Introduction to Many-Body Perturbation Theory: Interacting Fermions

Mikhail Katsnelson

Radboud Universiteit
Nijmegen, Nederland

Crystal: a system of many electrons and nuclei

An explanation should be as simple as possible but not simpler (A. Einstein)

Adiabatic approximation (Born and Oppenheimer)
$m<<M$
Electrons are separated from nuclei (or ionic cores)

Phonons (Born and von Karman, Debye, Peierls)
Atomic subsystem is replaced by almost ideal Bose-gas of phonons

Electrons: Band theory (Bloch, Peierls, A. Wilson)
Supposed to be noninteracting Fermi particles
It cannot be justified easily… but it works (semiconductors, "Fermiology",….) Why???

Fermi liquid theory: one-to-one correspondence between bare particles and quasiparticles (Landau)
Microscopic justification (Migdal and Galitskii, Luttinger and Ward…)
Normally all the many-body effects are just some (smooth) renormalizations of the parameters – except high-frequency properties (plasmons etc.)

"A standard model" of crystals: ideal gas of phonons + Landau Fermi-liquid of electrons

How to calculate excitation spectra of strongly correlated systems?

(Magnetism, superconductivity, charge ordering, Mott insulators, Kondo effect....)

Excitations:

1. Dynamical quasiparticles (from the poles of Green function)
2. Statistical quasiparticles (Landau theory of normal Fermi-liquid)
3. Kohn-Sham quasiparticles (DF theory)

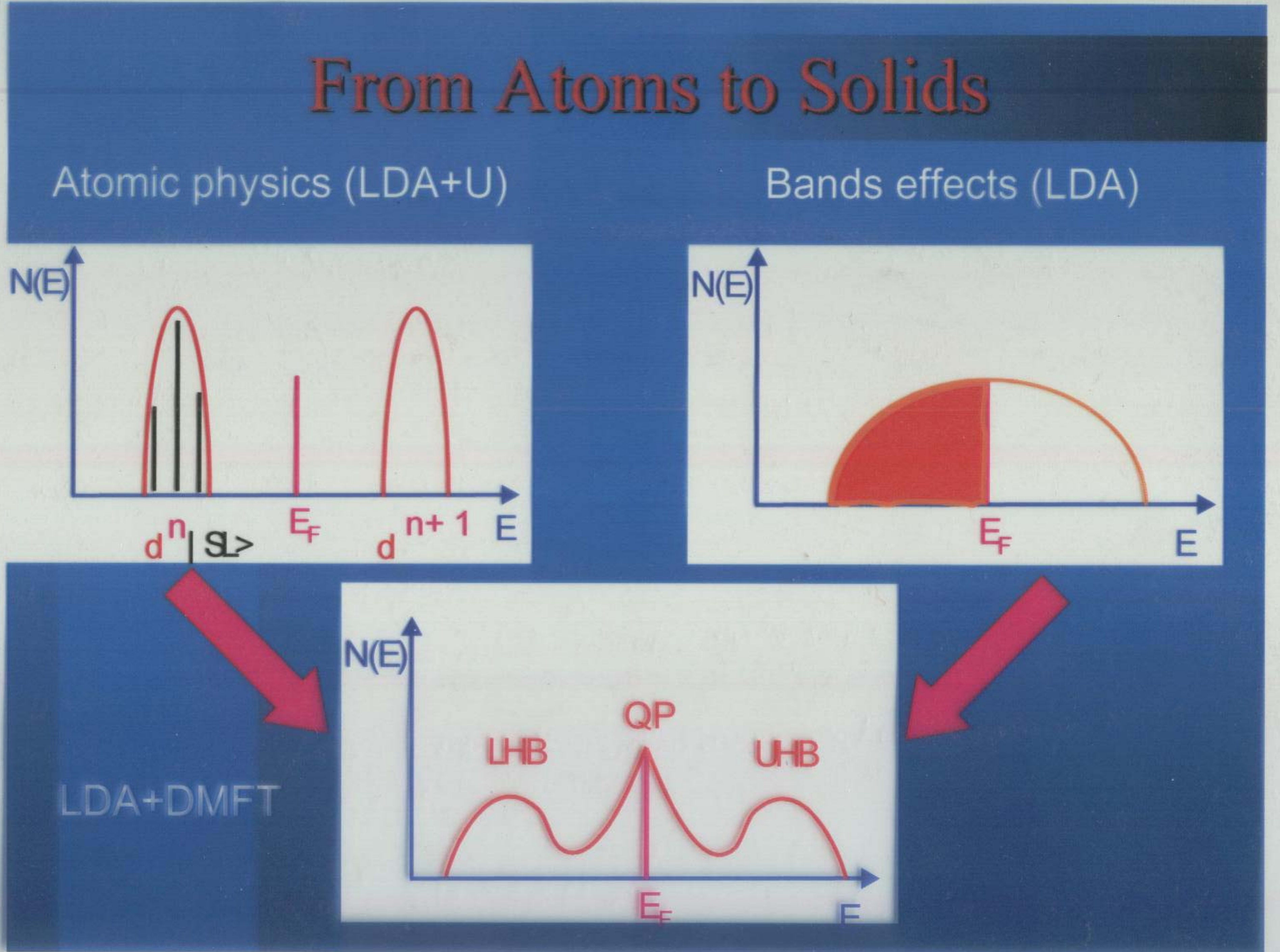
Only last way is convenient for *ab initio* calculations! But: they are only auxilary quantities to find the total energy!

1. Time-dependent DF: calculation of dynamical responce functions

2. GF-functional: to find Green function $G(\mathbf{k}, E)$ based on "traditional" many-particle theory (Gell-Mann – Bruckner - Migdal – Galitskii – Beliaev...) and new development (DMFT, QMC...)

$A(\mathbf{k}, E) = -(1/\pi)\,\mathrm{Im}\,G(\mathbf{k}, E)$

Photoemission experiments


From Atoms to Solids
Atomic physics (LDA+U)
Bands effects (LDA)
N(E)
d^n | SL>
E_F
d^{n+1}
E
N(E)
E_F
E
N(E)
LHB
QP
UHB
E_F
E
LDA+DMFT

Time-dependent DF: *formally* exact approach
In reality: LDA as a starting point + RPA-like approximations

LDA++ : on-site interactions and local correlations:
Σ is only *energy* dependent
Advantages: exact solution of local many-body problem (QMC, ED)

LSDF	LDA++
Density functional	Baym-Kadanoff functional
Density ρ	Green function G
Potential v_{xc}	Self-energy $\Sigma(E)$
$\Omega = \Omega_{sp} - \Omega_{dc}$	$\Omega = \Omega_{sp} - \Omega_{dc}$
$\Omega_{sp} = \sum_{\lambda<\lambda_F} \varepsilon_\lambda$	$\Omega_{sp} = -Tr \ln\left[-G^{-1}\right]$
$\Omega_{dc} = \int dr v_{xc} \rho - E_{xc} + E_{Hart}$	$\Omega_{dc} = Tr \Sigma G - \Phi$
	(Φ is the Luttinger-Ward GF)
Temperature in Fermi functions	Matsubara frequencies: real temperature for collective degrees of freedom

LDA+DMFT

- Tetrahedron BZ-integration and IPT for GF (Anisimov-Poteryaev-Kotliar)
- DMFT cavity scheme for real system (Katsnelson&Lichtenstein)
- Self-consistent charge density and Etot in LDA+DMFT (Savrasov-Kotliar)
- FLEX and multi-orbital QMC schemes (Katsnelson&Lichtenstein)
- Magnetic interactions in DMFT (Katsnelson&Lichtenstein)
- Long-range Coulomb interactions (Chitra-Sun-Kotliar)
- Short-range Spin-Orbital-Charge fluctuations: DCA , Cluster-DMFT, CDMFT (Jarrell, Katsnelson&Lichtenstein, Kotliar et. al.)

LSDA	LDA++
Density functional	Baym-Kadanoff functional
Density $\rho(\mathbf{r})$	Green-Function $G(\mathbf{r},\mathbf{r}',E)$
Potential $V_{xc}(\mathbf{r})$	Self-energy $\Sigma_i(E)$
$E_{tot} = E_{sp} - E_{dc}$	$\Omega = \Omega_{sp} - \Omega_{dc}$
$E_{sp} = \sum_{\lambda<\lambda_F} \varepsilon_\lambda$	$\Omega_{sp} = -Tr \ln[-G^{-1}]$
$E_{dc} = E_H + \int \rho V_{xc} d\mathbf{r} - E_{xc}$	$\Omega_{dc} = Tr \Sigma G - \Phi_{LW}$
Temperature:	Matsubara frequencies: real-T
in the Fermi function	for collective excitations

Hamiltonian:

$$H = \sum_{12} t_{12} c_1^+ c_2 + \frac{1}{2} \sum_{1234} \langle 12|v|34\rangle \cdot$$
$$\cdot c_1^+ c_2^+ c_4 c_3$$

$1 \equiv i_1 \lambda_1 \sigma_1$ site + orbital + spin indices

Green's function:

$$G(\xi, \xi') = -\langle T_\tau c(\xi) c^+(\xi') \rangle$$

$\xi \equiv \vec{r}\,\tau \qquad 0 < \tau \leq \beta = \frac{1}{T}$ is imaginary time

T_τ - time-ordering operator:

$$T_\tau [A(\xi_1) B(\xi_2)] = \begin{cases} A(\xi_1) B(\xi_2), & \tau_1 > \tau_2 \\ -B(\xi_2) A(\xi_1), & \tau_1 < \tau_2 \end{cases}$$

A, B - fermionic operators

Equilibrium case:

$$G(\vec{r}_1\tau_1, \vec{r}_2\tau_2) = G(\vec{r}_1, \vec{r}_2; \tau_1 - \tau_2)$$

$$\hat{G}(\tau) = T \sum_{\omega} \hat{G}(i\omega) e^{-i\omega\tau}$$

$$\hat{G}(i\omega) = \int_0^{\beta} d\tau\, \hat{G}(\tau) e^{i\omega\tau}$$

$$\omega_n = \pi(2n+1)/\beta, \quad n = 0, \pm 1, \ldots$$

Matsubara frequencies

For bosonic operators (e.g., $A = c_1^{+} c_2$)

$\omega_n = 2\pi n/\beta, \quad n = 0, \pm 1 \ldots$ – the only difference!

λ-representation:

$$\hat{\psi}(\vec{r}) = \sum_{\lambda} \varphi_{\lambda}(\vec{r}) \hat{c}_{\lambda}$$

$$G_{\lambda\lambda'}(\tau, \tau') = \int d\vec{r}\, d\vec{r}\,' \varphi_{\lambda}(\vec{r}) \varphi^{*}_{\lambda'}(\vec{r}\,') \cdot$$

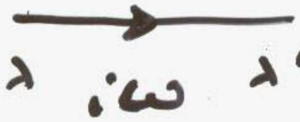
$$\cdot G(\vec{r}\tau, \vec{r}\,'\tau')$$

Graph: $\lambda \xrightarrow[i\omega]{} \lambda' \equiv -G_{\lambda\lambda'}$

Zero-order Green's function

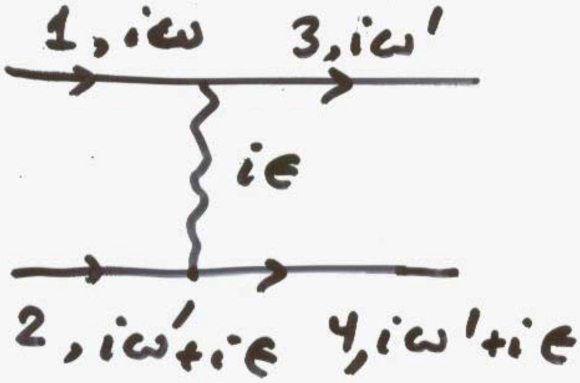
(noninteracting fermions)

$$H_0 = \sum_{12} t_{12}\, c_1^+ c_2 \qquad \hat{G}_0 = \frac{1}{i\omega - \hat{t}}$$



$\equiv -(G_0)_{\lambda\lambda'}$

Interaction line:

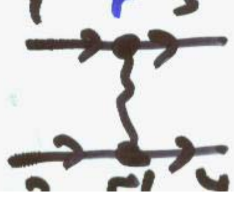


$\equiv -\langle 12 | v | 34 \rangle$

does not depend on energies!

Conservation of energies (Σ energies of →● lines = Σ energies of ●→ lines)

→•→ is local in $\vec{r}$-space:



$$\equiv - \int d\vec{r}\, d\vec{r}\,'\; \psi_1^*(\vec{r})\, \psi_3(\vec{r})\, v(\vec{r}-\vec{r}\,')\, \psi_2^*(\vec{r}\,') \ldots \psi_4(\vec{r}\,')$$

Green's function contains spectral information, e.g. for ARPES; STM...

$$\hat{G}(i\omega) = \int_{-\infty}^{\infty} dx \, \frac{\hat{A}(x)}{i\omega - x}$$

$\hat{A}(x)$: spectral density - supposed to be measurable quantity (with some matrix elements)

$$\hat{G}(i\omega) \to \hat{G}(\omega + i\delta)\big|_{\delta \to +0}$$

$$\hat{A}(x) = -\frac{1}{\pi} \operatorname{Im} \hat{G}(x + i\delta)$$

Problem of analytical continuation!

