Lecture 4.

Scattering from magnetic impurities

Kondo effect on magnetic impurities.
Abrikosov-Suhl resonance.
Spin-orbit interaction.
Spin relaxation.

Electron with spin

Hamiltonian in magnetic field (non-relativistic)

$$\mathcal{H} = -\frac{\hbar^2}{2m}\left(\nabla - \frac{ie}{\hbar c}\vec{A}\right)^2 + V(r) \underbrace{- \frac{1}{2} g \mu_B \vec{\sigma}\cdot\vec{H}}_{\text{Zeeman term}}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Pauli matrices

Non-relativistic also means: no SO interaction

If $\vec{H} \parallel z$

$$\vec{\sigma}\cdot\vec{H} = \sigma_z H = \begin{pmatrix} H & 0 \\ 0 & -H \end{pmatrix}$$

Up and down spin are separated

If $\vec{H}$ is not along z: wave function is an eigenfunction of $(\vec{\sigma}\cdot\vec{H})$ operator

Scattering from magnetic impurities

Spin-dependent part

$$V_s(\vec{r}) = -\frac{J}{n}\sum_i \vec{\sigma}\cdot\vec{S}_i\,\delta(\vec{r}-\vec{R}_i) \qquad n=\frac{N_i}{\Omega}$$

$\vec{S}_i$ are not uniformly oriented

For one impurity:

If we take $\vec{S}_i$ along z axis:

$$V_{s\uparrow}(\vec{r}) = -\frac{JS_z}{n}\delta(\vec{r}-\vec{R}_i)$$

$$V_{s\downarrow}(\vec{r}) = +\frac{JS_z}{n}\delta(\vec{r}-\vec{R}_i)$$

$\Rightarrow$ spin-dependent scattering

Scattering from one impurity

Amplitude of scattering $\alpha \to \alpha'$: $\qquad (\alpha = \uparrow, \downarrow)$

$$t_{\alpha'\alpha} = -\frac{J}{n}(\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha}$$

– one electron is scattered from impurity

Probability of scattering to all possible states (Born approximation)

$$W = \frac{1}{2}\left(\frac{J}{n}\right)^2 \sum_{\alpha\beta} \sigma^i_{\alpha\beta}\,\sigma^j_{\beta\alpha}\,S_i S_j = \frac{1}{2}\left(\frac{J}{n}\right)^2 \sum_{\alpha}(\sigma^i\sigma^j)_{\alpha\alpha} S_i S_j =$$

$$= \frac{1}{2}\left(\frac{J}{n}\right)^2 \sum_{\alpha} \left(\delta_{ij} + i\epsilon_{ijk}\sigma^k\right)_{\alpha\alpha} S_i S_j =$$

$$= \left(\frac{J}{n}\right)^2 \vec{S}^2 = \underbrace{\left(\frac{J}{n}\right)^2 S(S+1)}$$

Orders of magnitude:

Potential scattering $V(r) \sim \epsilon_F$

Spin-dependent scattering $J < V$ or $J \ll V$.

Beyond Born approximation

Perturbation theory.

1) Transitions $\vec{k}\alpha \to \vec{k}_1\alpha_1$ (intermediate) $\to \vec{k}'\alpha'$ (final)

$$t^{(a)}_{\alpha'\alpha} = \left(\frac{J}{n}\right)^2 \sum_{\alpha_1} \int \frac{d^3k_1}{(2\pi)^3} \frac{(\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha_1}(\vec{\sigma}\cdot\vec{S})_{\alpha_1\alpha}}{\varepsilon(k) - \varepsilon(k_1)} (1 - f_{k_1})$$

where $\varepsilon(k) = \frac{\hbar^2 k^2}{2m}$

2) Transitions $\vec{k}_1\alpha_1 \to \vec{k}'\alpha'$ and then $\vec{k}\alpha \to \vec{k}_1\alpha_1$

$$t^{(b)}_{\alpha'\alpha} = -\left(\frac{J}{n}\right)^2 \sum_{\alpha_1} \int \frac{d^3k_1}{(2\pi)^3} \frac{(\vec{\sigma}\cdot\vec{S})_{\alpha_1\alpha}(\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha_1}}{\varepsilon(k_1) - \varepsilon(k')} f_{k_1}$$

