Goethe-Universität Frankfurt
Fachbereich Physik

Institut für Theoretische Physik
Dr. Harald O. Jeschke
Dr. Francesc Salvat-Pujol

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Exercises for Computational Methods in Solid State Theory
SS 2013

Exercise Set 7

(Due date: Tuesday, July 2, 2013)

Exercise 7 (**Susceptibility in random phase approximation**) (10 points)

a) We again use the one band tight binding model we determined for $Sr_2CuO_2Cl_2$ (you can get a simple program from `http://itp.uni-frankfurt.de/~jeschke/CMSST2013/exercise7_ressources/`). Write a program to determine the 2D Fermi surface of $Sr_2CuO_2Cl_2$ at $k_z = 0$ and plot it. Repeat that for 5%, 10% and 20% hole doping.

b) Calculate the noninteracting susceptibility of κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ via

(1)
$$\chi^{pq}_{st}(\vec{q},\omega) = -\frac{1}{NN_{\vec{k}}}\sum_{\vec{k},\mu\nu}\left[f(\varepsilon_\nu(\vec{k}+\vec{q})) - f(\varepsilon_\mu(\vec{k}))\right]\frac{a^s_\mu(\vec{k})a^{p*}_\mu(\vec{k})a^q_\nu(\vec{k}+\vec{q})a^{t*}_\nu(\vec{k}+\vec{q})}{\omega+\varepsilon_\nu(\vec{k}+\vec{q})-\varepsilon_\mu(\vec{k})+i0^+}.$$

where p, q, s, t are orbital indices, μ, ν are band indices and the a^s_μ correspond to the components of the eigenvectors of the tight binding Hamiltonian; $\varepsilon_\nu(\vec{k})$ are the band energies. Use the tight binding model provided at `http://itp.uni-frankfurt.de/~jeschke/CMSST2013/exercise7_ressources/`. Plot the static, homogeneous noninteracting susceptibility

(2)
$$\chi_S(\vec{q}) = \frac{1}{2}\sum_{sp}\chi^{pp}_{ss}(\vec{q},\omega=0),$$

along the path Γ-X-M-Γ with $X = (0,\pi,0)$ and $M = (0,\pi,\pi)$ in the Brillouin zone.

c) Calculate the RPA enhanced transversal susceptibility $\chi^{+-}_{RPA}(\vec{q},\omega)$. Plot $\chi^{+-}_{RPA}(\vec{q},\omega=0)$ along the same path through the Brillouin zone.