Correlated Electron Systems

3) Screening and electron-phonon coupling in Metals

Literature
N. W. Ashcroft, D. N. Mermin, *Solid State Physics*
S. J. Blundell, Magnetism in Condensed Matter

Screening in metals

Test charge will cause electrons to redistribute

-> screen potential of test charge

- Different from dielectrics which only change the magnitude of the potential

Screening over finite length scale

- Electrons cannot localize on top of test charge (this would be to high a kinetic energy because of Heisenberg uncertainty principle)

Free electron gas

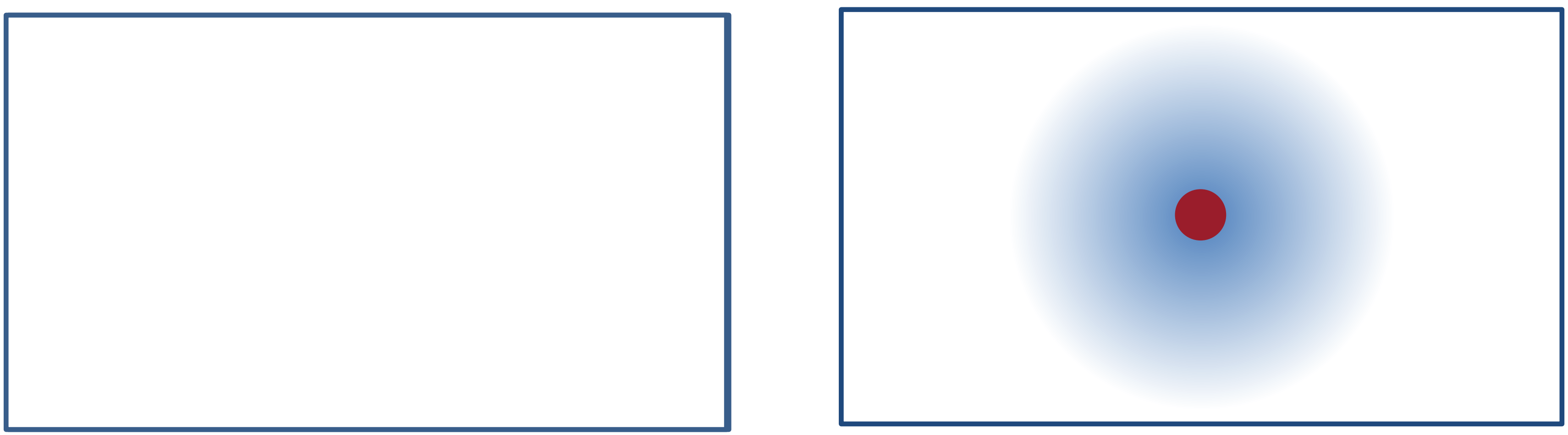
$$\nabla^2 V_0(\boldsymbol{r}) = -\frac{\rho_0(\boldsymbol{r})}{\epsilon(\boldsymbol{r})}$$

Free electron gas „Jellium“

$$\rho_0 = 0$$

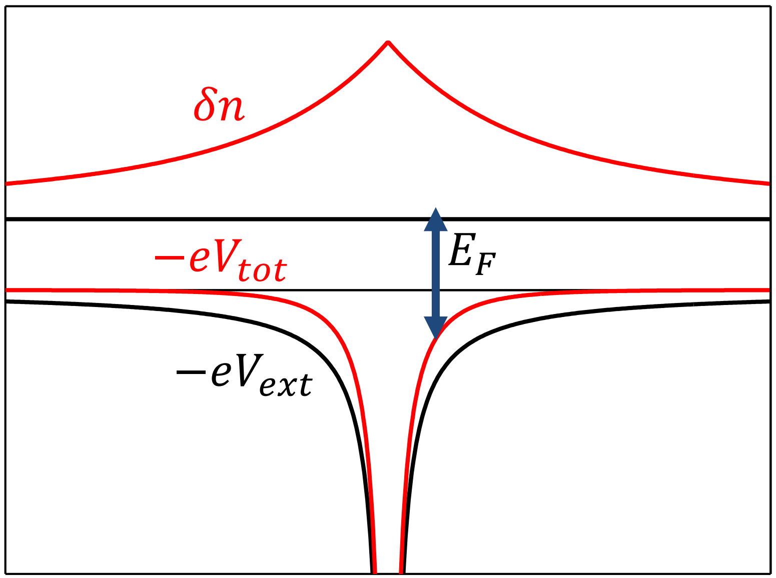
Test charge $\delta\rho(r)$

$$\nabla^2 \delta V(r) = \delta\rho(r)$$



Thomas Fermi - static

Local shift of Fermi energy



Yukawa potential

$$V(r) = \frac{Q}{r}\, e^{-q_{TF}\, r}$$

Slowly varying potetial

- Local shift of levels

$$E(\boldsymbol{k},\boldsymbol{r}) = E_0(\boldsymbol{k}) - eV_{tot}(\boldsymbol{r})$$

