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Exercises for Computational Methods in Solid State Theory
SS 2014

Exercise Set 7

(Due date: Monday, July 14, 2014)

Exercise 9 (**Susceptibility in random phase approximation**) (10 points)

a) Use the one band tight binding model we determined for $Sr_2CuO_2Cl_2$. Write a program to determine the 2D Fermi surface of this compound at $k_z = 0$ and plot it. Repeat that for 5%, 10% and 20% hole doping.

b) Calculate the static non-interacting susceptibility of $Sr_2CuO_2Cl_2$ via

(1)
$$\chi^{pq}_{st}(\vec{q}) = -\frac{1}{N}\sum_{\vec{k},\mu,\nu} a^{s}_{\mu}(\vec{k}) a^{p*}_{\mu}(\vec{k}) a^{q}_{\nu}(\vec{k}+\vec{q}) a^{t*}_{\nu}(\vec{k}+\vec{q}) \frac{f(E_\nu(\vec{k}+\vec{q})) - f(E_\mu(\vec{k}))}{E_\nu(\vec{k}+\vec{q}) - E_\mu(\vec{k})},$$

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. The $E_\nu(\vec{k})$ are the band energies. The calculation should be done at a temperature of $\beta = 40\ \mathrm{eV}^{-1}$.

Plot the static homogeneous non-interacting susceptibility

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

along the path Γ-X-M-Γ with reduced coordinates $X = (0.5, 0, 0)$ and $M = (0.5, 0.5, 0)$ in the Brillouin zone.

c) Calculate the RPA interacting susceptibilities $(\chi^{RPA}_{charge})^{pq}_{st}$ and $(\chi^{RPA}_{spin})^{pq}_{st}$ from

(3)
$$\left[(\chi^{RPA}_{spin})^{pq}_{st}\right]^{-1} = [\chi^{pq}_{st}]^{-1} - (U_{spin})^{pq}_{st}$$

(4)
$$\left[(\chi^{RPA}_{charge})^{pq}_{st}\right]^{-1} = [\chi^{pq}_{st}]^{-1} + (U_{charge})^{pq}_{st}.$$

Here $(U_{charge})^{pq}_{st} = (U_{spin})^{pq}_{st} = U$, for which an appropriate value has to be chosen.

Plot the RPA spin and charge susceptibilities along the same path through the Brillouin zone.