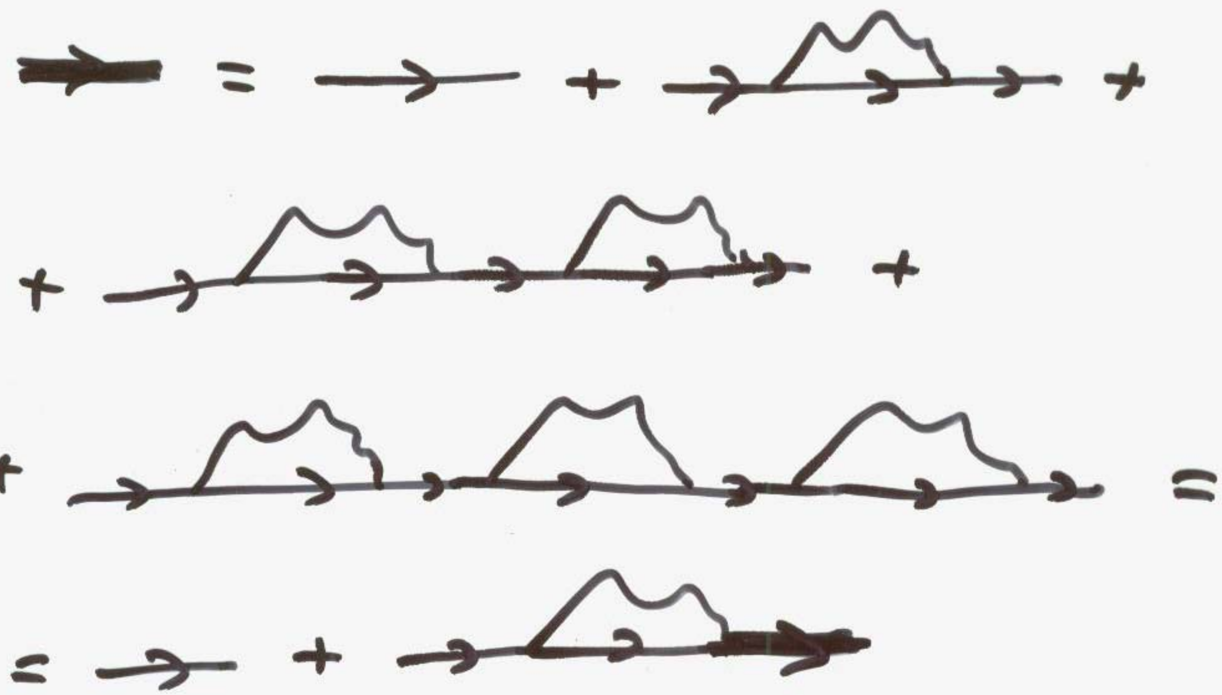
Perturbation theory: just simple replacement of arguments

Numerics, such as QMS: maxent, etc.

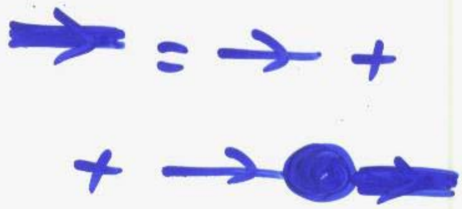
(may be nontrivial!)

To find GF perturbatively:

<u>all</u> connected diagrams + Dyson equation

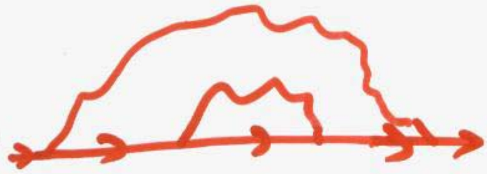
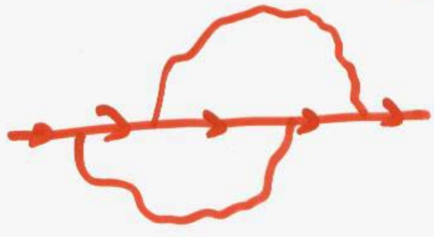


$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{\Sigma} \hat{G}$$



 $= -\Sigma$ sum of all diagrams which cannot be cut by a single line

$\Sigma^{(1)} =$  Hartree +  Fock

$\Sigma^{(2)} =$  + 

etc

Two-particle Green's functions

Optics; magnetic susceptibility; ...

Kubo formula:

External field h

$$\hat{H}' = -\hat{B} \cdot h$$

We need to calculate response $\hat{A}$

$h \to 0$ (linear response):

$$\delta \langle \hat{A} \rangle = \hat{\chi}_{AB} * \hat{h} \qquad \hat{h} \sim e^{-i\omega t};$$

$$\hat{\chi}_{AB}(\omega) = \int_0^\beta d\tau \int_{-\infty}^{\infty} dt \, e^{-i\omega t} \cdot$$

$$\cdot \langle \hat{A}(t - i\tau) \hat{B} \rangle$$

$$\hat{A}(\lambda) = e^{\lambda \hat{H}} \hat{A} e^{-\lambda \hat{H}}$$

Optics: $\hat{A} = \hat{B} = \sum_{12} j_{12} c_1^+ c_2$

$\hat{j}$-current operator

Magnetism: $\hat{A} = \hat{S}^-$; $\hat{B} = \hat{S}^+$

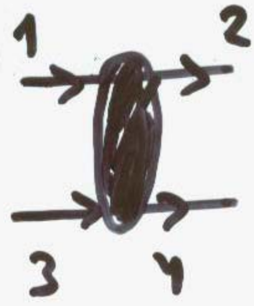
In all cases: $\langle c_1^+ c_2 \, c_3^+ c_4 \rangle$ correlator

Diagram technique: calculate at Matsubara frequences and then

$$\hat{\chi}(i\omega_n = 2\pi i n T) \Rightarrow \hat{\chi}(\omega + i\delta)\big|_{\delta\to+0}$$

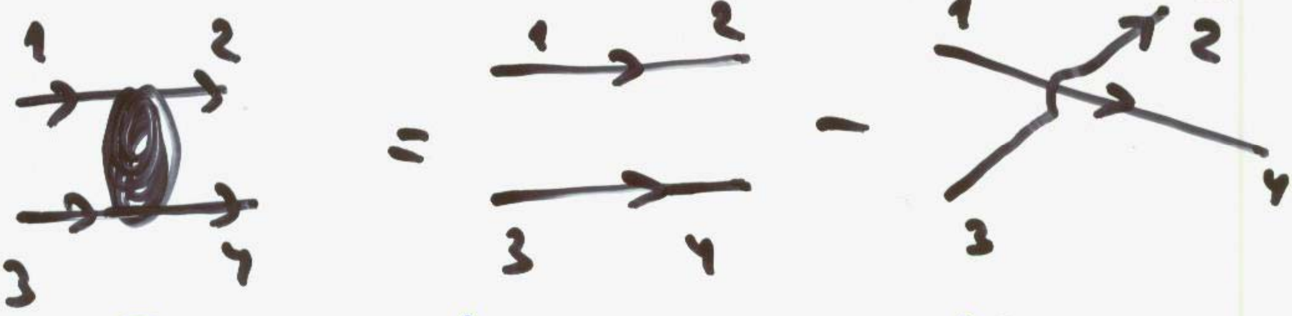
$$G^{II}_{1234} = \langle T_\tau\, c_1^+ c_2 c_3^+ c_4 \rangle$$

$1 \equiv i, \lambda, \sigma, \tau$, etc.



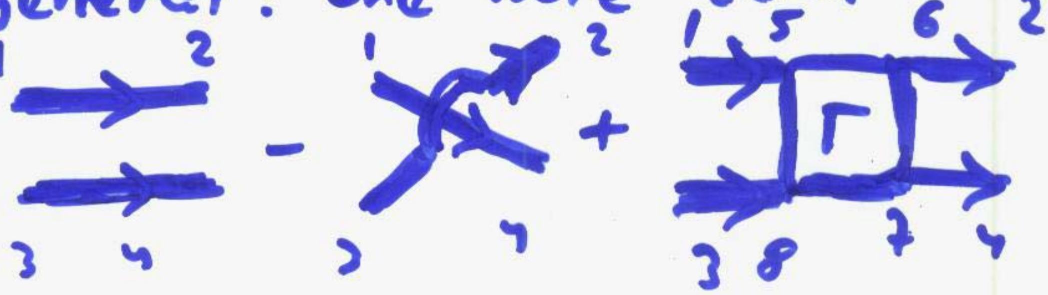
No interaction, Wick theorem:

$$G^{II}_{1234} = G_{12}G_{34} - G_{14}G_{23}$$



In general: one more term

$G^{II}_{1234} =$

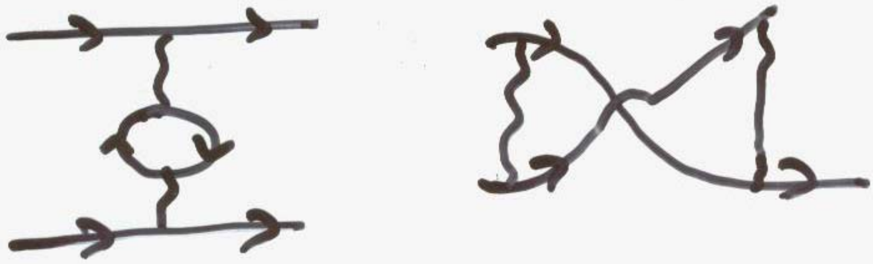


$$G_{12}G_{34} - G_{14}G_{23} + \sum_{5678} G_{15}G_{38}\Gamma_{5678} \times G_{62}G_{74}$$

Γ is called vertex (four-leg verte

Examples:

first order

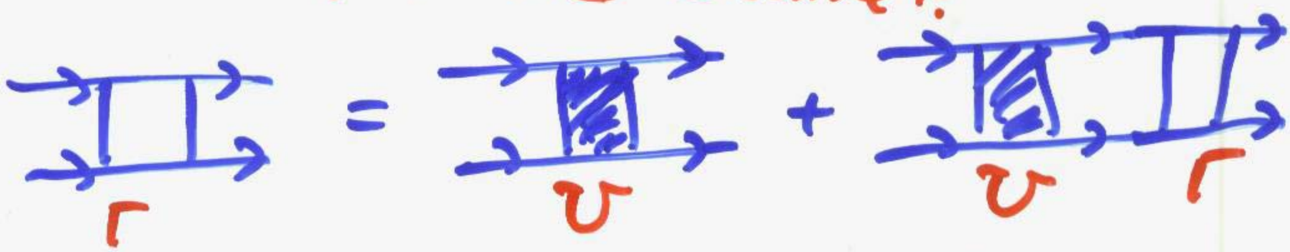


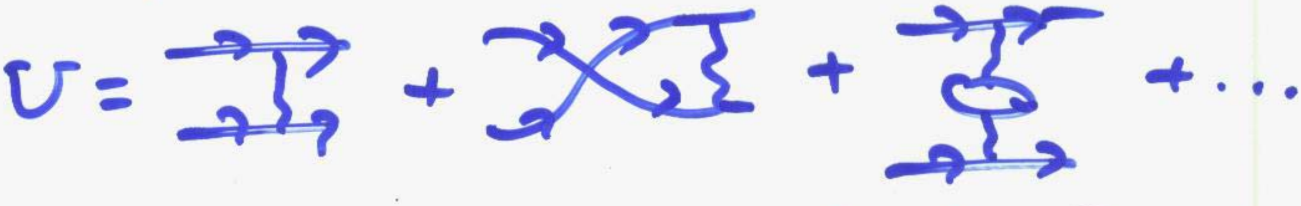
and many others

Analog of Dyson equation:

Bethe-Salpeter equation

Particle-particle channel:



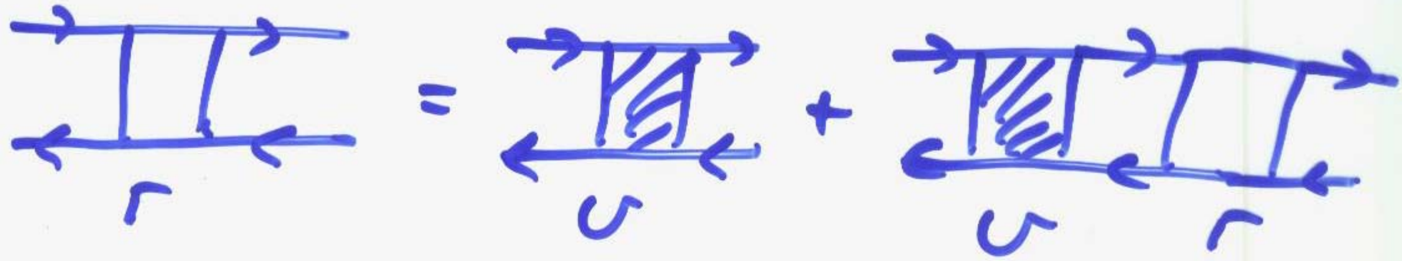


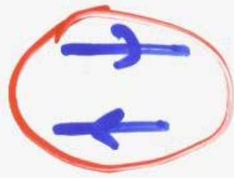
but not  or  ...

$$\hat{\Gamma} = \hat{U} + \hat{U}\hat{G}\hat{G}\hat{\Gamma}$$

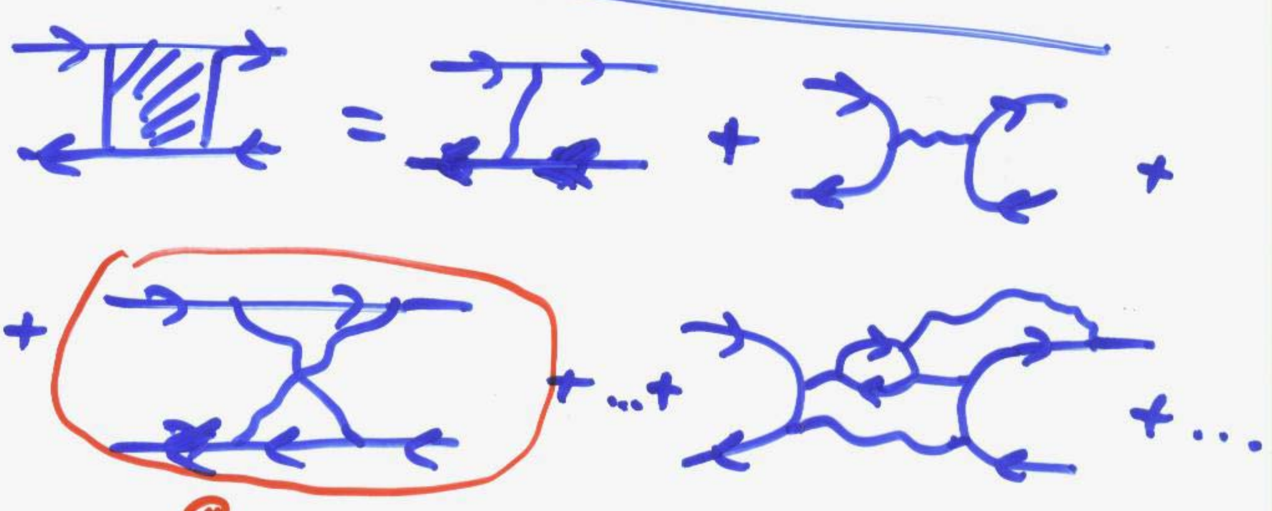
$\hat{U}$ - irreducible vertex (in p-p channel)

Particle-hole channel (more convenient for optics, magnetic susceptibility etc.)