- Local change in density

$$\delta n = e\, g(E_F)(\delta V + V_{ext})$$

- Poisson‘s equation

$$\nabla^2 \delta V = e/\epsilon_0\, \delta n$$

- Solved in q-space (FT)

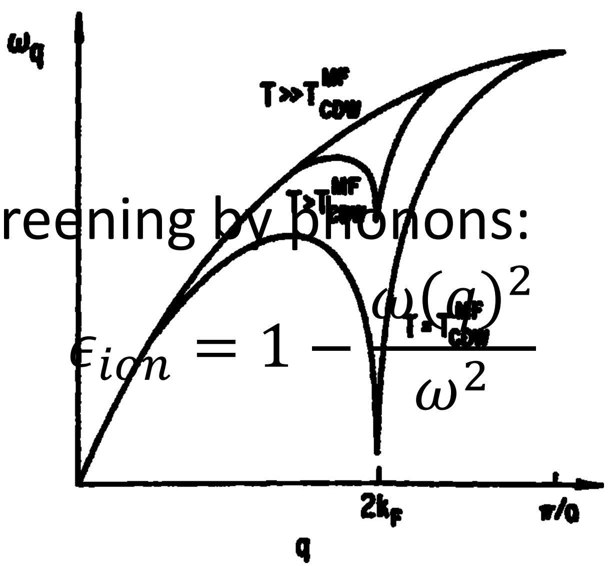
$$V_{tot} = V_{ext}\frac{q^2}{q^2 + q_{TF}^2}$$

$$q_{TF} = \frac{1}{\pi^2}\frac{me^2}{\epsilon_0 \hbar^2} k_F \approx \frac{2.95A^{-1}}{\sqrt{r_s a_0}}$$

Electron-Phonon Interaction

- Phonons as plasma oscillations Ω_p screened by electrons

$$\omega(q)^2 = \frac{\Omega_p^2}{\epsilon_{el}(q)} = \frac{\Omega_p^2}{1 + q_{TF}^2/q^2}$$



- screening by phonons:

$$\epsilon_{ion} = 1 - \frac{\omega(q)^2}{\omega^2}$$

Screening by (slow) ions which are screened themselves

$$V_{tot} = \frac{1}{\epsilon_{ion}}\left(\frac{1}{\epsilon_{el}}\, V_{ext}\right)$$

Combined dielectic

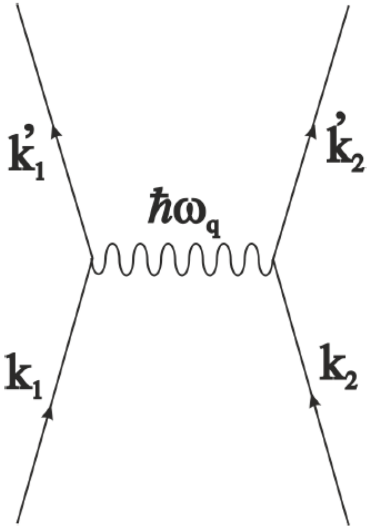
$$\frac{1}{\epsilon} = \frac{1}{\epsilon_{ion}}\frac{1}{\epsilon_{el}} = \left(\frac{\omega^2}{\omega^2 - \omega(q)^2}\right)\left(\frac{q^2}{q^2 + q_{TF}^2}\right) = \frac{q^2}{q^2 + q_{TF}^2}\left(1 - \frac{\omega(q)^2}{\omega^2 - \omega(q)^2}\right)$$

