Kondo necklace model

Heavy Fermion Compounds

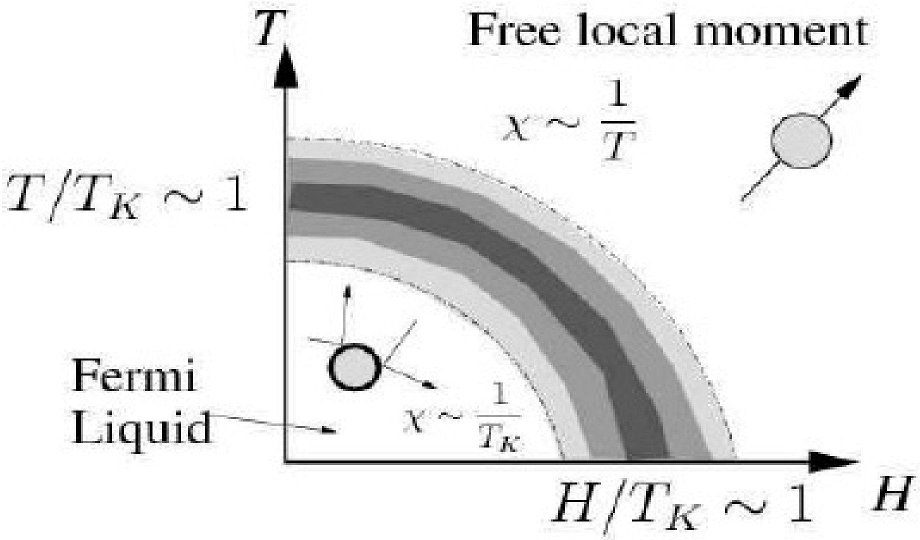
Containing conduction and localized electrons (Lanthanides $CeAl_3$ or actanides): (1975)

$Ce \quad 4f_1 \qquad 4f_{13} \quad Yb \qquad U \quad 5f_2$

- Density of states as much as 1000 times larger than free electron

$$\chi = cte \qquad C_V \propto T$$

$$\gamma = \mathrm{Lim}_{T\to 0}\left(\frac{C_V}{T}\right) = \frac{\pi^2 k_B^2}{3}\rho^*$$



$$\rho(T) = \rho_0 + AT^2$$

$$\frac{1}{\tau} \propto (J\rho + 2(J\rho)^2 ln\frac{D}{T}$$

High temperature and local moments systems.