$$\sum_{\alpha_1} (\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha_1}(\vec{\sigma}\cdot\vec{S})_{\alpha_1\alpha} = (\sigma^i\sigma^j)_{\alpha'\alpha} S_i S_j = \left(\delta_{ij} + i\epsilon_{ijk}\sigma^k\right)_{\alpha'\alpha} S_i S_j =$$

$$= \underbrace{\delta_{\alpha'\alpha} S(S+1) + (\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha}}$$

$$\sum_{\alpha_1} (\vec{\sigma}\cdot\vec{S})_{\alpha_1\alpha} (\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha_1} = (\sigma^j\sigma^i)_{\alpha'\alpha} S_i S_j =$$

$$= (\delta_{ij} + i\epsilon_{jik}\sigma^k)_{\alpha'\alpha} S_i S_j = \underset{\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim}{\delta_{\alpha'\alpha} S(S+1) - (\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha}}$$

Elastic scattering : $\varepsilon(k) = \varepsilon(k')$

$$t^{(2)}_{\alpha'\alpha} = t^{(a)}_{\alpha'\alpha} + t^{(b)}_{\alpha'\alpha} =$$

$$= \left(\frac{J}{n}\right)^2 \sum_{\alpha_1} \int \frac{d^3k_1}{(2\pi)^3} \frac{(\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha_1}(\vec{\sigma}\cdot\vec{S})_{\alpha_1\alpha}(1-f_{k_1}) + (\vec{\sigma}\cdot\vec{S})_{\alpha_1\alpha}(\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha_1} f_{k_1}}{\varepsilon(k) - \varepsilon(k_1)} =$$

$$= \left(\frac{J}{n}\right)^2 \int \frac{d^3k_1}{(2\pi)^3} \left[\frac{\delta_{\alpha'\alpha} S(S+1)}{\varepsilon(k)-\varepsilon(k_1)} + \frac{2f_{k_1}-1}{\varepsilon(k)-\varepsilon(k_1)} (\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha} \right] =$$

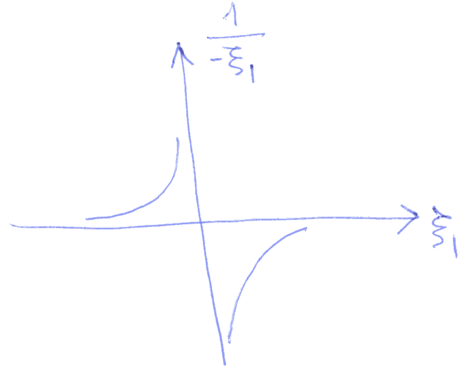
$$\simeq \frac{1}{2}\left(\frac{J}{n}\right)^2 \int_{-\mu}^{\mu} \nu(\xi_1)\, d\xi_1 \left[\frac{\delta_{\alpha'\alpha} S(S+1)}{\xi - \xi_1} + \frac{2f(\xi_1)-1}{\xi-\xi_1} (\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha} \right]$$

where $\xi = \varepsilon(k) - \mu$

$\xi_1 = \varepsilon(k_1) - \mu$

$$f(\xi) = \frac{1}{e^{\xi/T}+1} \Rightarrow 2f(\xi) - 1 = -\tanh\frac{\xi}{2T}$$

$$I_1 = \int_{-\mu}^{\mu} \frac{\nu(\xi_1)\, d\xi_1}{\xi - \xi_1} \sim \frac{\xi}{\mu}$$