Electron-Phonon Interaction

- Electron-electron interaction

$$v_{kk'} = \frac{4\pi e^2}{q^2 \epsilon} = \frac{4\pi e^2}{q^2 + q_{TF}^2}\left(1 - \frac{\omega(q)^2}{\omega^2 - \omega(q)^2}\right)$$

$$q = k - k' \qquad \omega = \epsilon_k - \epsilon_k'$$



- Change of electronic energy

$$\Delta\epsilon_k = \int \frac{d\boldsymbol{k}'}{(2\pi)^3} v_{kk'}$$

- Phonon coupling constant

$$\lambda = \int \frac{dS'}{8\pi^3 v(k')} \frac{4\pi e^2}{(k - k')^2 + q_{TF}^2}$$

Electron-Phonon Interaction

- Fermi energy not affected
- Changes $\hbar\omega_D$ around ϵ_F
- $\epsilon_k - \epsilon_F = \frac{\epsilon_k^{TF} - \epsilon_F}{1+\lambda}$
- Corrections vanish outside $\hbar\omega_D$

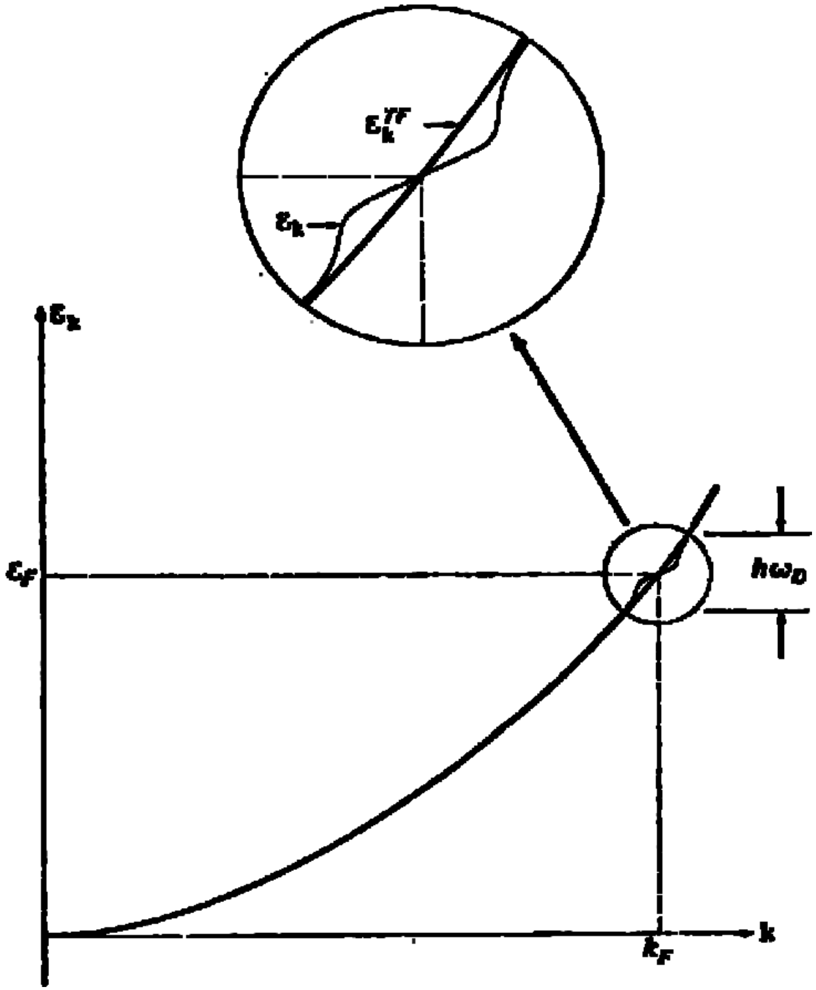
$$\epsilon_k - \epsilon_F = (\epsilon_{TF} - \epsilon_F) * \\ * \left[1 + O\left(\frac{\hbar\omega_D}{\epsilon_k - \epsilon_F}\right)\right]^2$$