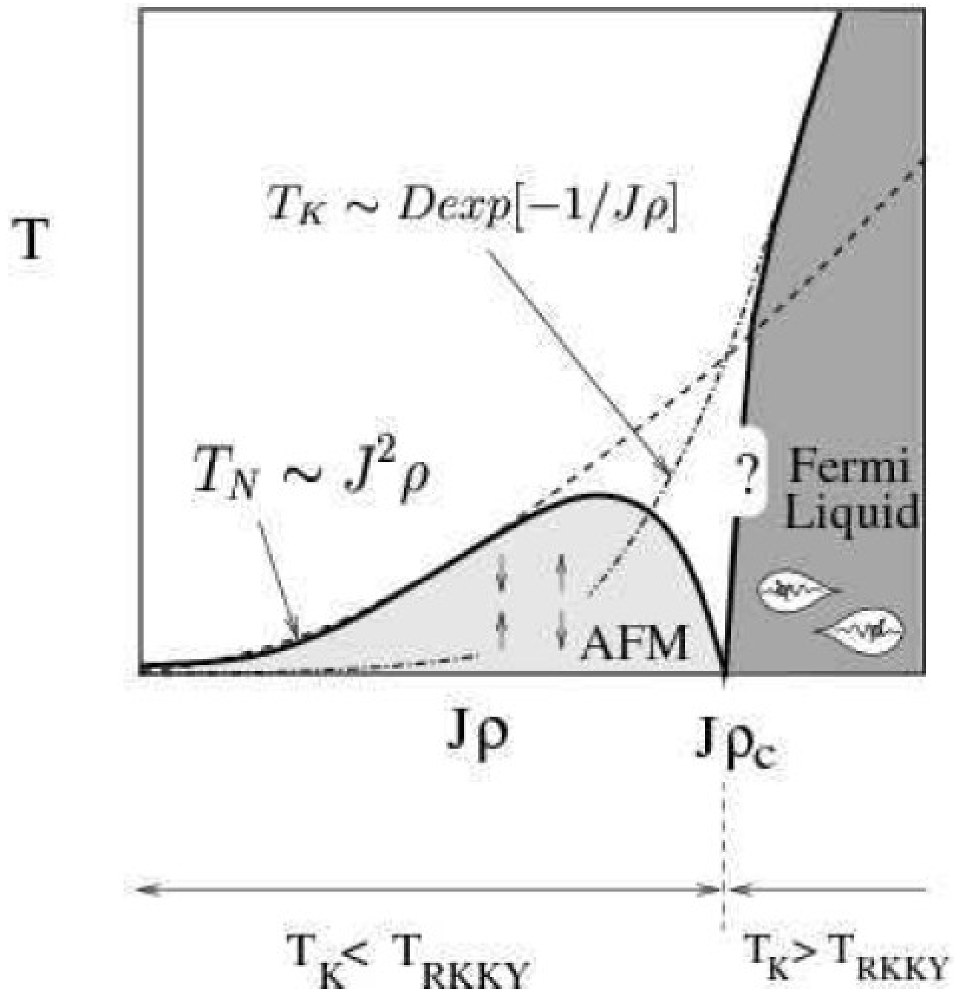
$$\chi = \frac{M^2}{3T}$$

$$M^2 = (g_J \mu_B)^2 J(J+1)$$

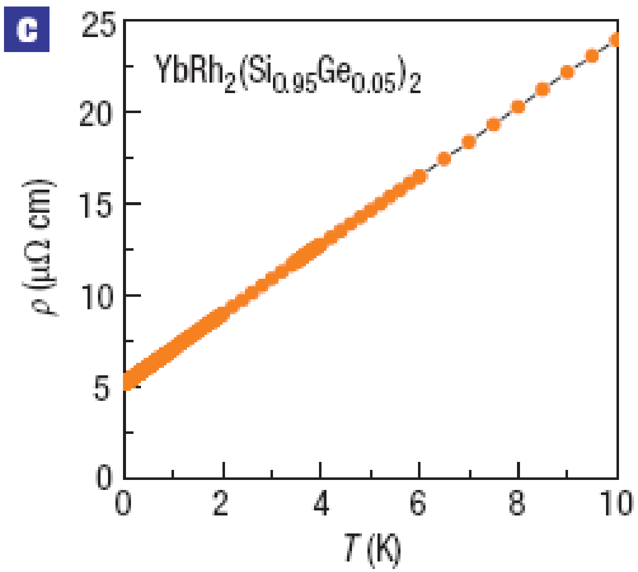
Drude peak in the optical conductivity

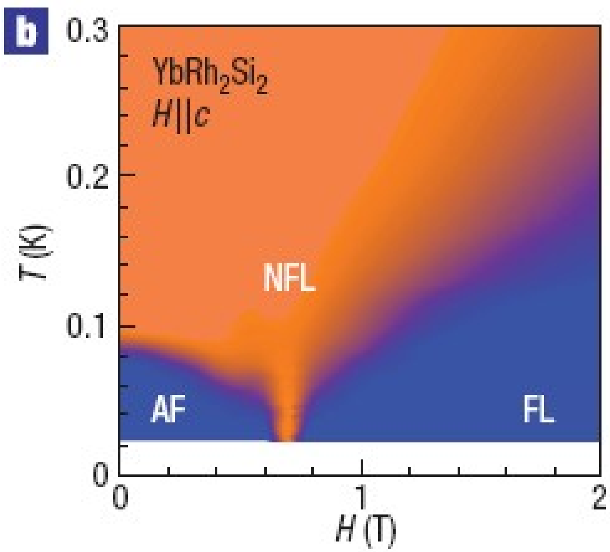
$$\int_{|\omega| \leq T_K} \frac{d\omega}{\pi} \sigma_{qp}(\omega) = \frac{ne^2}{m^*}$$

