How to plot magnetic calculation in non-magnetic BZ

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The general expression for the GS is

$$G_{\mathbf{k}_0}(\omega)=\sum_i \int d\mathbf{r}d\mathbf{r}' e^{-i\mathbf{k}_0\mathbf{r}}\psi_{i\mathbf{k}}(\mathbf{r})\frac{1}{\omega-\epsilon^i_{\mathbf{k}}}\psi^*_{i\mathbf{k}}(\mathbf{r}')e^{i\mathbf{k}_0\mathbf{r}'} \quad (1)$$

with k_0 an arbitrary momentum. Here

$$\psi_{i\mathbf{k}}(\mathbf{r})=\sum_{i\mathbf{K}} A^{\mathbf{k}}_{i\mathbf{K}}\chi_{\mathbf{k}+\mathbf{K}}(\mathbf{r}) \quad (2)$$

are Kohn-Sham solutions, and χ are basis functions. We hence have

$$G_{\mathbf{k}_0}(\omega)=\sum_i\sum_{\mathbf{K}_1,\mathbf{K}_2}\langle e^{-i\mathbf{k}_0\mathbf{r}}|\chi_{\mathbf{k}+\mathbf{K}_1}(\mathbf{r})\rangle A^{\mathbf{k}}_{i\mathbf{K}_1}\frac{1}{\omega-\epsilon^i_{\mathbf{k}}}A^{\mathbf{k}*}_{i\mathbf{K}_2}\langle\chi_{\mathbf{k}+\mathbf{K}_2}(\mathbf{r}')|e^{i\mathbf{k}_0\mathbf{r}'}\rangle \quad (3)$$

For plane wave basis, the matrix elements are

$$\langle e^{-i\mathbf{k}_0\mathbf{r}}|\chi_{\mathbf{k}+\mathbf{K}}(\mathbf{r})\rangle=\delta_L(\mathbf{k}+\mathbf{K}-\mathbf{k}_0)$$

where δ_L requires that $\mathbf{k}+\mathbf{K}=\mathbf{k}_0$ up to reciprocal vector of the non-magnetic unit cell!

In order to avoid computing annoying matrix elements, we will use the same expression also in the LAPW basis set. We just need to generalized it for the non-orthogonal basis set. The generalization is

$$G_{\mathbf{k}_0}(\omega)=\sum_{\mathbf{K}_1,\mathbf{K}_2,i}\delta_L(\mathbf{k}+\mathbf{K}_1-\mathbf{k}_0)A^{\mathbf{k}}_{i\mathbf{K}_1}\frac{1}{\omega-\epsilon^i_{\mathbf{k}}}A^{\mathbf{k}*}_{i\mathbf{K}_2}\delta_L(\mathbf{k}+\mathbf{K}_2-\mathbf{k}_0)\langle\chi_{\mathbf{k}+\mathbf{K}_1}|\chi_{\mathbf{k}+\mathbf{K}_2}\rangle \quad (4)$$

In order to plot fat-bands (with character), we can express G inside the muffin thin sphere in the following way

$$G^{L_1L_2}_{\mathbf{k}_0}(\omega)=\sum_{\mathbf{K}_1\mathbf{K}_2,i}\delta_L(\mathbf{k}+\mathbf{K}_1-\mathbf{k}_0)A^{\mathbf{k}}_{i\mathbf{K}_1}a^{\kappa_1}_{L_1}(\mathbf{k}+\mathbf{K}_1)\frac{1}{\omega-\epsilon^i_{\mathbf{k}}}A^{\mathbf{k}*}_{i\mathbf{K}_2}a^{\kappa_2*}_{L_2}(\mathbf{k}+\mathbf{K}_2)\delta_L(\mathbf{k}+\mathbf{K}_2-\mathbf{k}_0)\langle u^{\kappa_1}_{l_1}|u^{\kappa_2}_{l_2}\rangle \quad (5)$$

which can also be written as

$$G^{L_1L_2}_{\mathbf{k}_0}(\omega)=\sum_{i\kappa_1\kappa_2}\mathcal{A}^{\kappa_1}_{iL_1}(\mathbf{k})\frac{1}{\omega-\epsilon^i_{\mathbf{k}}}\mathcal{A}^{\kappa_2*}_{iL_2}(\mathbf{k})\langle u^{\kappa_1}_{l_1}|u^{\kappa_2}_{l_2}\rangle \quad (6)$$

with

$$\mathcal{A}^{\kappa}_{iL}(\mathbf{k})=\sum_{\mathbf{K}}\delta_L(\mathbf{k}+\mathbf{K}-\mathbf{k}_0)A^{\mathbf{k}}_{i\mathbf{K}}a^{\kappa}_L(\mathbf{k}+\mathbf{K}) \quad (7)$$

This expression is used to compute partial density of states in QTL and DMFT, except that δ_L-functions then requires that $\mathbf{k}=\mathbf{k}_0$ and $\mathbf{K}$ can be any reciprocal vector.

For magnetic calculation, we need to perform calculation in bigger unit cell. Hence we have shorter reciprocal vectors. Out of reciprocal vectors of the magnetic BZ, we need to find those which are reciprocal vectors of non-magnetic BZ. Then the sum over $\mathbf{K}$ above should be performed only over the non-magnetic reciprocal vectors. If $\mathbf{k}_0$ is in first-BZ of the magnetic unit cell, or is outside

it, a different set of reciprocal vectors will be summed over.