Reduced velocity

$$v(k) = \frac{1}{\hbar}\frac{d\epsilon}{dk} = \frac{1}{1+\lambda} v^0(k)$$

Increased DoS

$$g(E_F) = (1+\lambda) g^0(E_F)$$



Electron-Phonon Interaction

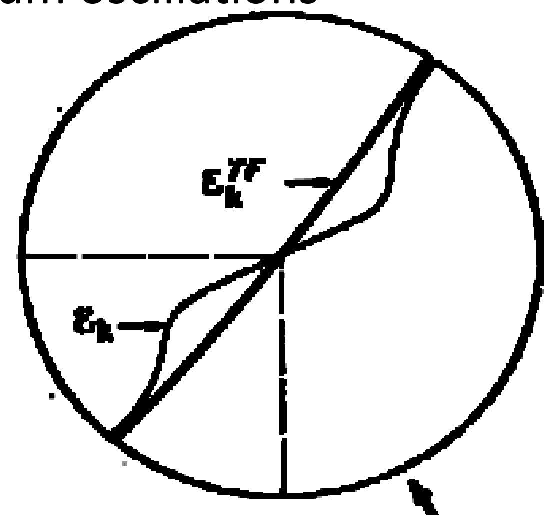
- Dominates deviations from nearly free electron results in most non-magnetic metals

$$m^* = m(1+\lambda)$$

- Relevant for (phonon) superconductivity

$$k_B T_c = 1.14\hbar\omega_D \exp\left(-\frac{1}{\lambda}\right)$$

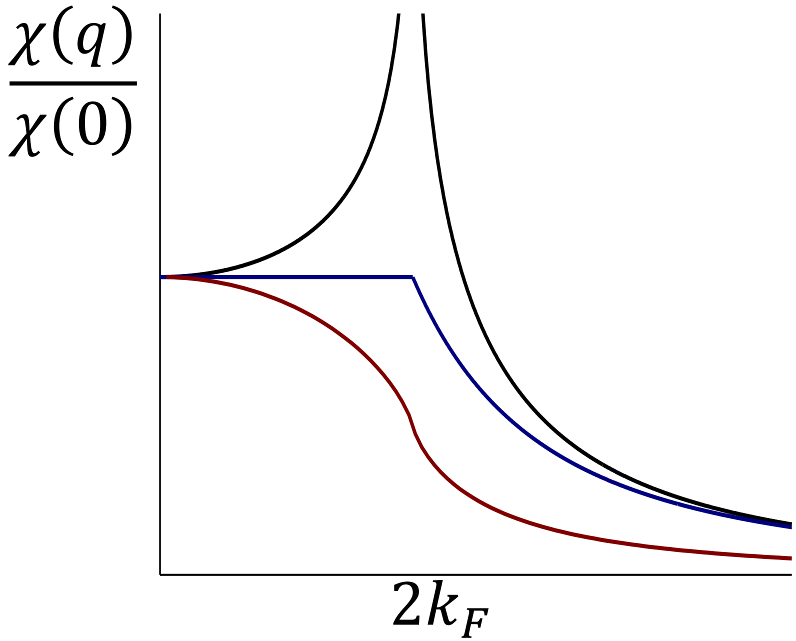
- Experiment:
- Phonon spectrum
- Tunneling spectroscopy
- Effective mass
  - Specfic heat
  - Quantum oscillations
  - ARPES



Dielectric Function $\epsilon(q)$

- Thomas Fermi

$$\epsilon(q) = 1 + \frac{q_{TF}^2}{q^2}$$



Linhard susceptibility

$$\chi(q) = -e^2 \int \frac{dk}{4\pi^3} \frac{f_{\boldsymbol{k}-\boldsymbol{q}} - f_{\boldsymbol{k}+\boldsymbol{q}}}{E(\boldsymbol{k}+\boldsymbol{q}) - E(\boldsymbol{k}-\boldsymbol{q})}$$

1D $\quad -\frac{1}{2\pi q} ln \left|\frac{s+1}{s-1}\right| \qquad s = \frac{q}{2k_F}$

2D $\quad -\frac{1}{2\pi}\left\{1 - \left(1 - \frac{4}{s^2}\right)\theta(s-1)\right\}$

3D $\quad -\frac{k_F}{2\pi^2}\left\{1 - \frac{s}{4}\left(1 - \frac{4}{s^2}\right)\ln\left|\frac{s+1}{s-1}\right|\right\}$