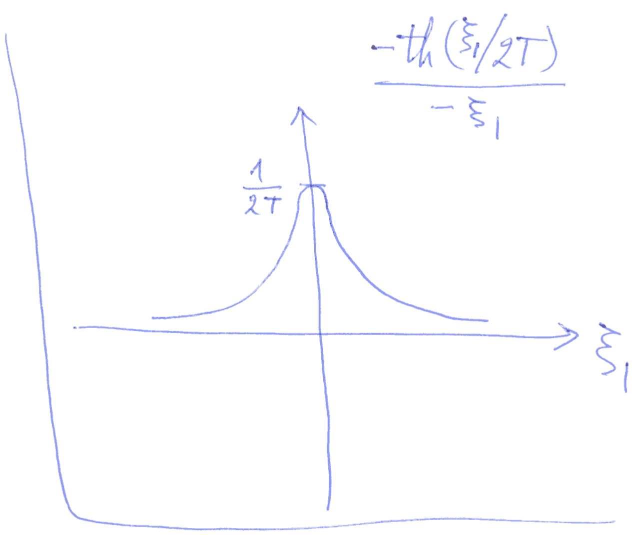
$\underline{\underline{\xi = 0}}$

$\nu(\xi \simeq 0) = \nu_F$

$$I_2 = \int_{-\mu}^{\mu} \frac{2f(\xi_1)-1}{\xi-\xi_1}\,\nu(\xi_1)\,d\xi_1 =$$

$$= \frac{1}{2}\int_{-\mu}^{\mu} \nu\, d\xi_1 \left[2f(\xi_1)-1\right] \times$$

$$\times\left(\underbrace{\frac{1}{\xi-\xi_1} - \frac{1}{\xi+\xi_1}}_{\text{antisym.}} + \underbrace{\frac{1}{\xi-\xi_1} + \frac{1}{\xi+\xi_1}}_{\text{sym.}}\right) =$$



$$= \int_0^{\mu} \nu\, d\xi_1 \frac{2\xi_1}{\xi^2-\xi_1^2}\left[2f(\xi_1)-1\right] \simeq 2\int_0^{1/2T} \frac{d\xi_1}{-\xi_1}\left(-\frac{\xi_1}{2T}\right)\nu(\xi_1) +$$

$$+2\int_{1/2T}^{\mu} \frac{\nu(\xi_1)\,d\xi_1}{\xi_1} \simeq 2\nu_F \ln\frac{\mu}{T}$$

$\xi = 0$

$$t_{\alpha'\alpha} = -\frac{J}{n}(\vec{\sigma}\cdot\vec{S})_{\alpha'\alpha}\left[1-\frac{J\nu_F}{n}\ln\frac{\mu}{\{|\xi|,T\}}\right]$$

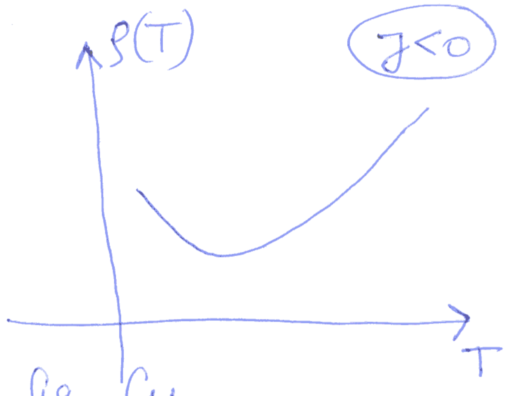
$\Leftarrow \xi \neq 0$

$|\xi| \ll \mu$

next-to-Born approximation
(2nd order of perturbation theory)

For conductivity: probability of scattering $W_{\alpha'\alpha} = |t_{\alpha'\alpha}|^2$

$$\Rightarrow \boxed{\rho = \rho_0 + \rho_1\left[1-\frac{2J\nu_F}{n}\ln\frac{\mu}{T}\right]}$$



Pure Au, Ag, Cu

J. Kondo (1964)

"Improved" perturbation theory:

Parquet diagrams, renormalization-group approximation

$$\boxed{t = -\frac{J}{h}\,\frac{\vec{\sigma}\cdot\vec{S}}{1+\frac{J}{h}\nu_F \ln\frac{\mu}{\{|\xi|,T\}}}}$$

A. Abrikosov (1965)

If $J<0$, there is a divergence in scattering amplitude

$$1-\frac{|J|\,\nu_F}{h}\ln\frac{\mu}{T}=0 \qquad \xi=0$$

$$\boxed{T_K \simeq \mu \exp\left(-\frac{h}{|J|\nu_F}\right)}$$ Kondo temperature

For $T \lesssim T_K$ perturbation theory does not work

Low-temperature limit: P. Nozières (1974)

<u>Other approaches:</u>

Numerical: K. Wilson (1979)

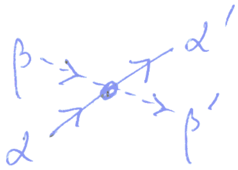
Exact solution: P. Wiegmann (1980)
N. Andrei (1980)

