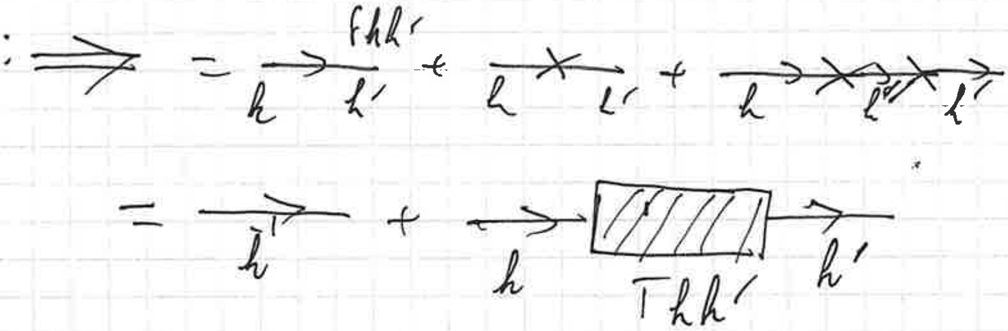
T-matrix formalism



We omit frequencies (elastic scattering)

$$g_{kk'} = g_0(k)\,\delta_{kk'} + g_0(k)\,V_{kk'}\,g_0(k') + \sum_{k''} g_0(k)\,V_{kk''}\,g_0(k'')\,V_{k''k'}\,g_0(k') + \dots$$

Graphically:



$$g_{kk'} = g_0(k)\,\delta_{kk'} + g_0(k)\,T_{kk'}\,g_0(k')$$

where $T_{kk'} = U_{kk'} + \sum_{k''} U_{kk''}\, g_0(k'')\, U_{k''k'} + \ldots$

$$T_{kk'} = V_{kk'} + \sum_{k''} V_{kk''}\, g_0(k'')\, T_{k''k'}$$

real space $\rightarrow$

$$g(\vec{r}, \vec{r}\,'; w) = g_0(\vec{r}, \vec{r}_0; w) + g_0(\vec{r}, \vec{r}_0)\, T(w)\, g_0(\vec{r}_0, \vec{r}\,'; w)$$

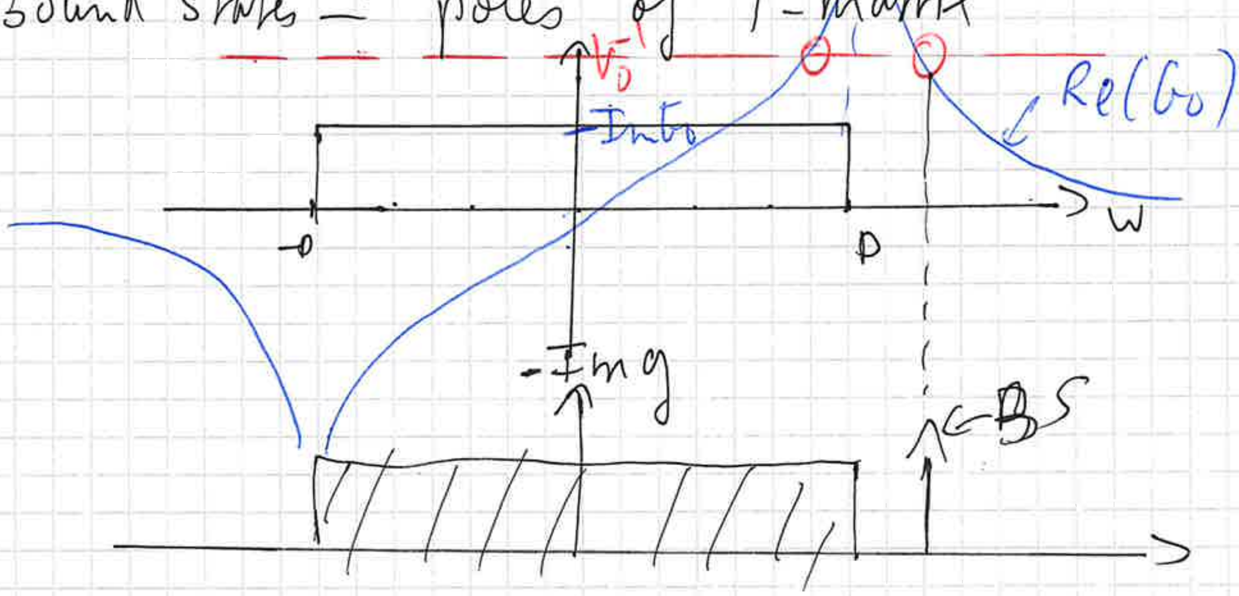
Potential scattering $V_{kk'} = V_0 \delta_{kk'}$ and $g_0(k) = \dfrac{1}{w - \varepsilon_k + i0^+}$