Singularity at $2k_F$

Friedel Oscillations

- Using Linhard susceptibility

$$\delta n(q) = \chi_0(q)V(q)$$

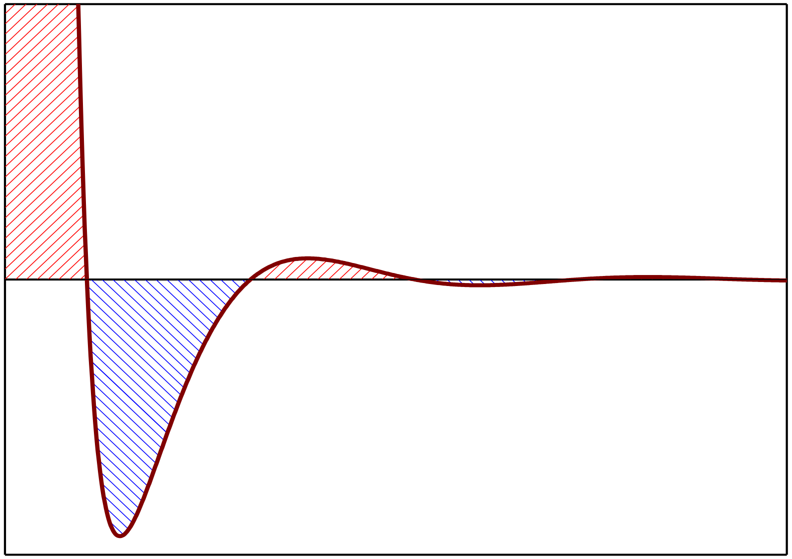
Fourier transform

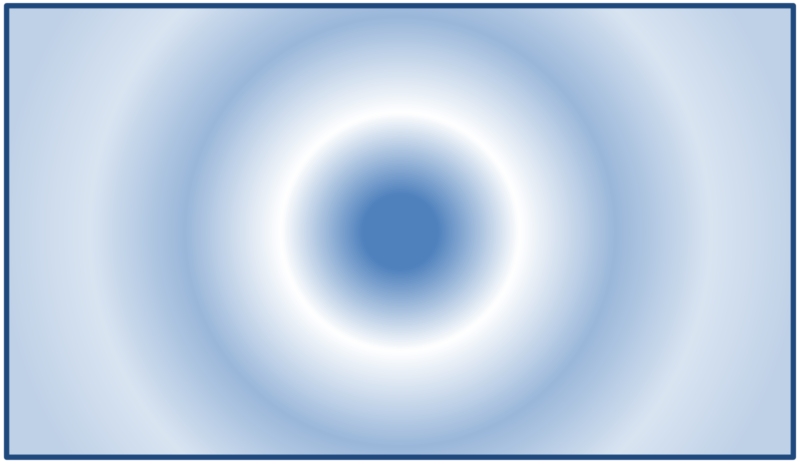
$$\delta n(r) = \int \frac{d^3q}{(2\pi)^3}\delta n(q)e^{i\boldsymbol{q}\boldsymbol{r}}$$

$$= \int_0^\infty \frac{dq}{2\pi^2}\frac{q}{r}\frac{1-\epsilon(q)}{\epsilon(q)}\sin(qr)$$

!Careful: singularity !

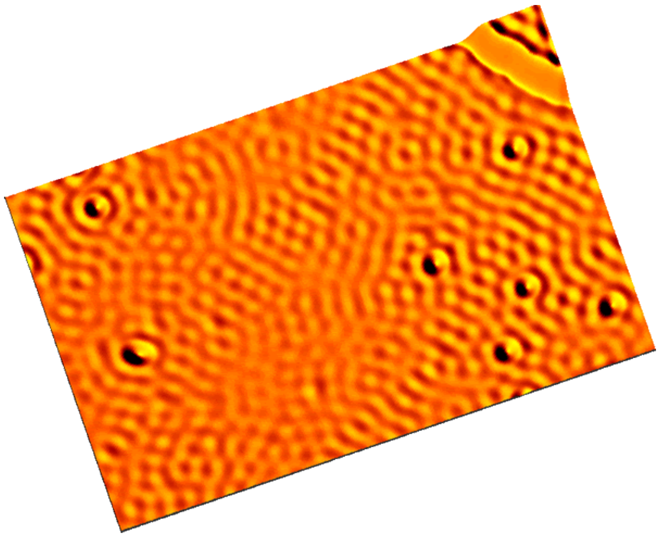
$$\delta n(r) \approx -\frac{\pi A\cos 2k_F r}{r^3}$$