Diagrams in Kondo problem

A. Abrikosov (1965)

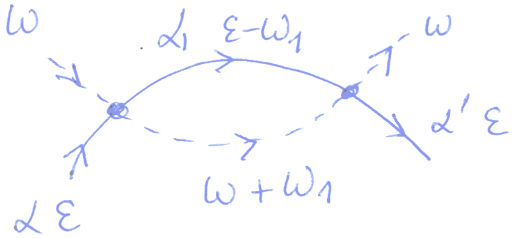
$\alpha \longrightarrow \alpha'$ $\qquad \dfrac{\delta_{\alpha\alpha'}}{\varepsilon - \varepsilon(k) + i\delta\, \mathrm{sign}\,(\varepsilon - \mu)}$ Green function of electrons

$\beta \longrightarrow \beta'$ $\qquad \dfrac{\delta_{\beta\beta'}}{\varepsilon - \varepsilon_0 + i\delta\, \mathrm{sign}\,(\varepsilon - \mu)}$ Green function of localized spin

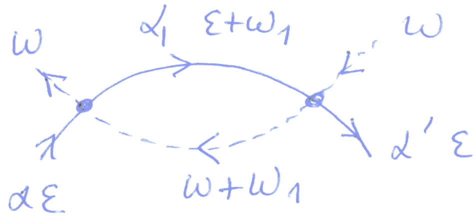


$-\dfrac{J}{n}\, \sigma^i_{\alpha'\alpha}\, S^i_{\beta'\beta}$ vertex

Vertex corrections (beyond Born appr.)



(a)



(b)

$\omega = \varepsilon_0$

$\varepsilon_0 > 0$

$$t^{(a)} = -i\left(\frac{J}{n}\right)^2 \int \frac{d\omega_1}{2\pi}\, \frac{d^3k_1}{(2\pi)^3} (\vec{\sigma}, \vec{S})^2\, \frac{1}{\varepsilon - \omega_1 - \varepsilon(k) + i\delta\, \mathrm{sign}\,(\varepsilon - \omega_1 - \mu)} \times$$

$$\times \frac{1}{\omega + \omega_1 - \varepsilon_0 + i\delta}$$

$$t^{(b)} = -i\left(\frac{J}{n}\right)^2 \int \frac{d\omega_1}{2\pi}\, \frac{d^3k_1}{2\pi}\, \sigma^i \sigma^j S^j S^i\, \frac{1}{\varepsilon + \omega_1 - \varepsilon(k) + i\delta\, \mathrm{sign}\,(\varepsilon + \omega_1 - \mu)} \times$$

$$\times \frac{1}{\omega + \omega_1 - \varepsilon_0 + i\delta}$$

$$t^{(a)} = \left(\frac{J}{h}\right)^2 \nu_F \left[S(S+1) - \vec{\sigma}\cdot\vec{S}\right] \ln \frac{\epsilon_F}{|\xi|}$$

$\xi = \varepsilon - \mu$

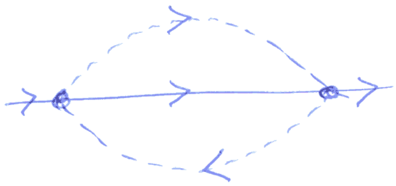
$$t^{(b)} = - \left(\frac{J}{h}\right)^2 \nu_F \left[S(S+1) + \vec{\sigma}\cdot\vec{S}\right] \ln \frac{\epsilon_F}{|\xi|}$$

$\Rightarrow$ Renormalized vertex:

$$\boxed{t = \frac{\frac{J}{h}\,\vec{\sigma}\cdot\vec{S}}{1 + \frac{J\nu_F}{h} \ln \frac{\epsilon_F}{|\xi|}}}$$

<u>Self-energy correction</u>

$$\Sigma(\varepsilon) = - i \,\text{sign}\, \varepsilon \, N_i \nu_F \, |t(\varepsilon)|^2$$