U cannot be cut on 

couple of anti-parallel lines!



irreducible in p-h channel but reducible in p-p channel!!!

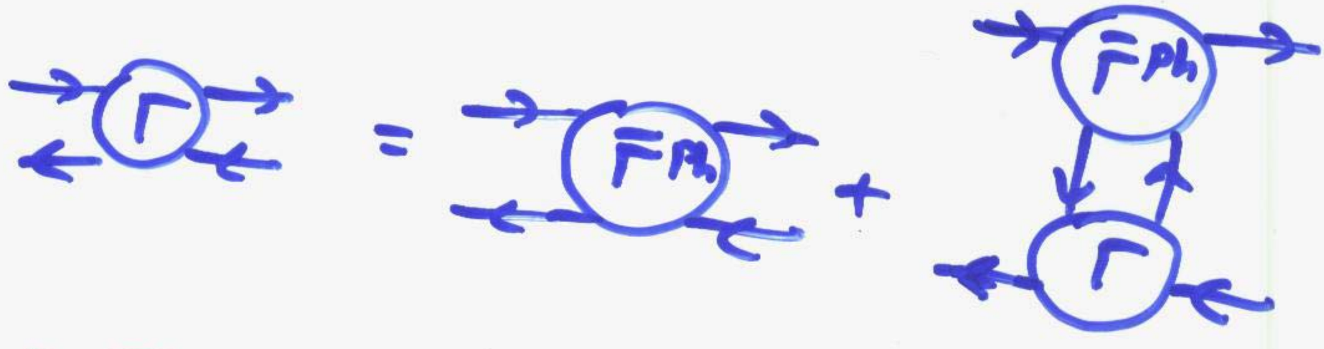
Parquet: irreducible in both channels

$\Gamma(12,34) \equiv -\Gamma_p(14,32)$ total vertex

$\Gamma^{ph}(12,34) = -\bar{\Gamma}^{(ph)}_{42,31}$ irreducible in p-h channel

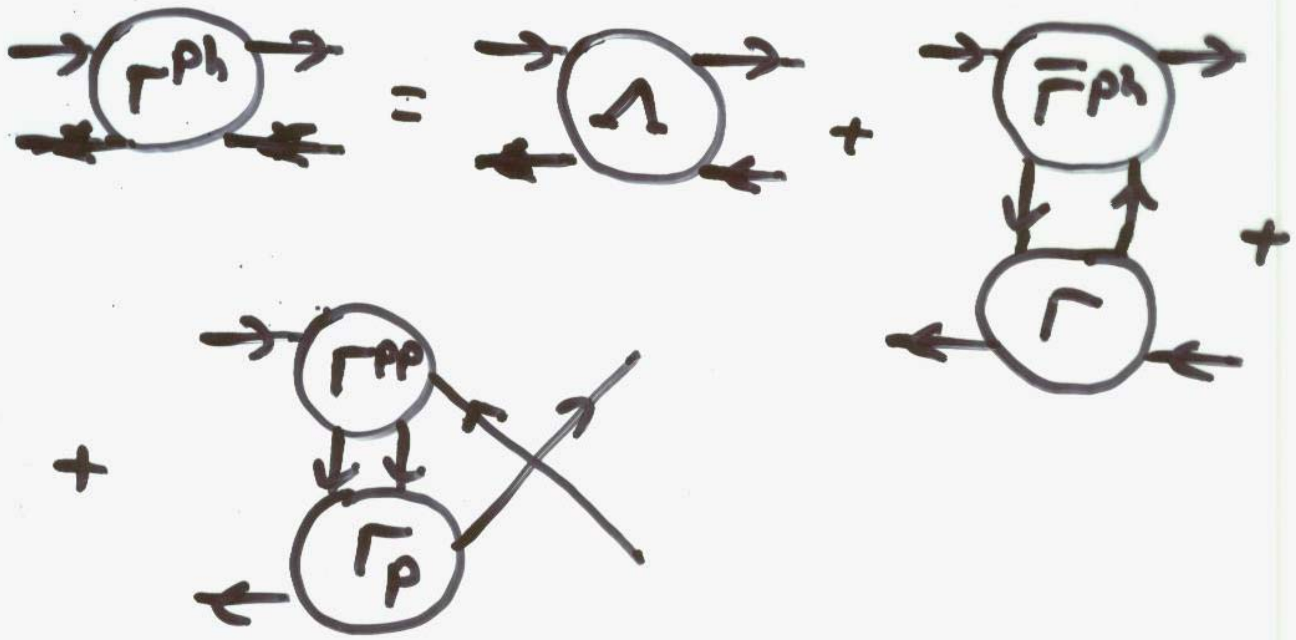
$\Gamma^{pp}(12,34)$ irreducible in p-p channel

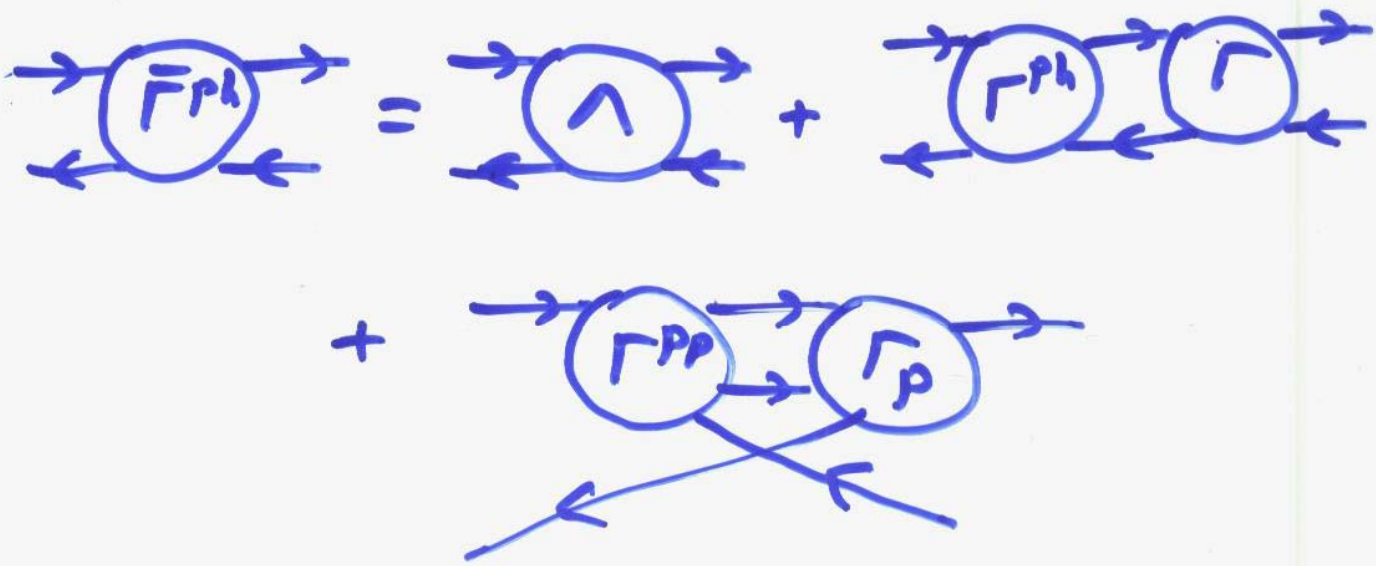
Bethe-Salpeter equations

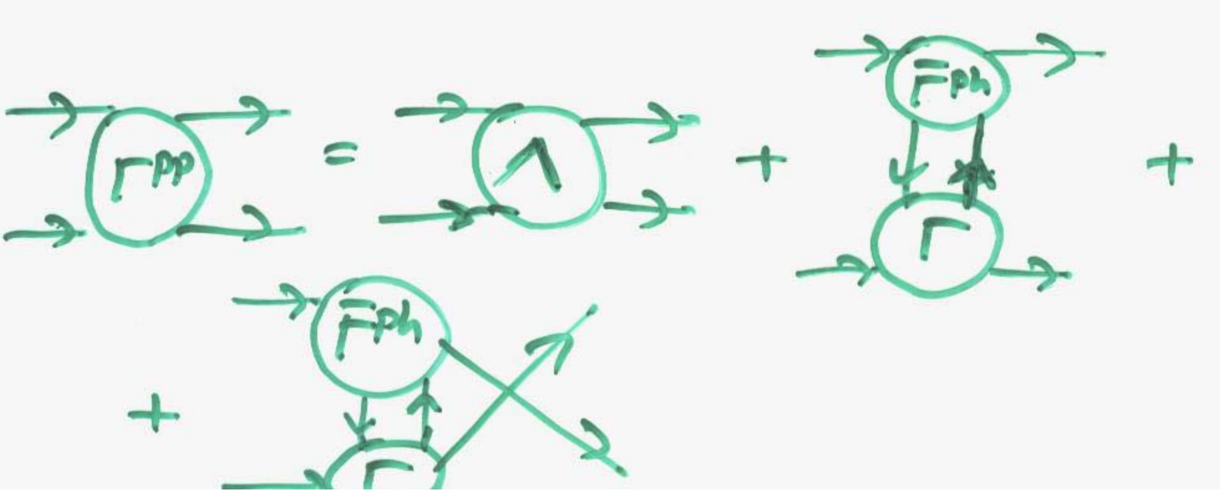


Rigorous: Double irreducible vertex

$$\Lambda(12;34) = -\Lambda(42;31) = -\Lambda_p(14;32)$$



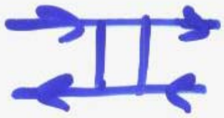




First-order diagrams

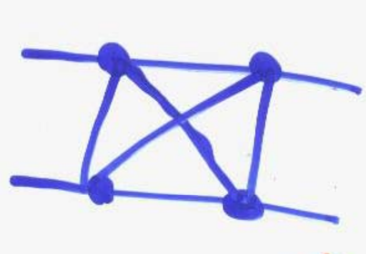
$\Lambda^{(0)} =$ 

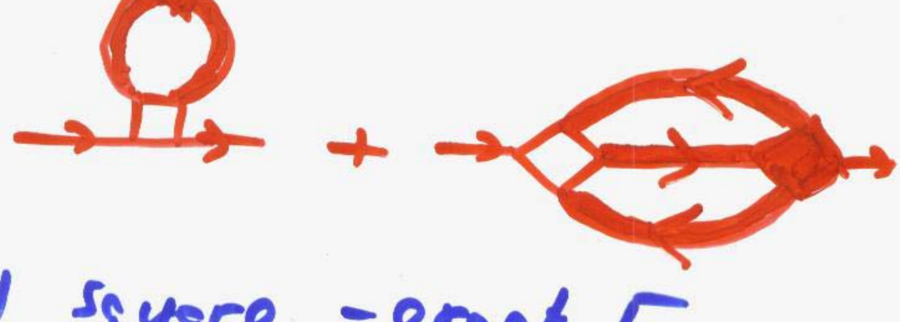
Parquet approximation (V. Sudakov 1956):

$\Lambda = \Lambda^{(0)} \equiv$ 

First neglected diagram:

(contact interaction, $v(\vec{r}-\vec{r}') \sim$
$\sim \delta(\vec{r}-\vec{r}')$, )

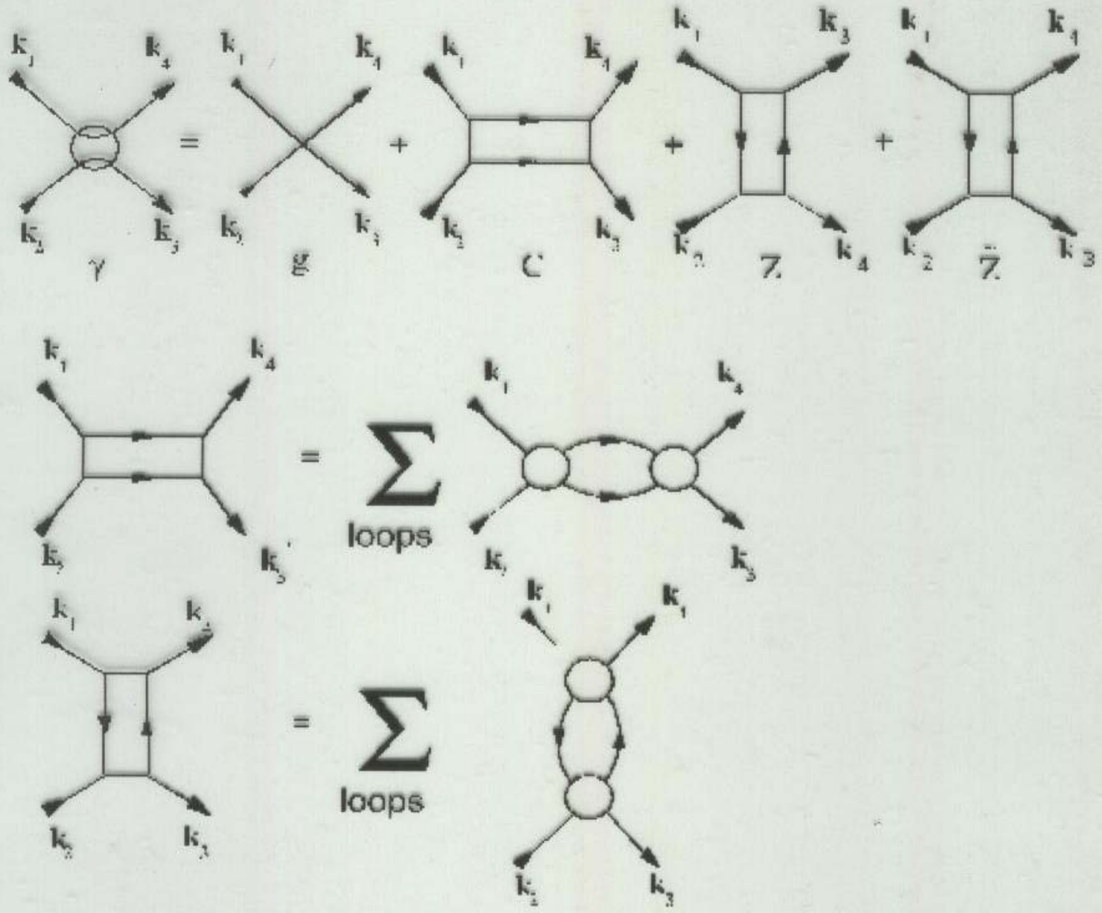
 $\sim v^4$ $\quad \Gamma \Rightarrow \Sigma$:

$\Sigma =$ 

Solid square - exact Γ

Empty square - $\Lambda^{(0)}$ (first order)

Parquet equations



Solution for 2D t-t' Hubbard model

(Irkhin, Katanin, Katsnelson 2001)

PR B <u>64</u>, 165107

Van Hove theorem

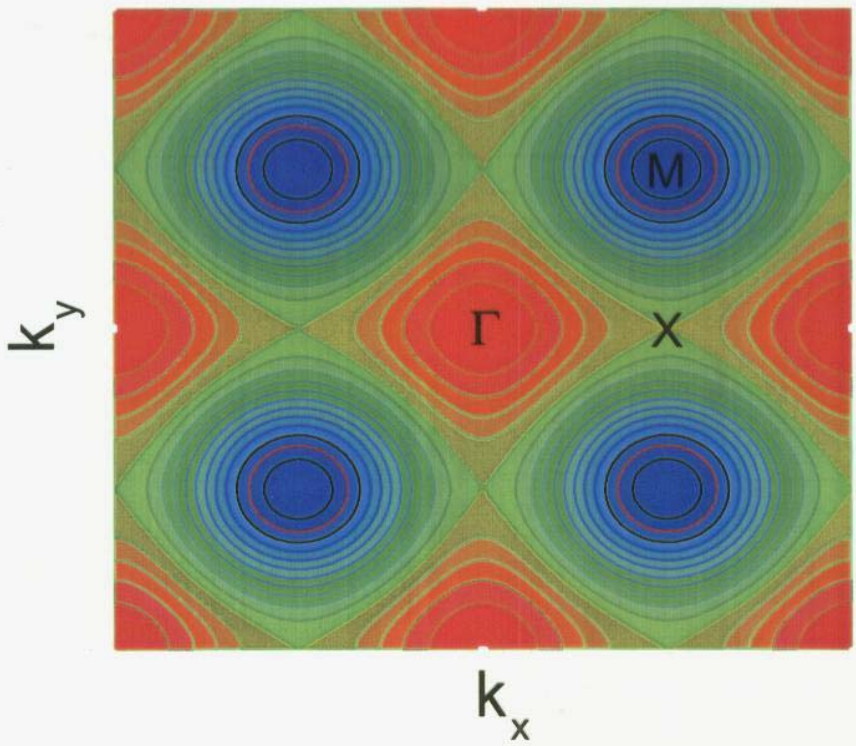
quantum mechanics + translational invariance + topology

$$E(\mathbf{k}) = E(\mathbf{k} + \mathbf{g})$$

any kind of elementary excitations in crystals
(phonons, electrons, magnons, etc.)

$$N(E) = \sum_{\mathbf{k}} \delta(E - E(\mathbf{k}))$$

Density of states:
In 2D and 3D cases there are saddle points where the topology of energy surfaces are changed $N(E)$ is singular in these points

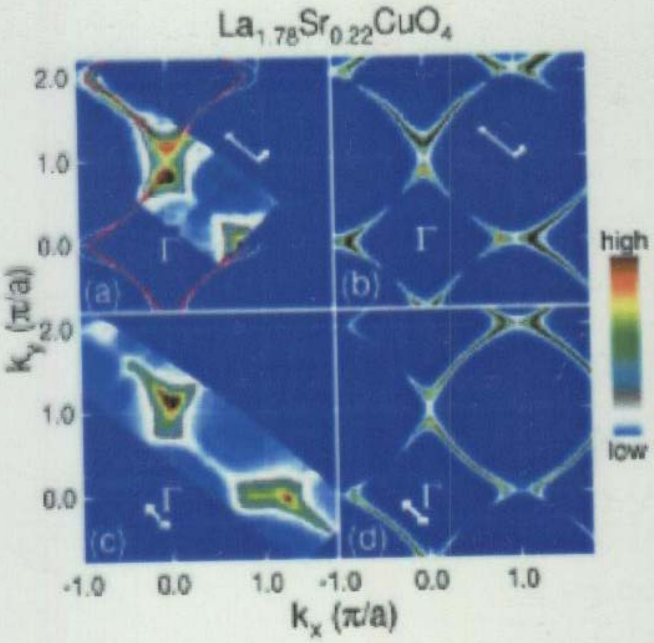


Van Hove singularities in quasi-2D strongly correlated systems and the problem of High-T_c superconductivity

ARPES experiments:

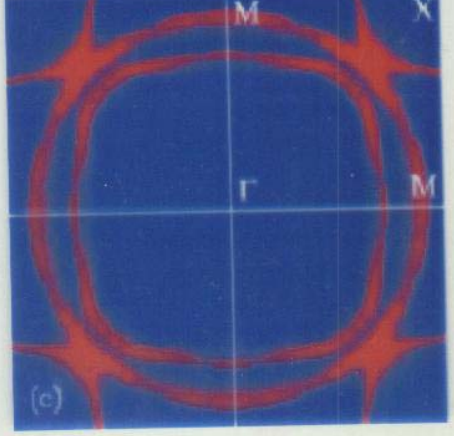
Cuprates: (T. Yoshida et. al. PRB-2001)

$La_{2-x}Sr_xCuO_4$



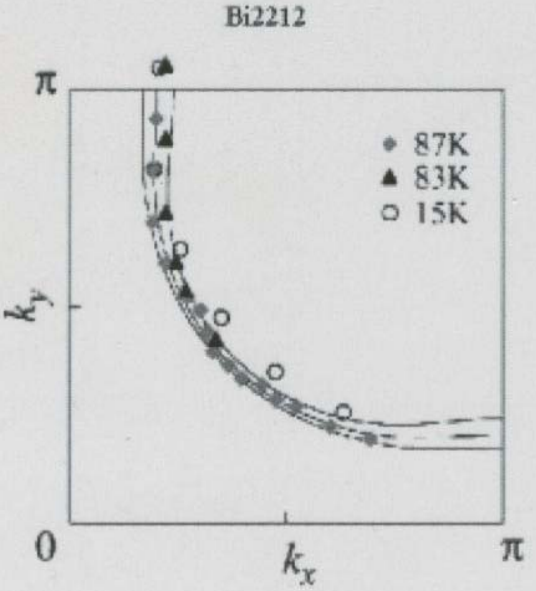
Ruthenates: (A. Damascelli et. al. PRL-2000)

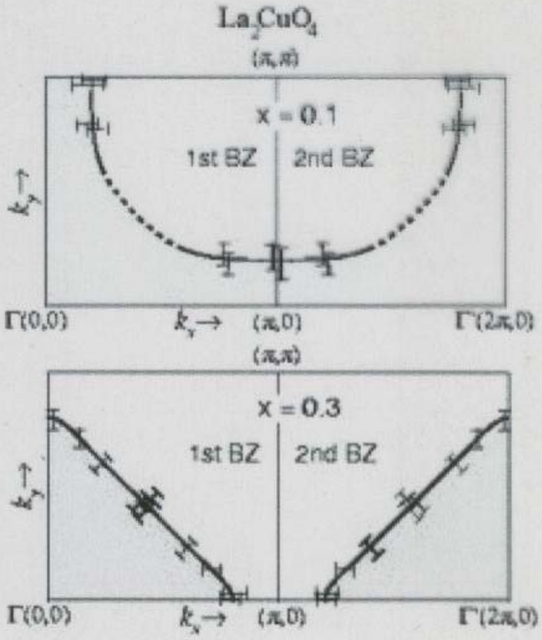
Sr_2RuO_4



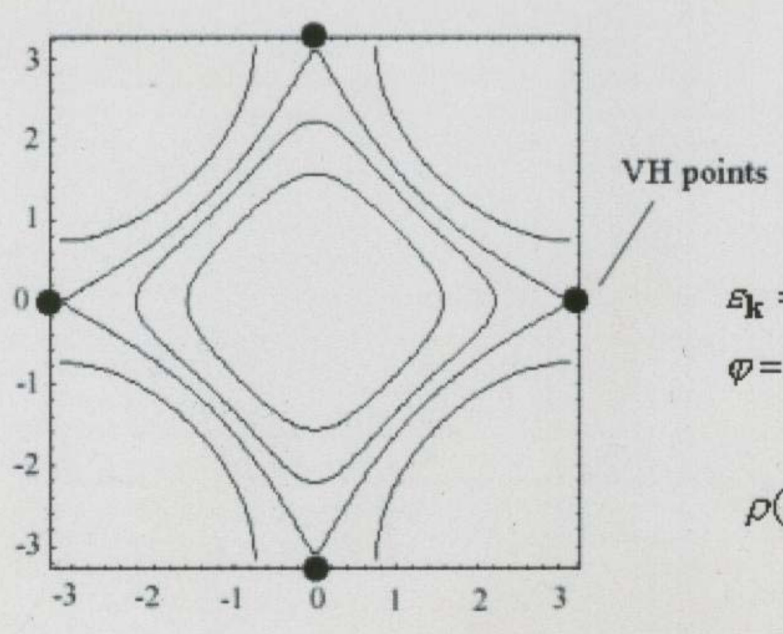
The Fermi surface of high-T_C compounds

From ARPES data:





Tight-binding (t-t' Hubbard) model:



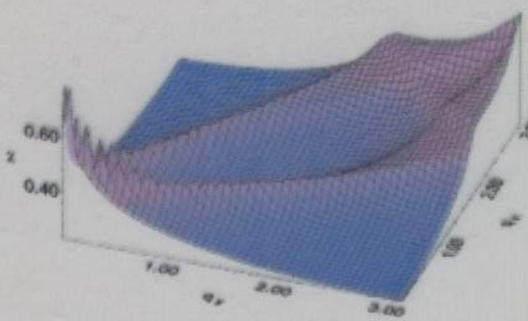
$$\varepsilon_{\mathbf{k}} = 2t(\sin^2 \varphi k_x^2 - \cos^2 \varphi k_y^2)$$

$$\varphi = (1/2)\arccos(2t'/t)$$

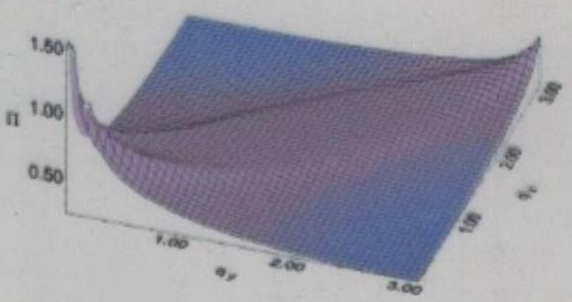
$$\rho(\varepsilon) \propto \ln |\varepsilon - \varepsilon_{\mathrm{VH}}|$$

VH singularities problem:

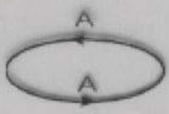
The competition between antiferromagnetism, superconductivity and ferromagnetism



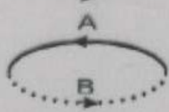
Susceptibility $\chi(\mathbf{q})$



Cooper response $\Pi(\mathbf{q})$

$L_1 =$ 

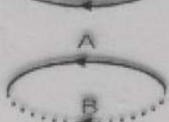
$\propto \ln\frac{\Lambda}{q_+} + \ln\frac{\Lambda}{q_-}$ Ferromagnetic response

$L_2 =$ 

$\propto \min\{\ln\frac{\Lambda}{q_+}, \ln\frac{\Lambda}{q_-}\}$ Antiferromagnetic response

$L_3 =$ 

$\propto \ln\frac{\Lambda}{q_+}\ln\frac{\Lambda}{q_-}$ Zero-momentum Cooper response

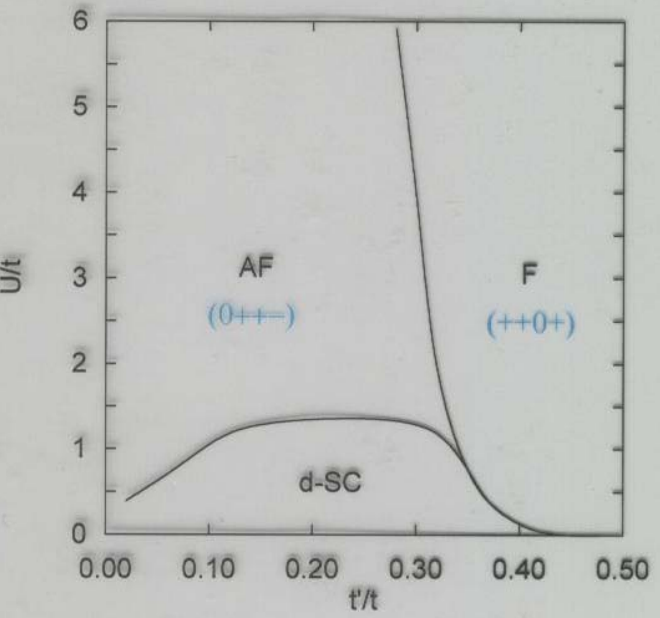
$L_4 =$ 

$\propto \min\{\ln\frac{\Lambda}{q_+}, \ln\frac{\Lambda}{q_-}\}$ π-Cooper response

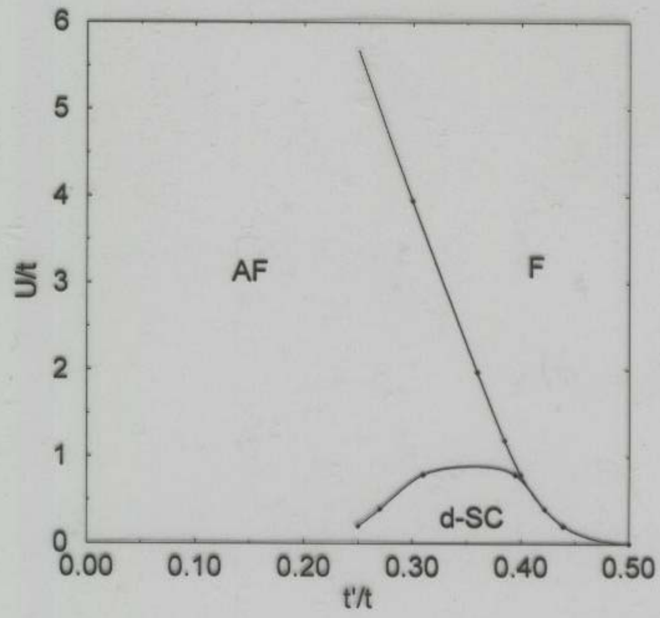
$$q_\pm = \sin\varphi k_x \pm \cos\varphi k_y$$

The phase diagram at vH band fillings

The two-patch equations



The parquet equations



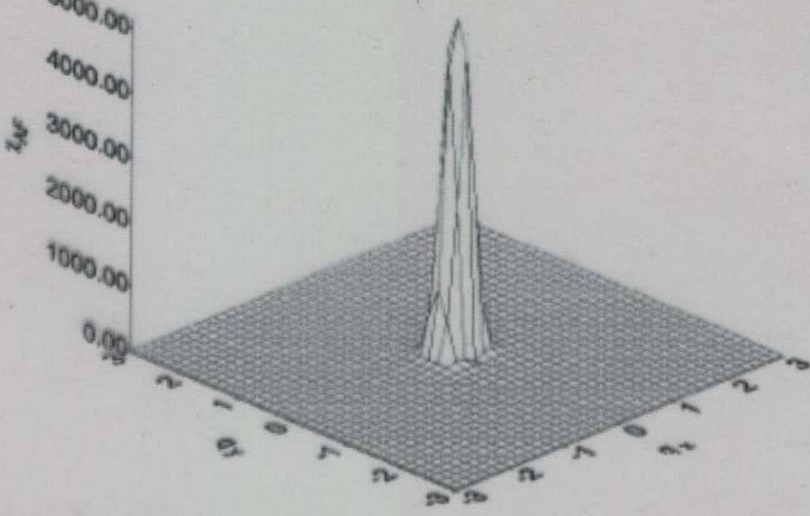
- The phase diagrams from the parquet and the two-patch equations are similar.