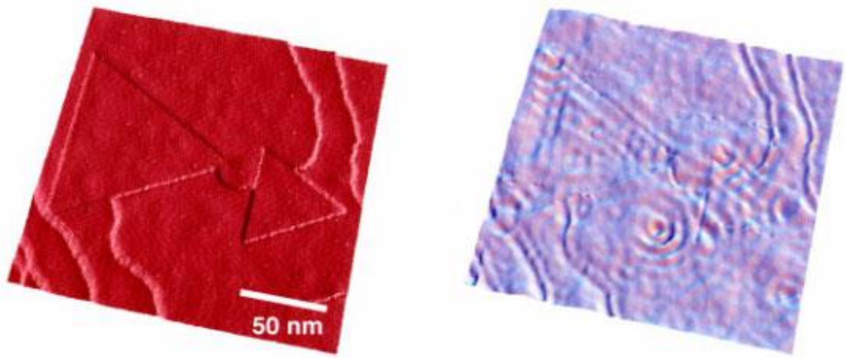


Friedel Oscillations Experiment

- STM – Pd on Au(111)



Suzuki, T., et al. *PRB*, *64*, 081403.



Topography

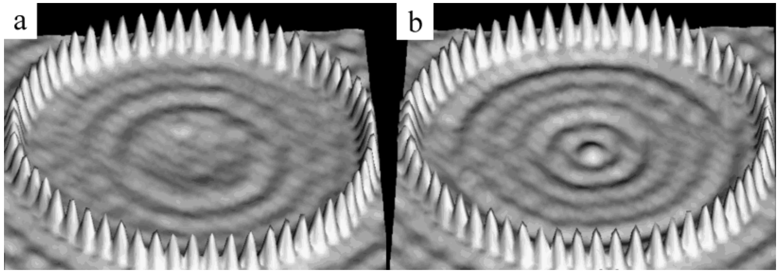
Local Density of States (LDOS)
(Friedel Oscillation)

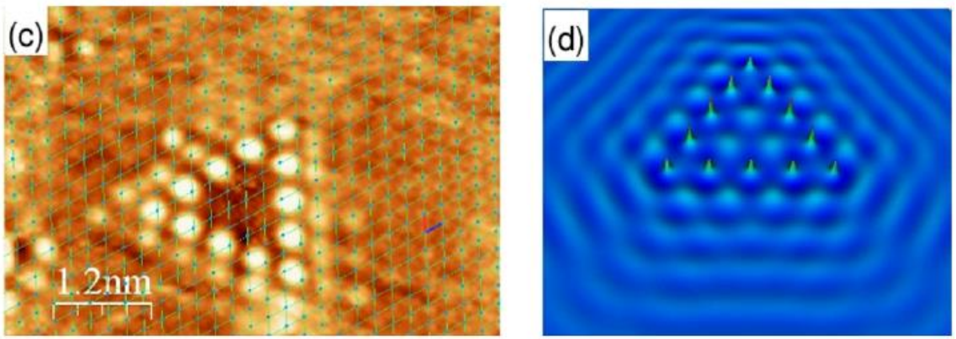
NTT report 2000

Friedel Oscillations Experiment

- Fancy structures
- Corall Fe on Cu(001)

- Self assembly
- Ni on Rh(111)





D. Eigler, IBM Almaden

Manai, G., et al. *PRL 101*(16), 165701.

Quasiparticle Interference

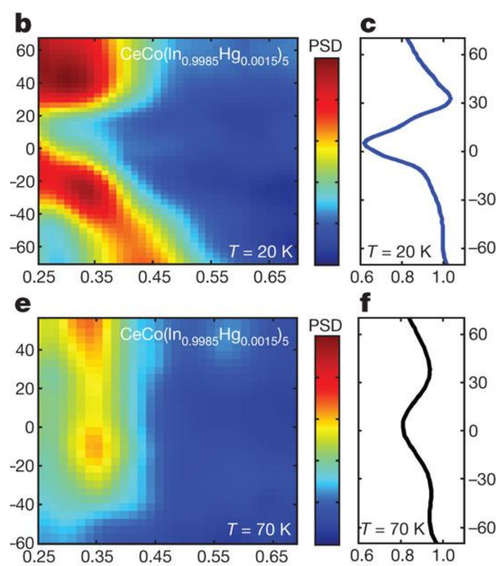
- Friedel oscillations on (surface) impurities
- Measured in LDOS (dI/dV)
- Analysis: Fourier Transform