$$T_{kk'} = V_0 \delta_{kk'} \Big(1 + \sum_{k''} V_0\, g_0(k'') + \ldots\Big) = \frac{V_0 \delta_{kk'}}{1 - V_0 \sum_k g_0(k)}$$

$$= \delta_{kk'} \left[V_0^{-1} - G_0 \right]^{-1}$$

where $G_0 = \sum_k g_0(k) \sim \rho_0 \ln \left| \dfrac{w+D}{w-D} \right|$

Bound states $\triangleq$ poles of T-matrix



2.2) Conventional SC (BdG formalism)

propagator $H_0 = \sum_k \Psi_k^\dagger \begin{bmatrix} \varepsilon_k & \Delta_k \\ \Delta_k^* & -\varepsilon_k \end{bmatrix} \Psi_k \qquad \Psi_k^\dagger = (c_{k\uparrow}^\dagger, c_{-k\downarrow})$

$$\hat{g}_0(k,\omega) = \frac{\omega \hat{\mathbb{1}} + \varepsilon_k \hat{\tau}_3 + \Delta_k \hat{\tau}_1}{\omega^2 - E_k^2} \qquad (\Delta \in \mathbb{R})$$

where $E_k = \sqrt{\varepsilon_k^2 + \Delta_k^2}$

Impurity

$$\sum_{k,k',\sigma} V_{kk'} c_{k\sigma}^\dagger c_{k'\sigma} = \sum_{k,k'} \Psi_k^\dagger \underbrace{V_0 \hat{\tau}_3}_{\hat{V}_{kk'}} \Psi_{k'}$$

Our previous T-matrix formalism applies (but with matrices)

$$\hat{g}_{kk'} = \hat{g}_k^0 + \hat{g}_k^0 \hat{T}_{kk'} \hat{g}_{k'}^0$$

with $\hat{T}_{kk'} = \hat{V}_{kk'} + \sum_{k''} \hat{V}_{kk''} [\hat{g}_{k''}^0] \hat{V}_{k''k'} + \dots$

$$= V_0 \hat{\tau}_3 \delta_{kk'} + V_0 \hat{\tau}_3 \left(\sum_k \hat{g}^0(k,\omega) \right) \hat{T}_{kk'}$$

$$\hat{T} = V_0 \tau_3 \left(\mathbb{1} + \sum_k \hat{g}^0(k,\omega) \hat{T} \right)$$

$$\boxed{\hat{T}(\omega) = V_0 \left(\mathbb{1} - V_0 \tau_3 \sum_k g_0(k,\omega) \right)^{-1} \tau_3}$$

$\hookrightarrow$ Poles of T : $\det \hat{T}(\omega) = 0$

$$\sum_{k'} \hat{g}_0 \simeq \rho_0 \int_{-D}^{D} d\varepsilon \left[\frac{\omega \hat{\mathbb{1}} + \varepsilon \hat{\tau}_3 + \Delta \hat{\tau}_1}{\omega^2 - \varepsilon^2 - \Delta^2} \right]$$

$$\simeq -(\omega \hat{\tau}_0 + \Delta \tau_1) \frac{\pi \rho_0}{\sqrt{\Delta^2 - \omega^2}} \qquad (\text{for } \Delta > |\omega|)$$

$$\Rightarrow T(\omega) = V_0 \left(\hat{\tau}_3 - \frac{\pi \rho_0 V_0 \omega \hat{\tau}_0}{\sqrt{\Delta^2 - \omega^2}} + \frac{\pi \rho_0 V_0 \Delta \hat{\tau}_1}{\sqrt{\Delta^2 - \omega^2}} \right) \frac{1}{\det T(\omega)}$$

$\det T(\omega) = 0 \iff 1 + (\pi \rho_0 V_0)^2 = 0 \to$ no poles for $|\omega| < \Delta$

we recover Anderson thm

2.3) Unconventional SC (d-wave) $\to$ nodes

Ex : $\Delta = \Delta(k)$ with $\Delta(\phi) = \Delta_0 \cos 2\phi$ (polar coord)

$$\hat{g}^{(0)} = \frac{\omega \hat{\tau}_0 + \varepsilon_k \hat{\tau}_3 + \Delta(\phi)\hat{\tau}_1}{\omega^2 - \varepsilon_k^2 - \Delta^2(\phi)}$$