Doniach's diagram



Quantum Criticality HF Metals

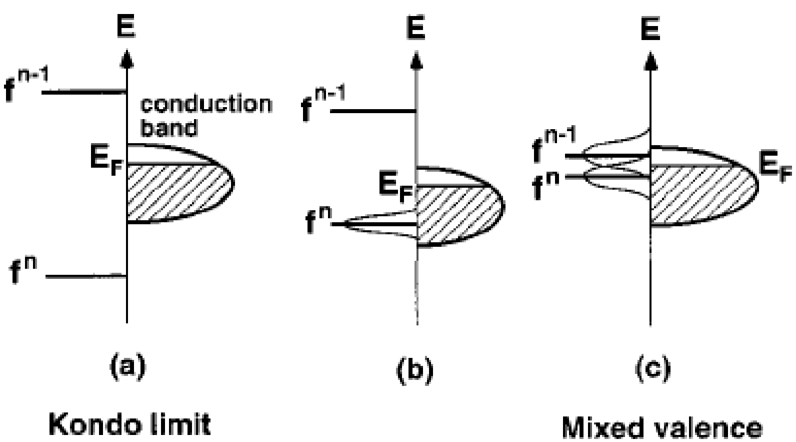




Models for heavy Fermion systems

- Periodic Anderson model and Kondo lattice model

$$H_{PAM} = -t \sum_{\langle ij \rangle} \sum_{\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + \sum_{i\sigma} \varepsilon_f n^f_{i\sigma} + V \sum_{\langle ij \rangle} \sum_{\sigma} (c^{\dagger}_{i\sigma} f_{j\sigma} + h.c.) + U \sum_{i} n^f_{i\uparrow} n^f_{i\downarrow}$$



width of virtual level $\Gamma_{eff} = \pi \rho(\varepsilon_F) V^2$

condition for arriving Kondo regime

$$U >> \Gamma_{eff}$$

Interactions in the Kondo lattice model

- RKKY interaction

In the weak coupling and AF coupling J/t<<1 RKKY interaction between localized spins occures

$$H_{RKKY} = \sum_{\langle ij \rangle} J_{RKKY} S_i . S_j$$

$$J_{RKKY} = \frac{-9\pi}{8} n_c^2 \left(\frac{J^2}{\varepsilon_F} \right) \left(2k_F \cos(2k_F r_{ij}) - \frac{\sin(2k_f r_{ij})}{r_{ij}} \right)$$

This interaction is long ranged and changes its sign depending on the distance between local spins

- Kondo singlet formation

in the strong coupling J/t>>1 that ground state is product state of singlet dimer between conduction electron and localized electron

Kondo necklace model

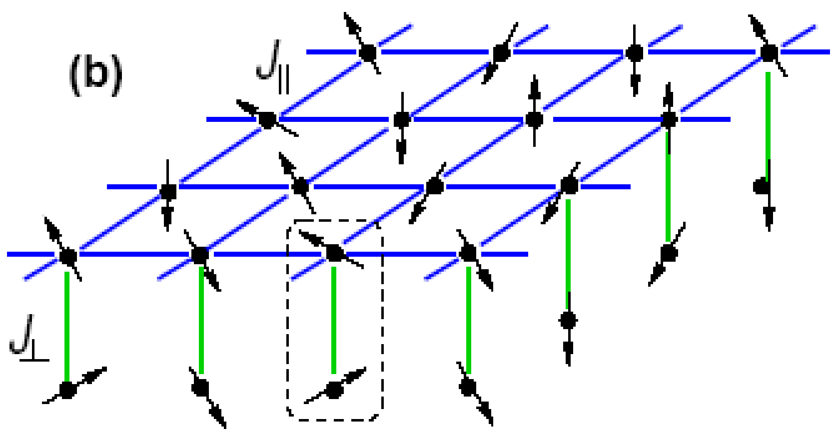
With Considering coulomb repulsion between conduction electrons at half filling conduction band

$$Nd_{1-x}Ce_xCuO_4$$

$$H_{UKLM} = \sum_{p,\sigma} \varepsilon_p c^{\dagger}_{p\sigma} c_{p\sigma} + J \sum_i S^c_i S^f_i + U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$$