- The system is ferromagnetic at t′/t~1/2, cf. Refs.

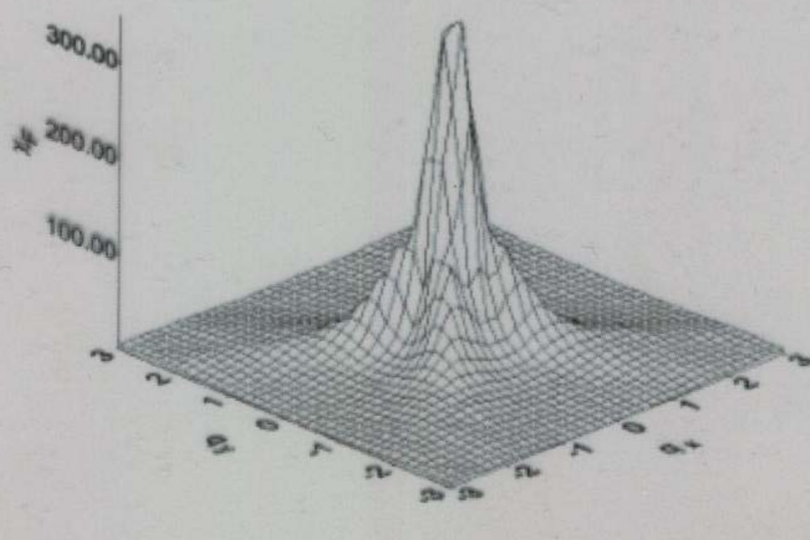
  M. Fleck, A. Oles and L. Hedin, Phys. Rev. B **56**, 3159 (1997) (T - matrix approach)
  R.Hlubina, S.Sorella and F.Guinea, Phys. Rev. Lett. **78**, 1343 (1997) (projected QMC)

The interplay of different channels of electron scattering is important to obtain correct phase diagram.

Parquet equations: the results



t'/t=0.15
U=3.95 t



Effect of external potential

$$V = \int dr\, \psi^+(r)\, V(r)\, \psi(r) = \sum_{12} c_1^+ V_{12}\, c_2$$

The effects $\sim V$:

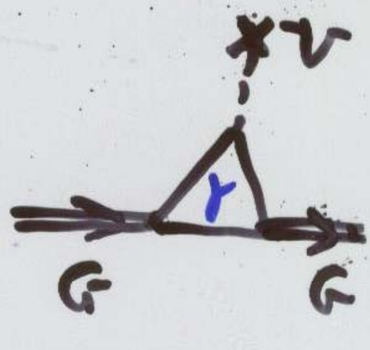
Noninteracting electrons

$$\delta \hat{G}^{-1} = -\hat{V} \qquad \left(\hat{G}^{-1} = i\omega - \hat{t}\right)$$

$$\left(\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{\Sigma} \hat{G}, \qquad \delta \hat{\Sigma} = -\hat{V}\right)$$

Interacting electrons:

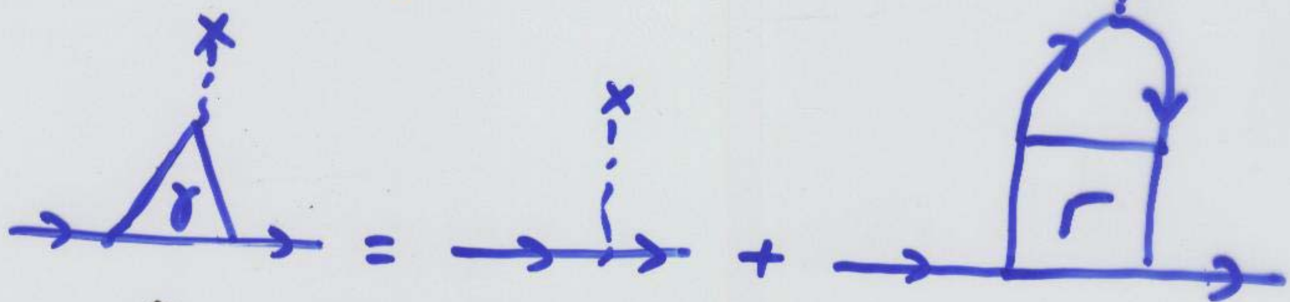
$\delta G =$



γ is called three-leg vertex

$$\boxed{\delta G = G \gamma V G} \qquad \boxed{\delta \hat{\Sigma} = -\hat{\gamma}\, \hat{V}}$$

Relation between 3-leg and 4-leg vertices:



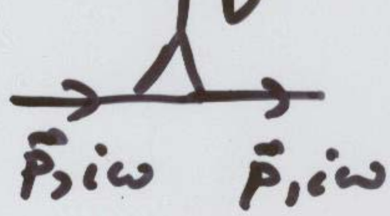
$$\hat{\gamma} = \hat{1} + \hat{\Gamma}\hat{G}\hat{G}$$

Ward identity

Homogeneous electron gas

$\hat{G} = \hat{G}(\vec{p}, i\omega)$

$V = \text{const}$ is equivalent to $i\omega \to i\omega - V$



$$\frac{\partial \hat{G}^{-1}}{\partial (i\omega)} = +\hat{\gamma}$$

$$\boxed{\frac{\partial G^{-1}(\vec{p}, i\omega)}{\partial (i\omega)} = \gamma(\vec{p}, i\omega; \vec{p}, i\omega; 0)}$$

Magnets: spin rotations, etc.

„Hubbard I" approximation

On-cite Coulomb interaction only

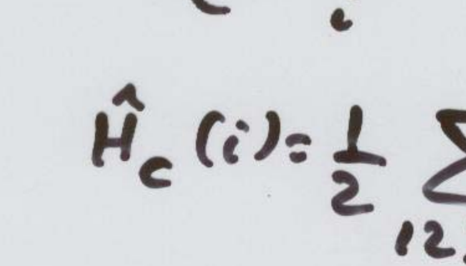
$$\hat{H}_c = \sum_i \hat{H}_c(i)$$

$$\hat{H}_c(i) = \frac{1}{2} \sum_{1234} U^{(i)}_{12,34}\, c^+_{i1} c^+_{i2} c_{i4} c_{i3}$$

Here $1 \equiv \lambda, \sigma,$ etc.

Hopping $H_t = \sum_{ij} t_{ij} c^+_i c_j$

as perturbation $(i \neq j)$



$t_{ij} = 0$ at $i = j$

But Coulomb lines should have all indices i the same!!! $\Rightarrow$ $\Gamma = 0$

$$\hat{G}^{-1}(i\omega, \vec{p}) = \hat{G}^{-1}_{atom}(i\omega) - \hat{t}(\vec{p})$$

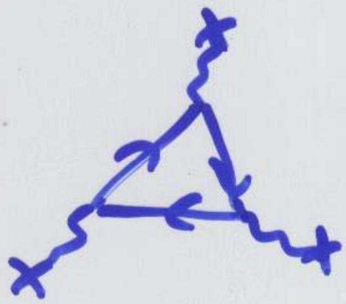
Rigorous at small t_{ij}!!!

Thermodynamic potential

$\delta\Omega$ = sum of all connected diagrams without legs with $1/n$ factor (n th order of perturbation)

Example: external potential, no interactions

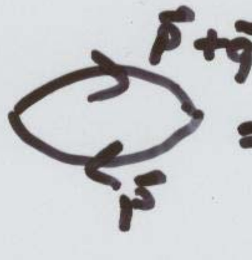
$\delta\Omega =$  $+ \frac{1}{2}$  $+$

$+ \frac{1}{3}$  $+ \ldots$

$$\delta\Omega^{(1)} = \sum_{\vec{p}} V_{\vec{p},\vec{p}}\, n^{(0)}_{\vec{p}}$$

$n^{(0)}_{\vec{p}} = \langle c^{+}_{\vec{p}} c_{\vec{p}} \rangle$ Green's function with coincident time

$$\delta\Omega^{(2)} = -\frac{1}{2}\sum_{\vec p \vec q} |V_{\vec p,\vec p+\vec q}|^2 \, \Pi_0(\vec q)$$

$\Pi_0 =$ 

$= -T\sum_{n}\sum_{\vec p} G_0(i\epsilon_n, \vec p+\vec q)\cdot$

$$\cdot G_0(i\epsilon_n, \vec p) = \sum_{\vec p} \frac{n_{\vec p} - n_{\vec p+\vec q}}{\epsilon_{\vec p+\vec q} - \epsilon_{\vec p}}$$

if $G_0(i\epsilon_n, \vec p+\vec q) = \dfrac{1}{i\epsilon_n - \epsilon_{\vec p+\vec q}}$

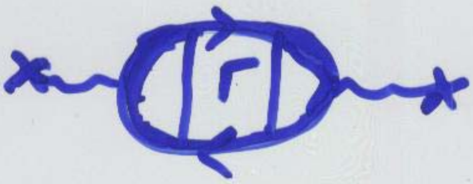
Effects of interaction

First order: $\delta\Omega^{(1)} =$  $=$

$$= \sum_{p} V_{p,p}\, n_{\vec p}$$

$n_{\vec p}$ is exact occupation number!

Second order:

$\delta\Omega^{(2)} = \frac{1}{2}$  $= \frac{1}{2} V * GG\Gamma GG * V$

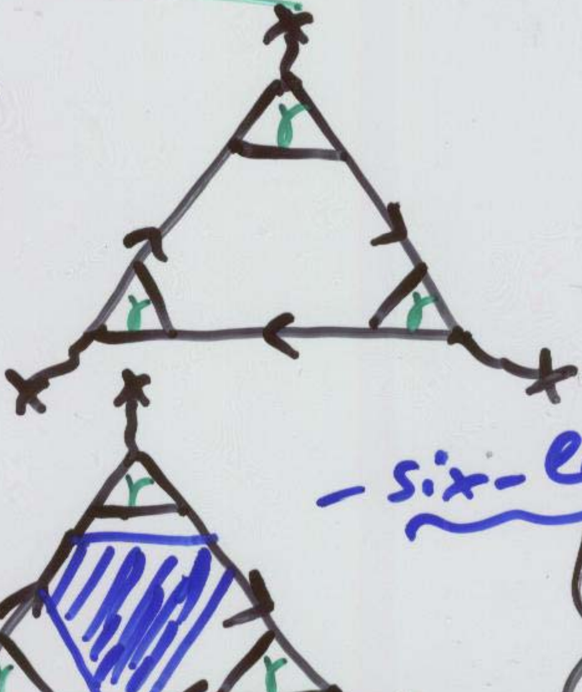
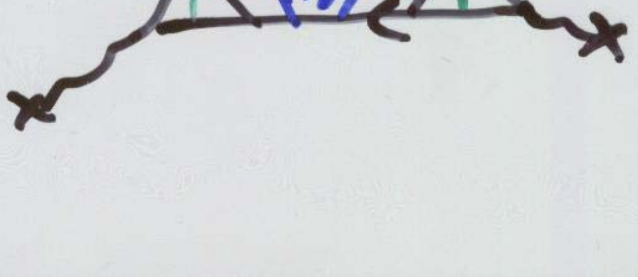
Equivalently:

$\delta\Omega^{(2)} = \frac{1}{2}$ 

$$\delta\Omega^{(2)} = \frac{1}{2}(\hat{\gamma} V) * GG * V$$

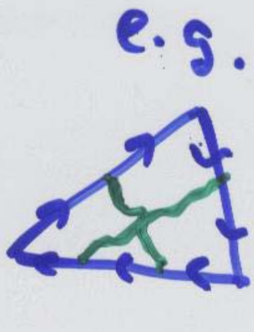
(γ is from only one side!!!)

Third order:

$\delta\Omega^{(3)} = \frac{1}{3} \Big\{$  $+$  $\Big\}$

– six-leg vertex!!!

e.g.



Applications: Exchange integrals

(Katsnelson & Lichtenstein)

Multi-band Hubbard Hamiltonian

$$H = \sum_{ij\sigma} c^{+}_{i\sigma} t_{ij} c_{j\sigma} + \sum_{i} H^{(i)}_{Coul}$$

matrix in orbital space!

Ferromagnet, ground state: all spins up! Rotation:

$$c_i \to \hat{U}(\theta_i, \varphi_i) c_i$$

$$U(\theta, \varphi) = \begin{pmatrix} \cos \theta/2 & \sin \theta/2 \, e^{-i\varphi} \\ -\sin \theta/2 \, e^{i\varphi} & \cos \theta/2 \end{pmatrix}$$

$H^{(i)}_{Coul}$ is rotationally invariant!