$\det T(\omega) = 0 \Rightarrow \frac{1}{2}\mathrm{Tr} \sum_k g^0(k) = \left\langle \frac{-i\omega}{\sqrt{\omega^2 - \Delta^2(\phi)}} \right\rangle_\phi + i \frac{\langle \Delta(\phi) \rangle}{\sqrt{\omega^2 - \Delta^2}}$ $\simeq 0$

$\hookrightarrow 1 - (\pi \rho_0 V_0)^2 \dfrac{\omega^2}{\langle \Delta^2(\phi)\rangle_\phi - \omega^2} = 0$

$\hookrightarrow$ This has solut° | Balatsky 95' | Salkola 96'

$\Rightarrow$ Analogy with the metallic case

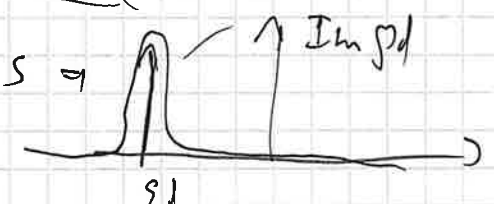
2024 $\Rightarrow$ Escape Anderson thm

2.4) Machida - Shibata BS (72 & Shiba 73')

Consider Anderson model at $U = 0$

$$H = H_0 + \varepsilon_d \hat{n}_d + \sum (V_{sd} c^\dagger_{k\sigma} d_\sigma + H.c)$$

$\hookrightarrow$ Energy dependent d.o.s $\to$



$$\hat{T}(\omega) = \tau_3 |V_{sd}|^2 \left[\omega - \varepsilon_d \tau_3 - |V_{sd}|^2 \tau_3 \sum_k \hat{G}_0(k|\omega)\tau_3\right]^{-1} \tau_3$$

$\det T(\omega) = 0$

$$\omega^2\left(1+\frac{2\Gamma}{\sqrt{\Delta^2-\omega^2}}\right)=\varepsilon_d^2+\Gamma^2$$

For $\Gamma \gg \Delta$, $\omega^* = \pm\Delta\left(1-2\frac{\Delta^2\Gamma^2}{(\Gamma^2+\varepsilon_d^2)^2}\right) \to$ gap edge!

However if $\Gamma \sim \Delta \to$ in gap states.

see Wiesendanger et al Nature 22'

III) Magnetic impurities in s-wave SCs

3.1) Yu-Shiba-Rusinov bound states

$$H_{imp} = J\,\vec{S}_{imp}\cdot\vec{\sigma}(\vec{r}_0) + K\,\delta(\vec{r}_0)$$

Hypothesis $|S_{imp}| \gg 1$ fluctuat° are negligible.
$\underset{S}{\shortparallel}$ favors $S^z = \pm S$

$$H_{imp} = (K-J)\,c^\dagger_\uparrow(\vec{r}_0)c_\uparrow(r_0) + (K+J)\,c^\dagger_\downarrow(r_0)c_\downarrow(\vec{r}_0)$$

$\hookrightarrow$ with spin, we need to work with a 4×4 Nambu matrices

$$H = \sum_k \Psi^\dagger_k H_{BdG} \Psi_k \quad \text{with } \Psi_k^T = (\psi_{\uparrow k}\ \psi_{\downarrow k}\ \psi^\dagger_{\downarrow -k}\ -\psi^\dagger_{\uparrow -k})$$

$$\left|\begin{array}{l} H_{BdG} = \varepsilon_k \hat{\tau}_z + \Delta\,\hat{\tau}_x \\ H_{imp} = (K\,\hat{\tau}_z + J\,\sigma^z)\,\delta(\vec{r}) \end{array}\right.$$

We can use again the $\hat{T}$ matrix results

$$T(\omega) = \left[\mathbb{1}_4 - V_{4\times4}\sum_k \hat{G}_0(k)\right]^{-1}\hat{V}_{4\times4}$$

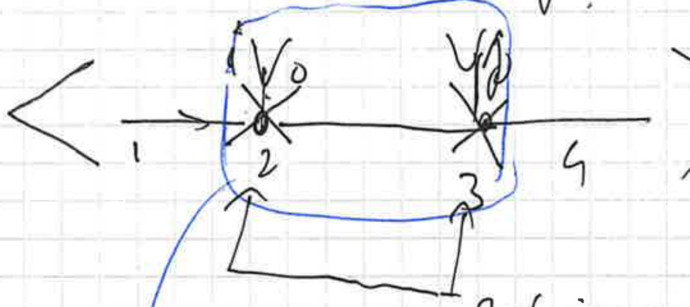
$$\boxed{E_S = \Delta\,\frac{1-\alpha^2+\beta^2}{\sqrt{4\alpha^2+(1-\alpha^2+\beta^2)^2}}}$$

$\alpha = \rho_0\pi J$
$\beta = \rho_0\pi K$
See slides

3.2) Finite concentrat° of impurities

Abrikossov-Gorkov - 1960' → average over impurities configurations.