At $U/t \gg 1$ UKLM model map to Kondo necklace model

$$H_{KNM} = J_{\|} \sum_{\langle ij \rangle} \tau_i . \tau_j + J_{\perp} \sum_i S_i . \tau_i$$



Anisotropic Kondo necklace model

- For considering crystal field and easy axis effect we introduce two global and local anisotropies:

$$H = J_{\perp} \sum_{\langle i,j \rangle} (\tau_i^x \tau_j^x + \tau_i^y \tau_j^y + \delta \tau_i^z \tau_j^z) + J \sum_{\langle i \rangle} (\tau_i^x S_i^x + \tau_i^y S_i^y + \Delta \tau_i^z S_i^z)$$

τ is the spin operator of itinerant electrons and S is the spin operator of localized one and the coupling constants $J, J_{\perp} < 0$ are antiferromagnetic type.

δ, Δ are anisotropies parameters

Bond operator Representation

Useful approach to the description of the disordered phase (Sachdev & Bhatt)

$$S^{\alpha}=\frac{1}{2}(s^{\dagger}t_{\alpha}+t_{\alpha}^{\dagger}s-i\,\varepsilon_{\alpha\beta\gamma}t_{\beta}^{\dagger}t_{\gamma})$$

$$\tau^{\alpha}=\frac{1}{2}(-s^{\dagger}t_{\alpha}-t_{\alpha}^{\dagger}s-i\,\varepsilon_{\alpha\beta\gamma}t_{\beta}^{\dagger}t_{\gamma})$$

$$\left[t_{\alpha},t_{\beta}^{\dagger}\right]=\delta_{\alpha\beta}$$

For satisfying the SU(2) algebra we should exert the following constraint for each site

$$s^{\dagger}s+t_{\alpha}^{\dagger}t_{\alpha}=1$$

We want to find one particle Green's function for triplet Bosons that its poles represent excitation energy.

Hamiltonian in the Bond operator Rep.

One particle parts of Hamiltonian:

$$H = \sum_{k,\alpha} A_{k,\alpha} t^{+}_{k,\alpha} t_{k,\alpha} + \sum_{k,\alpha} B_{k,\alpha} t^{+}_{k,\alpha} t^{+}_{-k,\alpha}$$

$$A_{k,z} = J_{\perp} + \delta J \xi_k \, , B_{k,z} = \delta J \xi_k$$

$$A_{k,x} = \frac{J_{\perp}}{2}(1+\Delta) + J\xi_k \, , B_{k,z} = J\xi_k$$

$$\xi_k = \frac{1}{2}(\cos(k_x) + \cos(k_y))$$

Other parts of Hamiltonian:

$$H_3 = \frac{t}{4} \sum_{\langle i,j \rangle} (i[(t_{i,x} + t^{\dagger}_{i,x})(t^{\dagger}_{j,y} t_{j,z} - t^{\dagger}_{j,z} t_{j,y}) + (t_{i,y} + t^{\dagger}_{i,y})(t^{\dagger}_{j,z} t_{j,x} - t^{\dagger}_{j,x} t_{j,z}) + \delta(t_{i,z} + t^{\dagger}_{i,z})(t^{\dagger}_{j,x} t_{j,y} - t^{\dagger}_{j,y} t_{j,x})] + h.c.)$$

$$H_4 = -\frac{t}{4} \sum_{\langle i,j \rangle} ((t^{\dagger}_{i,y} t_{i,z} - h.c.)(t^{\dagger}_{j,y} t_{j,z} - h.c.) + (t^{\dagger}_{i,x} t_{i,z} - h.c.)(t^{\dagger}_{j,x} t_{j,z} - h.c.) + \delta(t^{\dagger}_{i,x} t_{i,y} - h.c.)(t^{\dagger}_{j,x} t_{j,y} - h.c.))$$

Green's function formalism

Interacting one particle Green's function :

$$\Omega_{k,\alpha} = Z_{k,\alpha}\sqrt{(A_{k,\alpha} + \Sigma_{n,\alpha}(k,0))^2 - (B_{k,\alpha} + \Sigma_{a,\alpha}(k,0))^2}$$

$$G_\alpha(k,\omega) = \frac{Z_{k,\alpha}U^2_{k,\alpha}}{\omega - \Omega_{k,\alpha} + i\delta} - \frac{Z_{k,\alpha}V^2_{k,\alpha}}{\omega + \Omega_{k,\alpha} - i\delta}$$

$\Sigma_{n,\alpha}(k,0), \Sigma_{a,\alpha}(k,0)$ is normal and anomalous self energies and $Z_{k,\alpha}$ is renormalization constant.