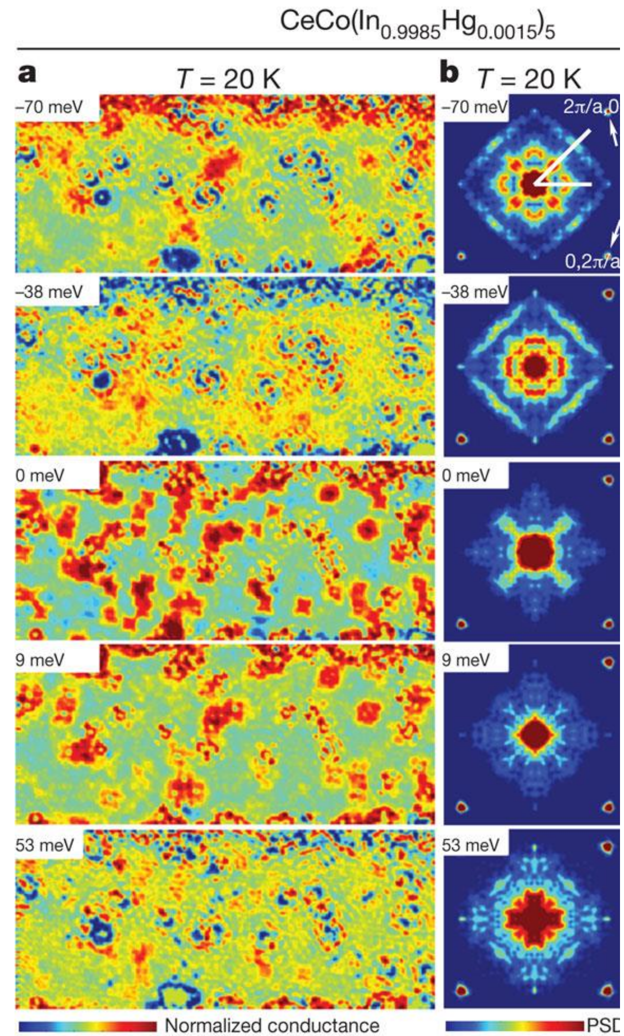
-> mapping the Fermi surfac

- Energy dependency

-> Mapping dispersion relations

Aynajian, P., et al. *Nature*, *486*, 201





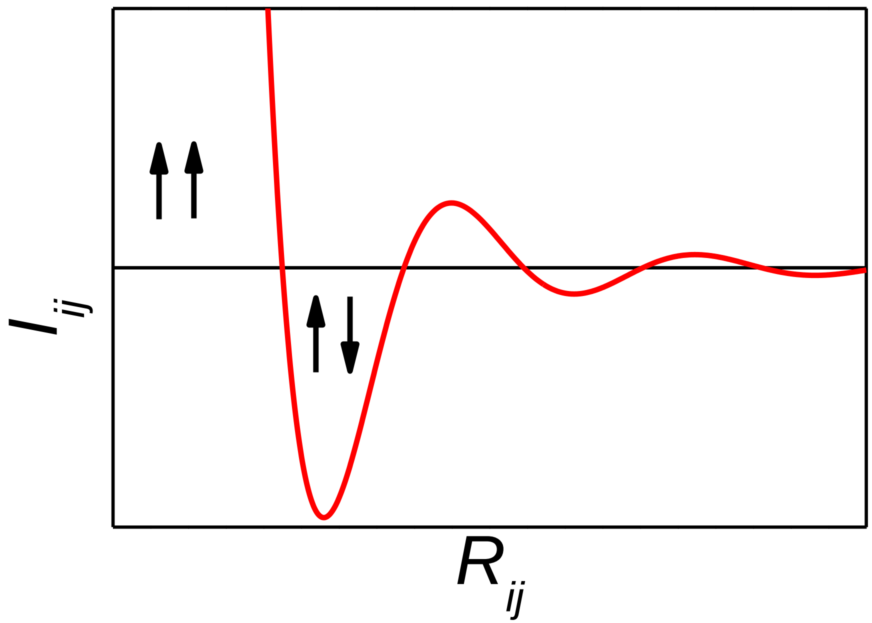
RKKY Interaction

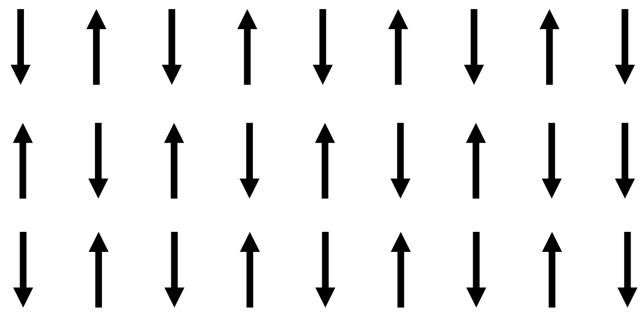
- Interaction J of conduction electrons with local moments (f-elctrons, nuclear moments) couples moments
- Spatially dependent coupling