Abrikosov-Suhl resonance

Spin-orbit interaction

Relativistic term in the Hamiltonian:

$$\mathcal{H}_{so} = \frac{\hbar^2}{2m^2c^2}\,\vec{\sigma}\cdot\left[\hat{\vec{K}}\times\nabla V\right]$$

$$\vec{H} = \frac{1}{c}\left[\vec{v}\times\vec{E}\right]$$

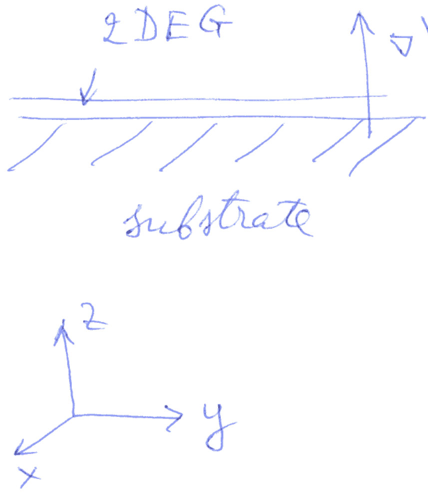
Potential $V(\vec{r})$ from

- crystal lattice
- impurities
- interfaces

Example: Electrons near the interface

$$\mathcal{H}_{so} = \frac{\hbar^2}{2m^2c^2}\,\frac{dV}{dz}\left(\vec{\sigma}\times\vec{K}\right)_z \to$$

$$\to \underbrace{\alpha_{so}\left(\sigma_y K_x - \sigma_x K_y\right)}_{\text{Rashba SO interaction}}$$



Spin relaxation: $t_{\uparrow\downarrow}$ – scattering with spin-flip.

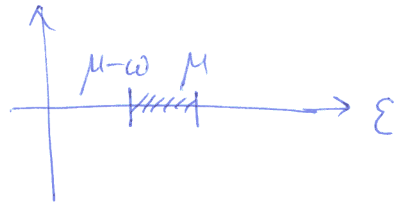
Conductivity

$$\sigma_0 = \frac{2e^2}{3\omega} \int \frac{d^3k}{(2\pi)^3} \frac{d\varepsilon}{2\pi} v^2 \, G(\vec{k}, \varepsilon+\omega) \, G(\vec{k}, \varepsilon)$$

Limit of $\omega \to 0$

$$\int \frac{d\varepsilon}{2\pi} \frac{1}{\varepsilon+\omega-\varepsilon_k+\frac{i}{2\tau}\,\mathrm{sign}(\varepsilon+\omega-\mu)} \cdot \frac{1}{\varepsilon-\varepsilon_k+\frac{i}{2\tau}\,\mathrm{sign}(\varepsilon-\mu)} \to$$

$$\to \int_{\mu-\omega}^{\mu} \frac{d\varepsilon}{2\pi} \underbrace{\frac{1}{\varepsilon+\omega-\varepsilon_k+\frac{i}{2\tau}}}_{G^R(\varepsilon+\omega)} \cdot \underbrace{\frac{1}{\varepsilon-\varepsilon_k-\frac{i}{2\tau}}}_{G^A(\varepsilon)} \simeq$$



$\mu-\omega < \varepsilon < \mu$

$$\simeq \frac{\omega}{2\pi} G^R(\vec{k},\mu) \, G^A(\vec{k},\mu)$$

$$\sigma_0 = \frac{e^2}{3\pi} \int \frac{d^3k}{2\pi} v^2 \frac{1}{\mu-\varepsilon_k+\frac{i}{2\tau}} \frac{1}{\mu-\varepsilon_k-\frac{i}{2\tau}} =$$

$$= \frac{e^2}{3\pi m} \int \nu(\varepsilon_k)\, d\varepsilon_k \frac{\varepsilon_k}{\left(\varepsilon_k-\mu-\frac{i}{2\tau}\right)\left(\varepsilon_k-\mu+\frac{i}{2\tau}\right)} =$$

$$\boxed{2\int \frac{d^3k}{(2\pi)^3} \to \int \nu \, d\varepsilon_k \qquad \frac{m v^2}{2} = \varepsilon_k}$$

$$= \frac{e^2}{3\cancel{\pi} m} \nu_F \varepsilon_F \frac{2\cancel{\pi}\cancel{i}}{\frac{\cancel{i}}{\tau}} = \frac{2e^2 \nu_F \tau \varepsilon_F}{3m} =$$

$$\sigma_0 = \frac{n e^2 \tau}{m}$$