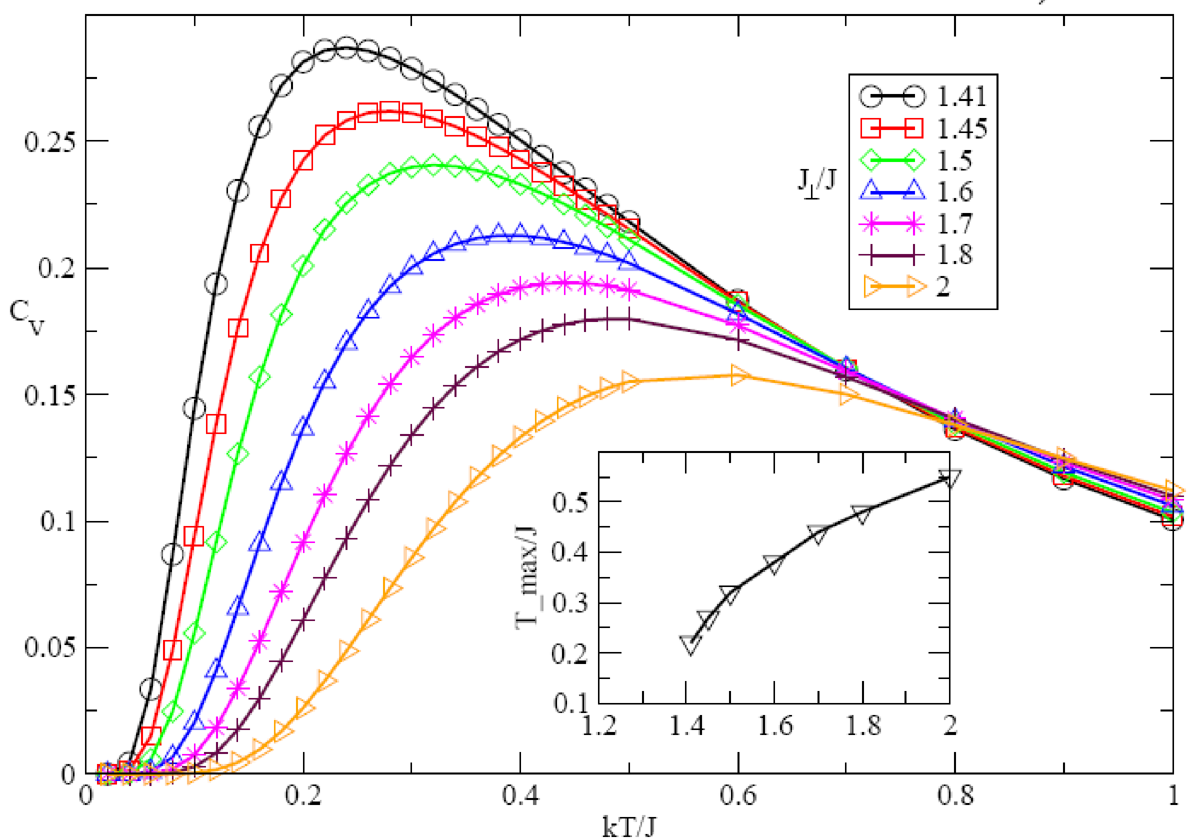
$$Z^{-1}_{k,\alpha} = 1 - \frac{\partial \Sigma_{n,\alpha}(k,0)}{\partial \omega}$$

Interacting Bogoliubov coefficients:

$$U^2_{k,\alpha}, V^2_{k,\alpha} = +,- \frac{1}{2} + \frac{A_{k,\alpha} + \Sigma_{n,\alpha}(k,0)}{2\Omega_{k,\alpha}}$$