Perturbation:

$$\boxed{H' = \sum_{ij} Tr_{\sigma} \{ c^{+}_{i} [U^{+}_{i} t_{ij} U_{j} - t_{ij}] c_{j} \}}$$

Spiral: $\Theta_i = \Theta = \text{const}$ $(\Theta \to 0)$

$\varphi_i = \vec{q}\vec{R}_i$

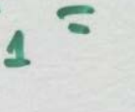
Up to Θ^2:

$$H' = \delta H_1 + \delta H_2$$

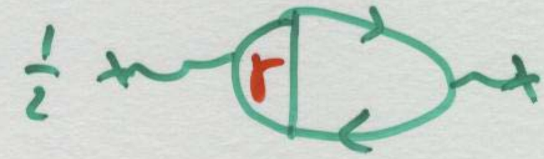
$$\delta H_1 = \sin^2\frac{\Theta}{2} \sum_{\vec{p}} \mathrm{Tr}_{\downarrow\sigma} \{[t(\vec{p}+\vec{q}) - t(\vec{p})] c^+_{\vec{p}} c_{\vec{p}}\}$$

$$\delta H_2 = \frac{1}{2}\sin\Theta \sum_{ij} \mathrm{Tr}_{\downarrow} \{t_{ij} c^+_{i\downarrow} c_{j\uparrow}\} [e^{i\vec{q}\vec{R}_i} - e^{i\vec{q}\vec{R}_j}]$$

First order in $\delta H_1 \sim \Theta^2$:

$\delta E_1 =$  $= \dfrac{\Theta^2}{4} \mathrm{Tr}_{\downarrow} \sum_{\vec{p}} [t(\vec{p}+\vec{q}) - t(\vec{p})] n_{\vec{p}}$

Second order in $\delta H_2 \sim \Theta$:

$\delta E_2 = \frac{1}{2}$  $= \dfrac{\Theta^2}{4} \mathrm{Tr}_{\downarrow}\, T \sum_{\omega} \sum_{\vec{p}} \gamma(p,q)$

$$\times G_\downarrow(p+q) [t(\vec{p}+\vec{q}) - t(\vec{p})] G_\uparrow(p)$$

$p \equiv \vec{p}, i\omega$

$q \equiv \vec{q}, 0$

<u>**Exact**</u> expression which should be compared with $\frac{\theta^2}{4}\left[J(\vec{q})-J(0)\right]$

Fourier component of exchange integrals

Approximations:

I. Σ is local $\hat{\Sigma}=\hat{\Sigma}(i\omega)$ and not on $\vec{p}$

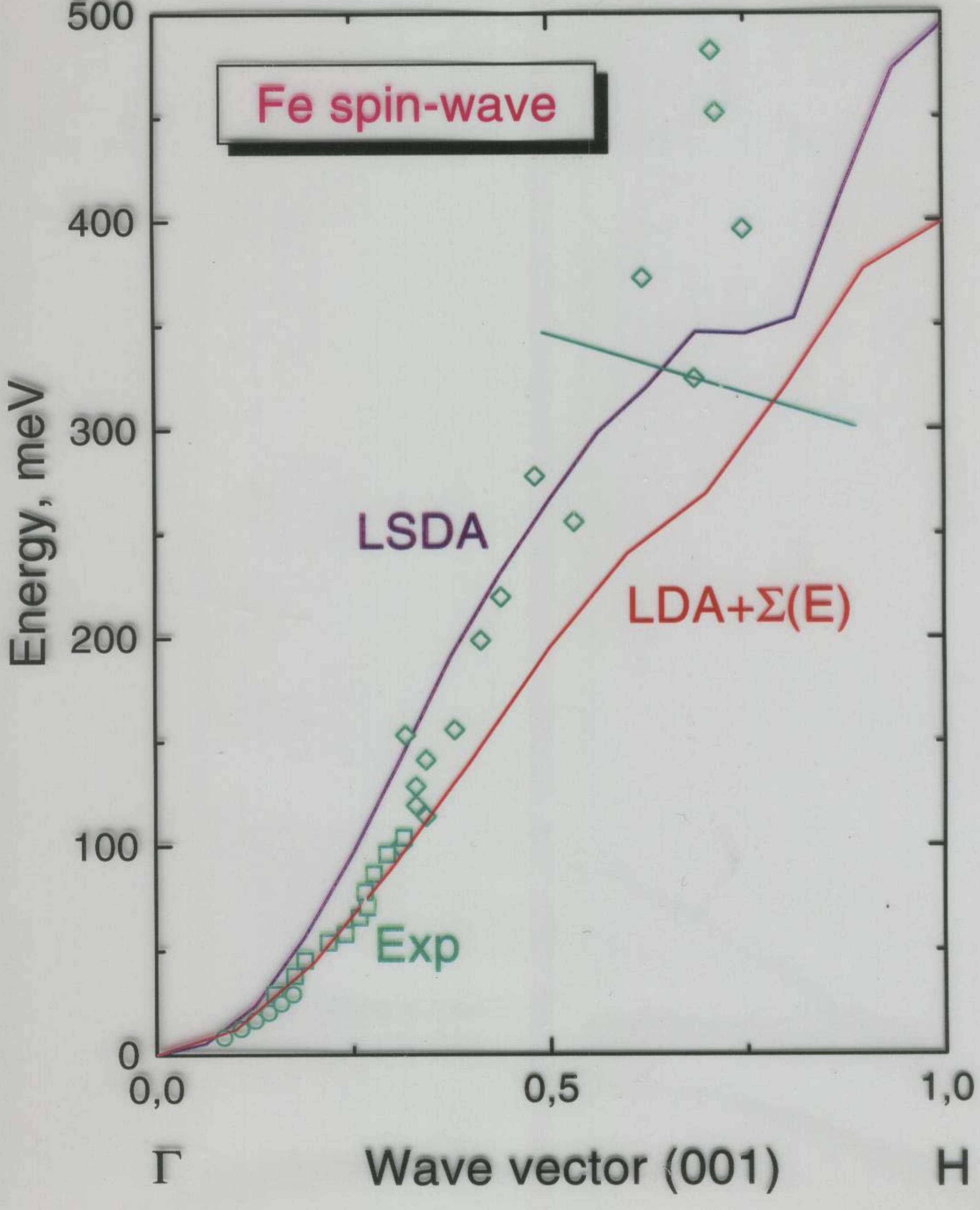
II Γ is local

$\Downarrow$

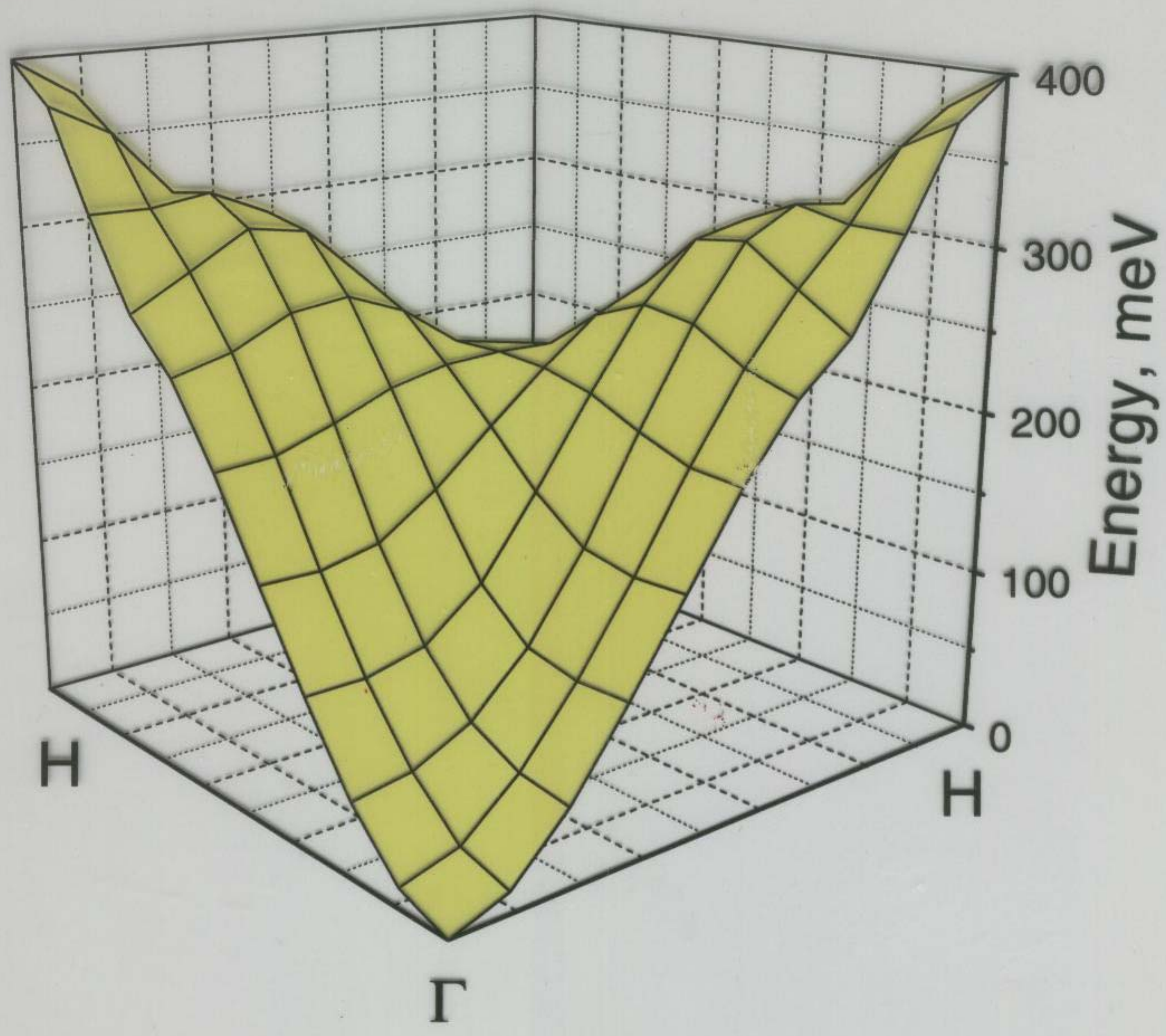
$$J_{ij} \sim -T\sum_{\omega} \mathrm{Tr}_L \left\{ G_{ij}^{\uparrow}\, \Delta\Sigma_i\, G_{ji}^{\downarrow}\, \Delta\Sigma_j \right\}$$

$$\Delta\Sigma_i \equiv \frac{1}{2}\left[\Sigma_i^{\uparrow}(i\omega)-\Sigma_i^{\downarrow}(i\omega)\right]$$

Important formula to calculate energy of magnetic excitations!



Fe spin-wave
500
400
300
200
100
0
Energy, meV
LSDA
LDA+Σ(E)
Exp
0,0
0,5
1,0
Γ
Wave vector (001)
H


400
300
200
100
0
Energy, meV
H
H
Γ

Thermodynamic potential as a functional of exact Green's function

(Luttinger & Ward; more general nonequilibrium case - Baym & Kadanoff)

Some properties of exact Green's function:

$$\hat{G}(z) = \int_{-\infty}^{\infty} dx \, \frac{\hat{A}(x)}{z-x}$$

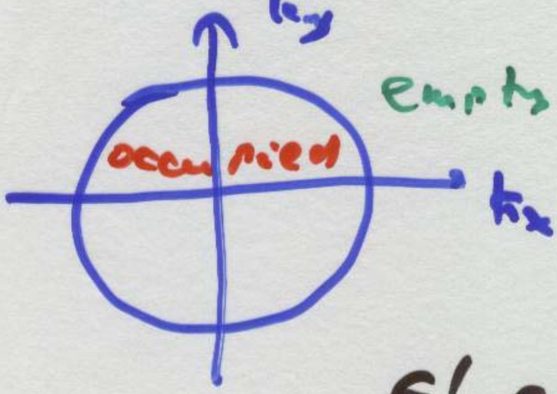
$\hat{A}(x)$ is positively defined matrix

$\hat{G}(z)$ is analytical in upper half plane

Fermi liquid:

Noninteracting particles, $T=0$

Fermi sphere



Collisions:

$$\epsilon_1 + \epsilon_2 = \epsilon_1' + \epsilon_2'$$

But: $\epsilon_1, \epsilon_2 \leq \epsilon_F$

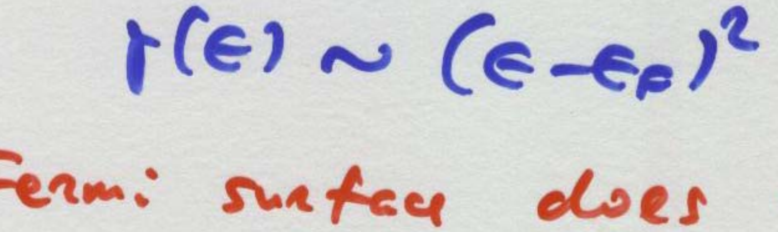
ϵ_1', ϵ_2' should be $\geq \epsilon_F$

(Pauli principle) $\Rightarrow$ decay rate

$$\gamma(\epsilon) \sim (\epsilon - \epsilon_F)^2 \quad T=0$$

Fermi surface does exist!!!

(Migdal 1957)



jump at $p = p_F$

$0 < Z < 1$

$$G_\lambda(E) = \frac{Z_\lambda}{E - \epsilon_\lambda} + G_\lambda^{incoh}(E)$$

$E \to 0$ (counted from Fermi ...

At $E \to 0$

$$-\,\mathrm{Im}\,\Sigma(E+i\delta) \sim \ldots E^2 + |E|^3$$

(positive!)

Analytic continuation:

$$|E|^3 = E^3 \,\mathrm{sgn}\, E = E^3\left[1 - 2\theta(-E)\right]$$

$$\theta(-E) = \begin{cases} 1, & E<0 \\ 0, & E>0 \end{cases}$$

But

$$\theta(-E) = \frac{1}{\pi}\,\mathrm{Im}\,\ln(E+i\delta)$$

$\mathrm{Re}\,\Sigma(E)$ contains $E^3 \ln|E|$ term

(Migdal 1962)

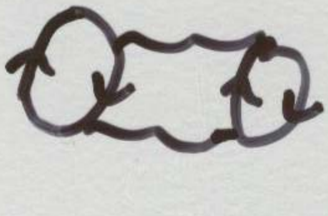
$\Downarrow$

$T^3 \ln T$ terms in heat capacity, etc.