$$I(R_i - R_j) \propto \frac{J^2}{\epsilon_F} F(2k_F|R_i - R_j|)$$

- oscillating

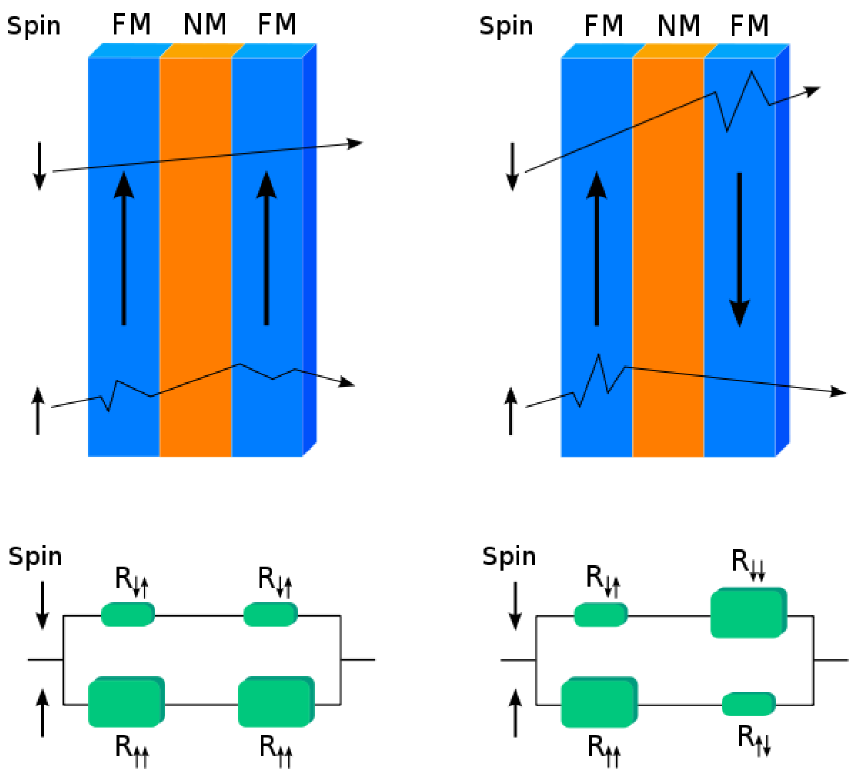
$$F(x) = \frac{x\cos x - \sin x}{x^4}$$

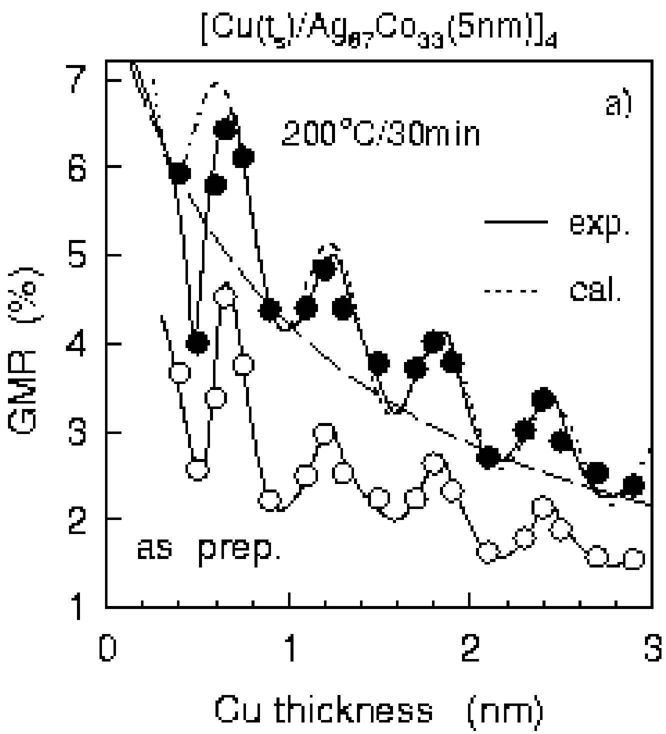




RKKY application

- GMR devices





Europhys. Lett, **37** (3)