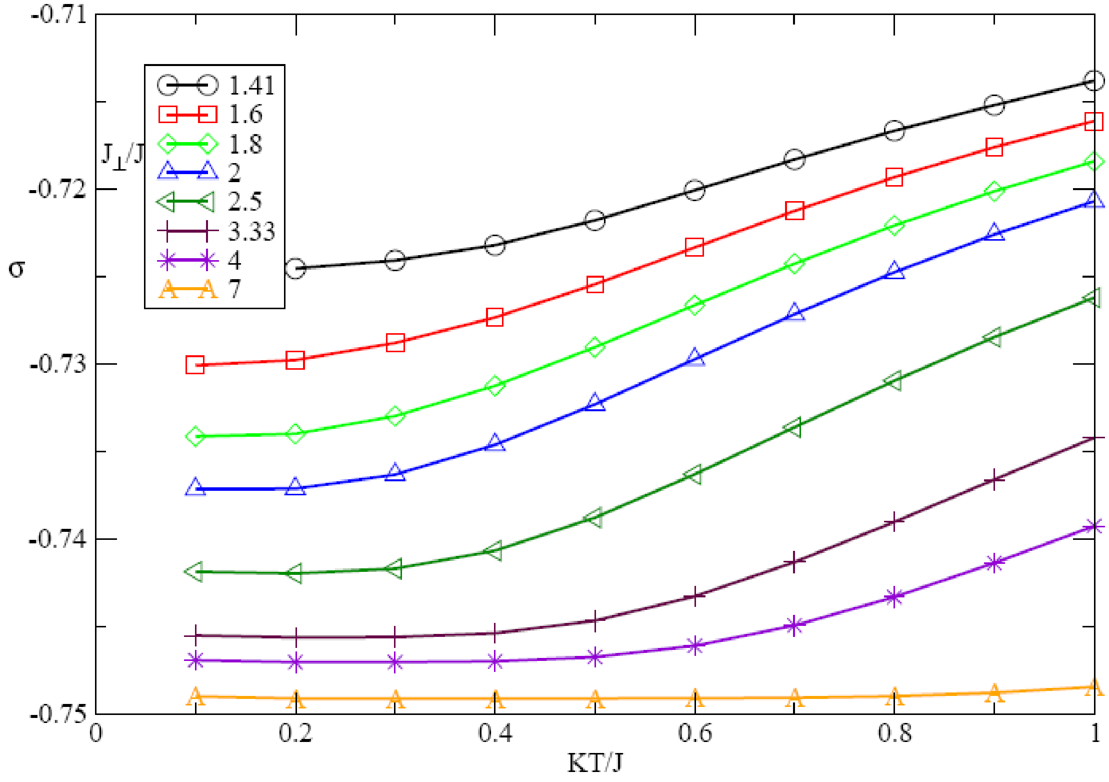
Specific Heat

$$E = \frac{N}{2}\int \frac{d^2k}{(2\pi)^2}\left(\sum_{\alpha=x,y}\frac{J_\perp(1+\Delta)}{2}\left[Z_{\mathbf{k},\alpha}U^2_{\mathbf{k},\alpha}n_B(\Omega_{\mathbf{k},\alpha}) - Z_{\mathbf{k},\alpha}V^2_{\mathbf{k},\alpha}n_B(-\Omega_{\mathbf{k},\alpha})\right] + J_\perp\ \left[Z_{\mathbf{k},z}U^2_{\mathbf{k},z}n_B(\Omega_{\mathbf{k},z}) - Z_{\mathbf{k},z}V^2_{\mathbf{k},z}n_B(-\Omega_{\mathbf{k},z})\right]\right),$$