$\Phi = \Phi[G]$ exist such that

$\Sigma = \frac{\delta \Phi}{\delta G}$ (Luttinger & Ward 1960)

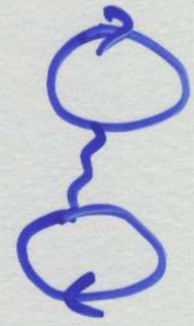
Sum all "sceleton" diagrams without free legs



sceleton (can be written in terms of exact G)

already part of Φ!!!

not sceleton

$\delta \Phi = \frac{1}{2}$ 

$\delta \Sigma = \frac{\delta \Phi}{\delta G} =$ 

$\delta \Phi = \frac{1}{2}$ 

$\delta \Sigma = \frac{\delta \Phi}{\delta G} =$ 

Already from the statement that Φ exists $\Longrightarrow$ Luttinger theorem

Volume of the Fermi surface does not depend on the interaction

Replace in all lines $i\epsilon \to i\epsilon + \mathrm{const}$

Φ will be the same:

$$\frac{\delta \Phi}{\delta \mathrm{const}} = \mathrm{Tr}\left[\int d\epsilon \, \frac{\delta \Phi}{\delta G} \frac{\partial G}{\partial \epsilon}\right] = 0$$

(for simplicity $T=0$ $T\sum_{\omega} \to \int \frac{d\omega}{2\pi}$)

$$\boxed{\mathrm{Tr} \int d\epsilon \, \Sigma \frac{\partial G}{\partial \epsilon} = 0}$$

since $\Sigma = \frac{\delta \Phi}{\delta G}$

Number of particles:

$$N = Tr\langle \psi^+\psi\rangle = Tr \int \frac{d\epsilon}{2\pi i}\, \hat{G}(\epsilon) e^{-i\epsilon\tau}\Big|_{\tau\to}$$

↑ real axis $\int$

$$\frac{\partial}{\partial\epsilon}\hat{G}^{-1} = 1 - \frac{\partial\hat{\Sigma}}{\partial\epsilon}$$

Integration by part:

$$0 = Tr\int\frac{d\epsilon}{2\pi i}\,\hat{\Sigma}\frac{\partial\hat{G}}{\partial\epsilon} = -Tr\int\frac{d\epsilon}{2\pi i}\,\hat{G}\frac{\partial\hat{\Sigma}}{\partial\epsilon} =$$

$$= -Tr\int\frac{d\epsilon}{2\pi i}\,\hat{G}\left(1-\frac{\partial}{\partial\epsilon}\hat{G}^{-1}\right) =$$

$$= -N + Tr\int\frac{d\epsilon}{2\pi i}\,\hat{G}\,\frac{\partial\hat{G}^{-1}}{\partial\epsilon}\, e^{-i\epsilon\tau}\Big|_{\tau\to+0}$$

$$N = Tr\int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi i}\,\frac{\partial \ln\hat{G}^{-1}}{\partial\epsilon}\, e^{-i\epsilon\tau}\Big|_{\tau\to-0}$$

Using analytic properties of $\hat{G}$:

$$N = -\frac{1}{\pi} Tr\left[\hat{\varphi}(-0) - \hat{\varphi}(-\infty)\right] =$$

↑ phases

$$= \sum_{\epsilon_i<0} 1$$

Q.E.D.

Thermodynamic potential:

$$\Omega = \Phi - \mathrm{Tr}[\hat{\Sigma}\hat{G}] - \mathrm{Tr}\ln[-\hat{G}^{-1}]$$

It is exact.

Approximations:

Satisfying $\Sigma = \frac{\delta\Phi}{\delta G}$ with some Φ - good

(Φ-derivable, conserving, consistent in Baym' sense, etc.)

Otherwise can be problem!

Exchange interactions in LDA++

Thermodynamic potential:

$$\Omega = \Omega_{sp} - \Omega_{dc}$$

$$\Omega_{sp} = -Tr\left\{\ln\left[\Sigma - G_0^{-1}\right]\right\}$$

$$\Omega_{dc} = Tr\Sigma G - \Phi$$

Dyson equation

$$G^{-1} = G_0^{-1} - \Sigma$$

Variational identity

$$\delta\Phi = Tr\Sigma\delta G$$

Local-force theorem

Variation of thermodynamic potential

$$\delta\Omega = \delta^*\Omega_{sp} + \delta_1\Omega_{sp} - \delta\Omega_{dc}$$

Luttinger theorem

$$\delta_1\Omega_{sp} = \delta\Omega_{dc} = Tr G\delta\Sigma$$

Local force - variations:

$$\delta\Omega = \delta^*\Omega_{sp} = -\delta^* Tr \ln\left[\Sigma - G_0^{-1}\right]$$

Spin-matrix structure

$$\Sigma_i = \Sigma_i^c + \Sigma_i^s \sigma$$

$$G_{ij} = G_{ij}^c + \mathbf{G}_{ij}^s \sigma$$

Effective spin Hamiltonian

Spin excitations

$$\delta\mathbf{e}_i = \delta\varphi_i \times \mathbf{e}_i$$

Magnetic torque:

$$\delta\Omega = \delta^*\Omega_{sp} = \mathbf{V}_i\delta\varphi_i$$

$$\mathbf{V}_i = 2Tr_{\omega L}\left[\mathbf{\Sigma}_i^s \times \mathbf{G}_{ii}^s\right]$$

Exchange interactions

$$\Omega_{spin} = -\sum_{ij} J_{ij}\mathbf{e}_i\mathbf{e}_j$$

$$J_{ij} = -Tr_{\omega L}\left(\Sigma_i^s G_{ij}^{\uparrow} \Sigma_j^s G_{ji}^{\downarrow}\right)$$

Spin wave spectrum

$$\omega_{\mathbf{q}} = \frac{4}{M}\sum_j J_{0j}\left(1 - \cos\mathbf{q}\mathbf{R}_j\right) \equiv \frac{4}{M}[J(0) - J(\mathbf{q})]$$

Exact for $\vec{q} \to 0$ in DMFT !

LDA+U functional

LSDA plus Local Coulomb interactions:

$$H = H_{dc}^{LDA} + \frac{1}{2}\sum_{i\{\sigma m\}} U^{i}_{m_1 m_2 m_1' m_2'} c^{+}_{im_1\sigma} c^{+}_{im_2\sigma'} c_{im_2'\sigma'} c_{im_1'\sigma}$$

LDA part with double-counting corrections:

$$H_{dc}^{LDA} = \sum_{ij\sigma\{m\}} h^{ij}_{m_1 m_2 \sigma} c^{+}_{im_1\sigma} c_{jm_2\sigma} - E_{dc}$$

Spin-polarized case:

$$E_{dc} = \frac{1}{2}\overline{U} n_d(1-n_d) - \frac{1}{2}\overline{J}[n_{d\uparrow}(1-n_{d\uparrow}) + n_{d\downarrow}(1-n_{d\downarrow})$$

Screened Coulomb Matrix

$$V_{ee}(\mid \mathbf{r}_1 - \mathbf{r}_1 \mid) = \sum_{kq} F^k Y_{kq}(\mathbf{r}_1) Y^*_{kq}(\mathbf{r}_2)$$

F^k - effective Slater parameters

$$\langle m, m'' \mid V_{ee} \mid m', m''' \rangle = \sum_k a_k(m, m', m'', m''') F^k$$

where $0 \leq k \leq 2l$ and

$$a_k(m, m', m'', m''') = \frac{4\pi}{2k+1} \sum_{q=-k}^{k} \langle lm \mid Y_{kq} \mid lm' \rangle \langle lm'' \mid Y^*_{kq} \mid lm''' \rangle$$

For f-electrons:

$$U = F^0, \ and \ J = \frac{1}{3}(\frac{2}{15}F^2 + \frac{1}{11}F^4 + \frac{50}{429}F^6).$$

Supercell LSDA calculation of U and J

(Gunnarrson-1989)

$$U = \varepsilon_{d\uparrow}(\frac{n}{2} + \frac{1}{2}, \frac{n}{2}) - \varepsilon_{d\uparrow}(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} - 1)$$

$$J = \varepsilon_{d\uparrow}(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} - \frac{1}{2}) - \varepsilon_{d\downarrow}(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} - \frac{1}{2})$$

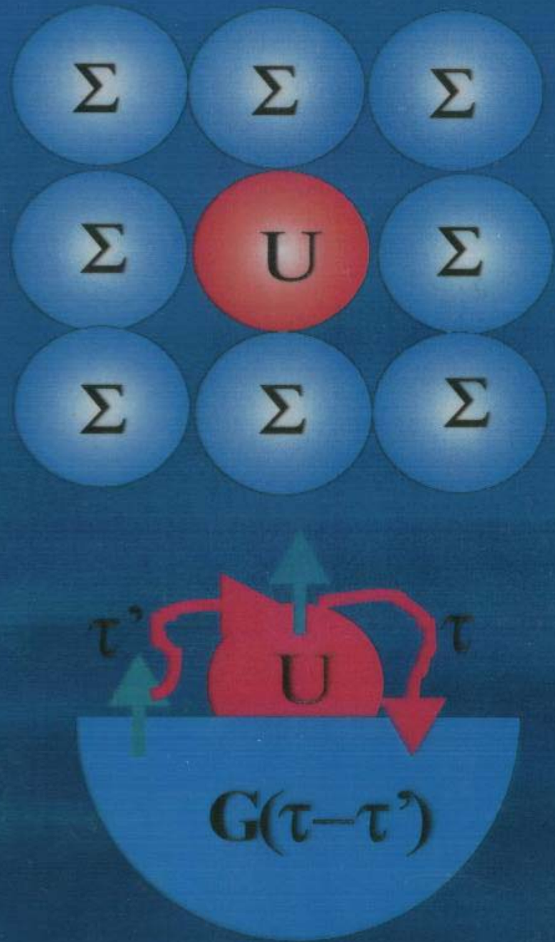
Dynamical Mean-Field Theory

$$S_{eff} = \int_0^\beta d\tau \int_0^\beta d\tau' Tr[\mathbf{c}^+(\tau)\mathcal{G}^{-1}(\tau,\tau')\mathbf{c}(\tau')] + \frac{1}{2}\sum_{m,m',\sigma}[U_{mm'}n_\sigma^m n_{-\sigma}^{m'} + (U_{mm'} - J_{mm'})n_\sigma^m n_\sigma^{m'}]$$

$$\mathbf{G}_\sigma(\tau - \tau') = -\frac{1}{Z}\int D[\mathbf{c},\mathbf{c}^+]e^{-S_{eff}}\mathbf{c}(\tau)\mathbf{c}^+(\tau')$$

$$\mathcal{G}_\sigma^{-1}(\omega n) = \mathbf{G}_\sigma^{-1}(\omega n) + \boldsymbol{\Sigma}_\sigma(\omega n)$$

$$\mathbf{G}_\sigma(\omega n) = \sum_{\mathbf{k}}[(i\omega n + \mu)\mathbf{1} - \mathbf{H}^{LDA}(\mathbf{k}) - \boldsymbol{\Sigma}_\sigma^{dc}(\omega n)]^{-1}$$



$$G^{-1}(\omega) = \mathcal{G}^{-1}(\omega) + \Sigma(\omega)$$

W. Metzner and D, Vollhardt, 1989
A. Georges and G. Kotliar, 1992

Spin-polarized multi-band FLEX approximation

The Hamiltonian and the screened Coulomb interaction:

$$H = H_t + H_U;$$

$$H_t = \sum t_{ij} c^+_{i,\sigma} c_{j\sigma}; H_U = \frac{1}{2} \sum \langle i_1 j_2 | U | i_1' \, j_2' \rangle c^+_{i_1,\sigma} c^+_{j_2,\sigma'} c_{j_2'\sigma'} c_{i_1'\sigma}$$

$$\langle 12 | U | 34 \rangle = \int dr dr' \Psi_1^*(r) \Psi_2^*(r') V(r-r') \Psi_3(r) \Psi_4(r')$$

FLEX is a conserving approximation, so it is consistent with macroscopical laws for conserving of number of particles, energy and momentum[1]

$$\Sigma(1,2) = \frac{\delta \Phi}{\delta G(2,1)}$$

T-matrix renormalization of effective interaction is used in the T-matrix-FLEX approximation[2]

[1]N.E.Bickers and D.J. Scalapino Ann. Phys., NY, 193, 206 (1989)
[2]M.I. Katsnelson and A.I.Lichtenstein J.Phys.Condens.Matter. 11, 1037 (1999)

Around mean-field limit of LDA+U

LDA+U in fully-localized limit (LDA+U-FLL) applied to Pu lead to magnetic solution

LDA+U in around mean-field limit (LDA+U-AMF):

$$U\, n_{m\uparrow} n_{m'\downarrow} = \underbrace{U\left(n_{m\uparrow}\langle n_{\downarrow}\rangle + \langle n_{\uparrow}\rangle n_{m'\downarrow} - \langle n_{\uparrow}\rangle\langle n_{\downarrow}\rangle\right)}_{\text{"mean-field"} = \text{LDA}} + \underbrace{U\left(n_{m\uparrow} - \langle n_{\downarrow}\rangle\right)\left(n_{m'\downarrow} - \langle n_{\downarrow}\rangle\right)}_{\text{LDA+U}}$$

$$E^{AFM} = \frac{1}{2} \sum_{\gamma_1\gamma_2\gamma_3\gamma_4} \delta n_{\gamma_1\gamma_2} \left[\langle \gamma_1, \gamma_3 | U | \gamma_2, \gamma_4 \rangle - \langle \gamma_1, \gamma_3 | U | \gamma_4, \gamma_2 \rangle\right] \delta n_{\gamma_{31}\gamma_4}$$

$$\delta n_{\gamma_1\gamma_2} = n_{\gamma_1\gamma_2} - n^{\sigma_1} \delta_{\gamma_1\gamma_2}, \quad n^{\sigma} = \frac{1}{2l+1} \sum_{m=-l}^{l} n_{m\sigma, m\sigma}$$

Spin-orbit generalization of T-matrix FLEX

Spin-orbit coupling: $G_{12}(\tau) = -\langle T_\tau c_1 c_2^+ \rangle$ where $1 = \{m, \sigma\}$

$$H_t = \sum t_{ij} c_i^+ c_j; \; H_U = \frac{1}{2} \sum \langle i_1 j_2 | U | i_1' j_2' \rangle c_{i_1}^+ c_{j_2}^+ c_{j_2'} c_{i_1'}$$