Idea :



imp config.

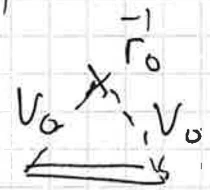
2 ≠ impurities

$$\langle V(2)V(3)\rangle g^{(0)}(3-2) = \sum V_0^2\, \delta(\vec r_2-\vec r_i)\,\delta(\vec r_3-\vec r_j)\, g^{(0)}(3-2)$$

$$= \sum_{k,k'} V_0^2\, e^{ik\vec r_2}\, e^{ik'\vec r_3} \underbrace{\sum_{i,j} \left\langle e^{-ikr_i}\, e^{-ik'r_j}\right\rangle}_{\delta_{r_i,r_j}\ \delta_{k,-k'}} g^{(0)}(3-2)$$

$$= \sum_k V_0^2\, e^{ik(\vec r_2-\vec r_3)}\, g^{(0)}(\vec 3-\vec 2)\, n_{imp}$$

$$= n_{imp} V_0^2 \sum_k g^{(0)}(k,\omega)$$



"Born approx. diagram"

→ neglect diagrams at $O(n_{imp}^2)$

$$G^{-1}(\vec k,\omega) = \omega \mathbb{1} - \varepsilon(k)\vec\tau_3 - \hat\Delta - \hat\Sigma$$

with $\hat\Sigma(\omega,k) = n_{imp}\int dk'\ U_{imp}(k-k')\,\hat G_0(k'',\omega)\,U_{imp}(k',\omega)$

Exact (Born) Green function becomes

$$G^{-1}(k,\omega) = \tilde{\omega}\mathbb{1} - \tilde{\varepsilon}(k)\hat{\tau}_3 - \hat{\tilde{\Delta}}\sigma_y\tau_y$$

with $\tilde{\omega}$, $\tilde{\Delta}$ renormalized parameters.

$$\begin{cases} \tilde{\omega} = \omega + \frac{1}{2}\left(\frac{1}{\tau_p} + \frac{1}{\tau_s}\right)\frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2 + \Delta_0^2}} \\ \tilde{\Delta} = \Delta + \frac{1}{2}\left(\frac{1}{\tau_p} - \frac{1}{\tau_s}\right)\frac{\tilde{\Delta}}{\sqrt{\tilde{\omega}^2 + \Delta_0^2}} \end{cases}$$

$\frac{1}{\tau_p} = n_{imp}\rho_0 \int d\hat{\Omega}\, |U_{pot}(k-k')|^2 \to$ potential scattering times

$\frac{1}{\tau_s} = n_{imp}\rho_0\, S(S+1) \int d\hat{\Omega}\, |J(k-k')| \to$ spin-flip scattering

if $\tau_s^{-1} = 0 \to \tilde{\omega}, \tilde{\Delta}$ same renormalized $\to$ Anderson recovered.

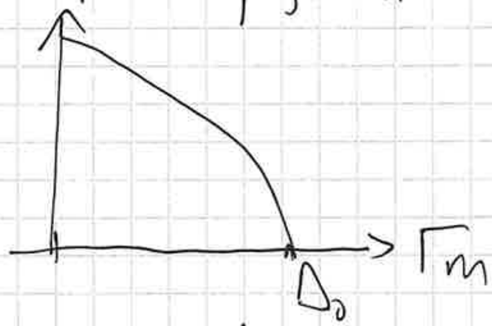
However if we consider magnetic impurities, the gap closes with $n_{imp}\nearrow$

universal AG curve

$$\psi\left(\frac{1}{2} + \frac{1}{2\pi\tau_s T_c}\right)$$

$$\boxed{\cancel{\psi\left(\frac{1}{2} + \frac{\Gamma}{\pi\Delta_0}\right)} - \psi\left(\frac{1}{2}\right) = \ln\frac{T_{c0}}{T_c}}$$

$\Gamma = n_{imp}\rho_0 V_m^2$



$\to$ ~~gapless SC for~~

Define $\alpha' = \tau_s^{-1} = \Delta_0 e^{-\pi/4}$
$\hookrightarrow$ gap of pure SC at $T=0$

If $\alpha_c = \tau_s^{-1} > \alpha' \to$ SC is destroyed

However as $\tau_s^{-1} \sim 0.912\,\alpha_c \to$ <u>Gapless SC</u>