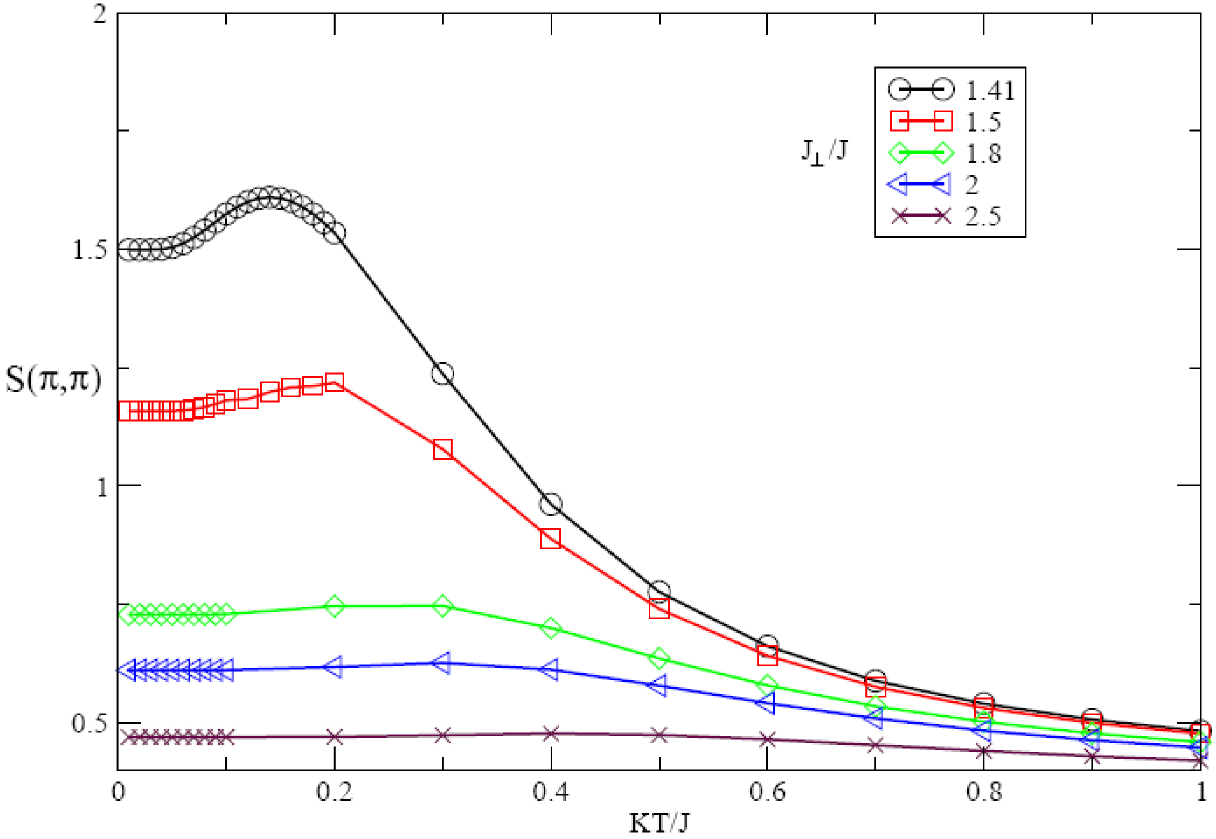
Local cite correlation

$$\sigma = \frac{1}{N}\sum_i \langle \tau_i S_i \rangle$$



Local spin structure factor

$$\chi_{\alpha,\alpha}(q,\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} \langle [S_\alpha(q,t), S_\alpha(-q,0)] \rangle$$



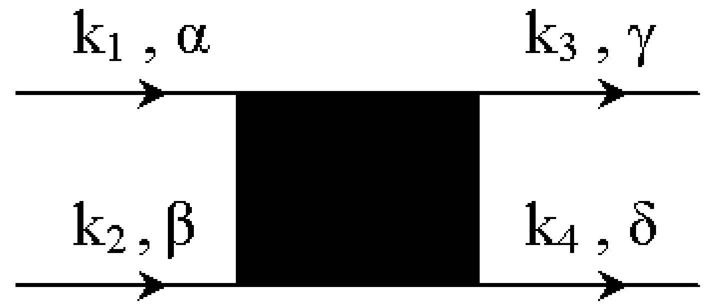
Calculating of hard core self energy

Brueckner approach [Fetter & Walecka] for finding self energy of hard core condition in the dilute Boson gas:

$$H_U = U \sum_{i,\alpha,\beta} t^{\dagger}_{\alpha i} t^{\dagger}_{\beta i} t_{\beta i} t_{\alpha i}$$