All PH channels are coupled

$$\langle 12 | U | 34 \rangle = \delta_{\sigma_1 \sigma_3} \delta_{\sigma_2 \sigma_4} \int dr dr' \Psi_1^*(r) \Psi_2^*(r') V(r - r') \Psi_3(r) \Psi_4(r')$$

Self energy in SO T-matrix FLEX approximation

$$\boxed{\Sigma = \Sigma^{(T-H)} + \Sigma^{(T-F)} + \Sigma^{(PH)}}$$

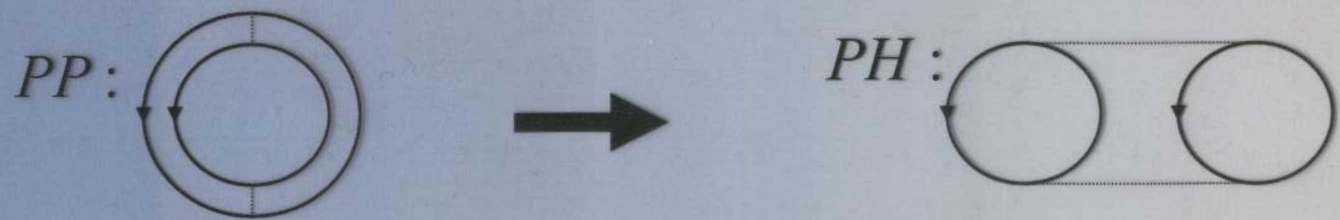
T-matrix renormalization of the electron-electron interaction

Bare interaction replaced by the T-matrix:

Hartree and Fock T-matrix contributions:

$$\Sigma_{12}^{(T-H)}(\tau) = \sum_{34} \langle 13 | T\ (\tau) | 24 \rangle G_{43}(-\tau) \qquad \Sigma_{12}^{(T-F)}(\tau) = -\sum_{34} \langle 14 | T\ (\tau) | 32 \rangle G_{34}(-\tau)$$

All second order contributions are included

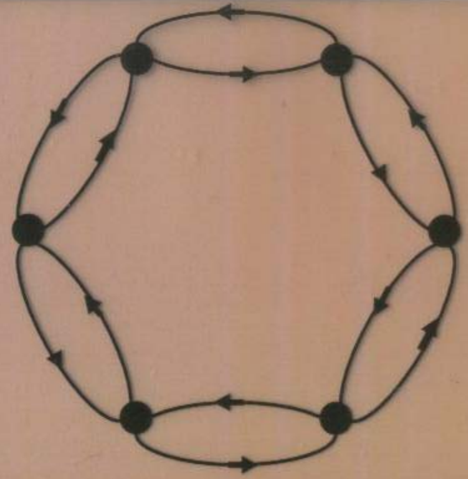


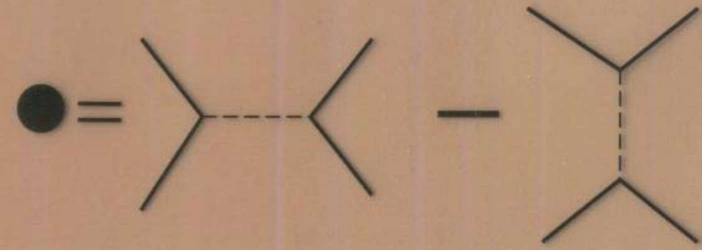
Static approximation for renormalized vertex is used for FLEX contributions:

$$\langle 13 | U | 24 \rangle \rightarrow \langle 13 | T\ (i\Omega = 0) | 24 \rangle$$

PH contribution with antisymmetric vertex

Summation over all possible rearrangements of direct and exchange vertices

$\Phi = \sum \frac{1}{n}$ 



$$\langle 12 | V | 34 \rangle = \langle 13 | U | 24 \rangle - \langle 13 | U | 42 \rangle$$

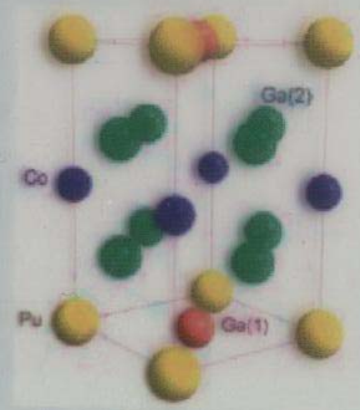
Self-energy: $\Sigma^{(Ph)}_{12}(\tau) = \sum_{34} W_{13,42}(\tau) G_{34}(\tau)$

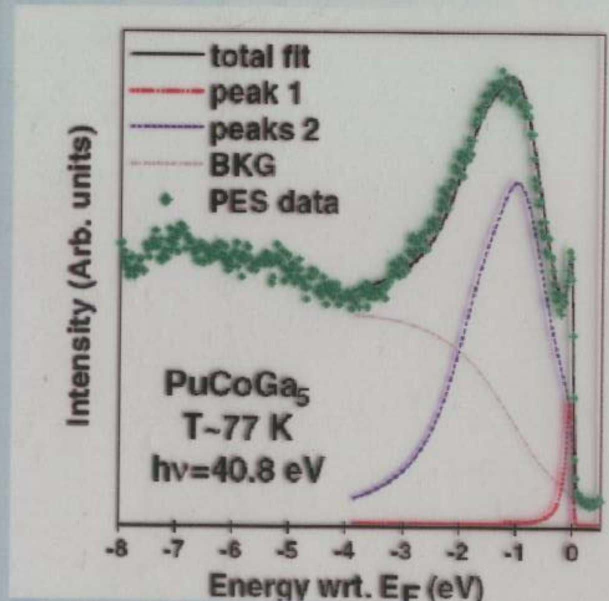
Fluctuation potential matrix: $\hat{W}(i\omega) = \hat{V} * \left(\hat{\chi}(i\omega) - \hat{\chi}^0(i\omega)\right) * \hat{V}$

$\chi^0_{12;34}(\tau) = G_{41}(-\tau) G_{23}(\tau)$ $\quad \hat{\chi}(i\omega) = \left(\hat{1} + \hat{\chi}^0(i\omega)\hat{V}\right)^{-1} \hat{\chi}^0(i\omega)$

$PuCoGa_5$ superconductor

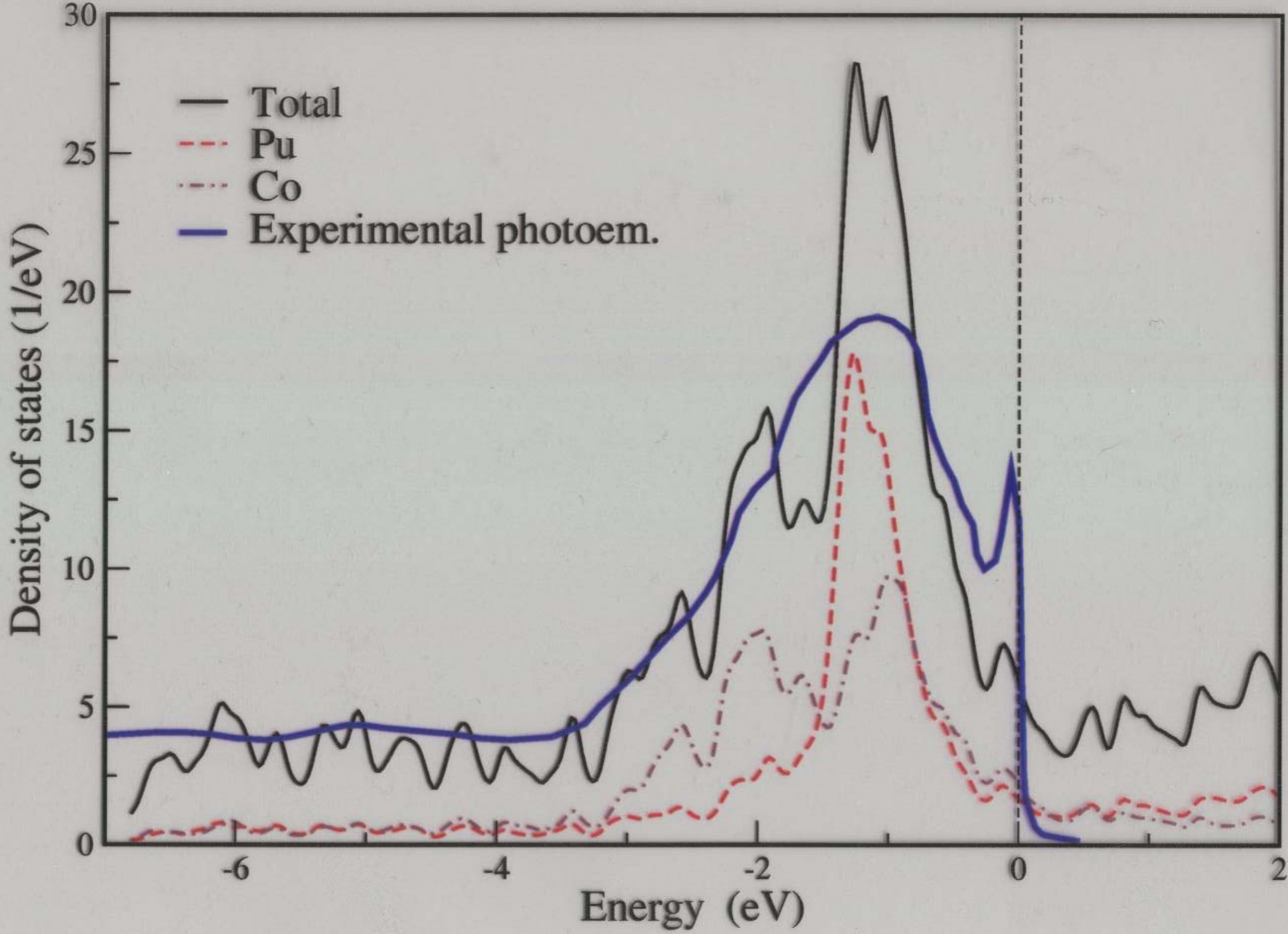
- The first Pu based superconductor with the highest T_c=18.5 K among actinide based superconductors (later discovered $PuCoRh_5$ with T_c=8.7 K)
- Unconvetional d-wave superconductivity (Curro *et al.* Nature **434**, 622 (2005)
- No magnetic order down to 0 K, local moment of 0.75 μ_B deduced from Curie-Weise behaviour of the suseptebility.
- Peak on E_F on the PES and γ(PuSe)=90 mJ/mol K2 hint on possible importance of correlations



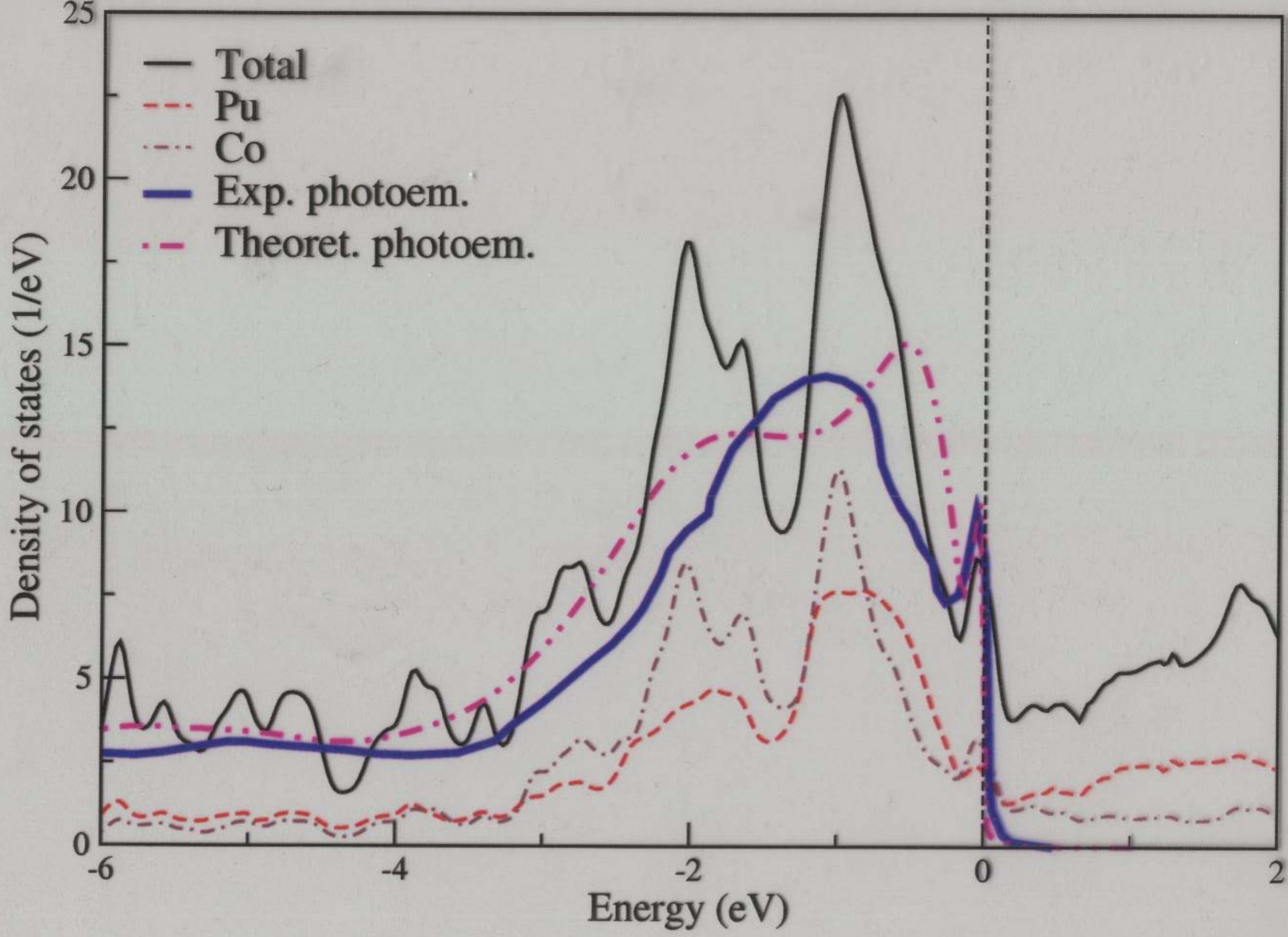


Joyce et al. PRL 91, 176401 (2003)

$PuCoGa_5$: LDA+U   U = 3eV J = 0.55eV



$PuCoGa_5$: LDA + DMFT



$PuCoGa_5$ spectral function in the DMFT