$, U$ □□

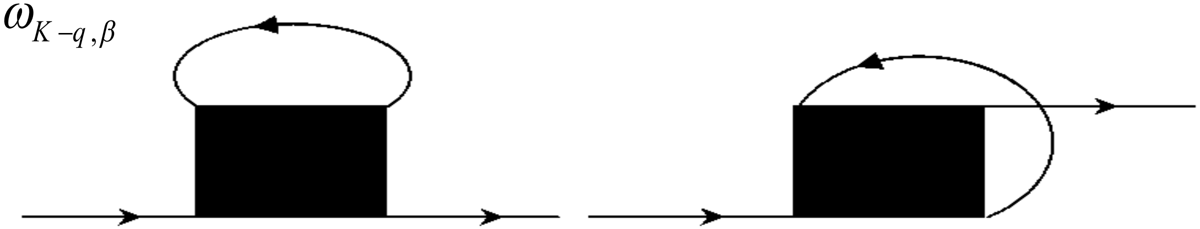
$$\Gamma^{\alpha\beta,\gamma\delta}(K = k_1 + k_2) \boxplus$$



Vertex function (Scattering amplitude)

$$\Gamma^{\alpha\beta,\alpha\beta}(K,\omega) = -\left(\frac{1}{N}\sum_{q} \frac{u^2_{q,\alpha} u^2_{K-q,\beta}}{\omega - \omega_{q,\alpha} - \omega_{K-q,\beta}}\right)^{-1}$$

Hard core part of self energy:

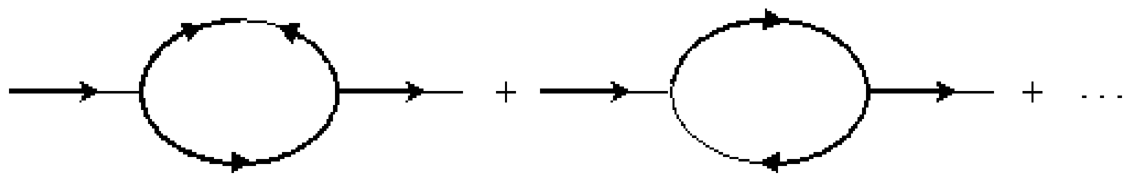


$$\Sigma^{\alpha}_{U}(k,\omega) = \frac{1}{N}\sum_{\beta,q} \Gamma^{\alpha\beta}(k+q, \omega - \omega_q) v^2_{q,\beta}$$

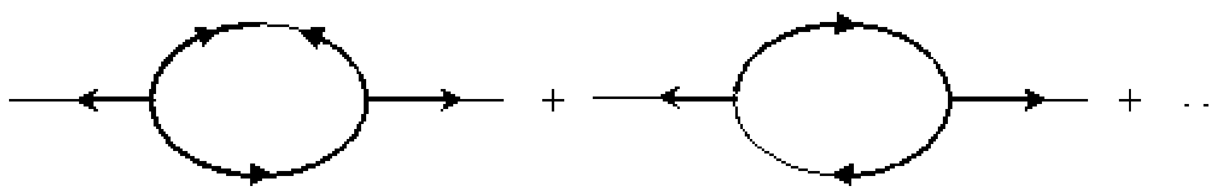
Effects of H_3, H_4 in the spectrum

Second order of perturbation theory and finding of anomalous and normal self energy:

$\Sigma_{n,3}(k,0)$



$\Sigma_{a,3}(k,0)$



By Splitting the quartic operator products into all possible pairs, we have for the following renormalized coefficients of noninteracting

$$A_{k,z} \to A_{k,z} + 2t\xi_k \frac{1}{N}\sum_q v^2_{q,x}\xi_q, \quad A_{k,\alpha=x,y} \to A_{k,\alpha=x,y} + t\xi_k \frac{1}{N}\sum_q (\delta v^2_{q,\alpha=x,y} + v^2_{q,z})\xi_q$$

$$B_{k,z} \to B_{k,z} - 2t\xi_k \frac{1}{N}\sum_q u_{q,x}v_{q,x}\xi_q, \quad B_{k,\alpha=x,y} \to B_{k,\alpha=x,y} - t\xi_k \frac{1}{N}\sum_q (\delta u_{q,\alpha=x,y}v_{q,\alpha=x,y} + u_{q,z}v_{q,z})\xi_q$$