How to plot magnetic calculation in non-magnetic BZ

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I. DERIVATION 1

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 recip-

rocal 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.

II. ALTERNATIVE DERIVATION

The green's function of LDA+DMFT in real space, expressed in terms of the Kohn-Sham states $\psi_{i\mathbf{k}}(\mathbf{r})$, is

$$G(\mathbf{r},\mathbf{r}') = \sum_{ij\mathbf{k}} \psi_{i\mathbf{k}}(\mathbf{r}) \left(\frac{1}{\omega+\mu-\varepsilon_{\mathbf{k}}-P_{\mathbf{k}}\Sigma} \right)_{ij} \psi^*_{j\mathbf{k}}(\mathbf{r}') \tag{8}$$

Below, we will use the notation

$$\left(\frac{1}{\omega+\mu-\varepsilon_{\mathbf{k}}-P_{\mathbf{k}}\Sigma} \right)_{ij} \equiv g_{\mathbf{k}ij} \tag{9}$$

Magnetic unit cell is bigger, and hence we can write Green's function on sublatice A, on sublatice B, and the off-diagonal Green's function. If the Green's function is written in the position representation within the unit cell, it is easy to derive the green's function in the non-magnetic unit cell. The result is

$$\begin{pmatrix} G_{\mathbf{k},AA} & G_{\mathbf{k},AB} \\ G_{\mathbf{k},BA} & G_{\mathbf{k},BB} \end{pmatrix} \rightarrow \tag{10}$$

$$G_{\mathbf{k}} = G_{\mathbf{k},AA} + G_{\mathbf{k},BB} + G_{\mathbf{k},AB}e^{i\mathbf{k}\delta} + G_{\mathbf{k},BA}e^{-i\mathbf{k}\delta} \tag{11}$$

Here δ is the vector connecting sublatice A and sublatice B. For the checkerboard AFM state, this vector is for example $(1,0,0)$.

We want to write the LAPW Green's function in terms of the four components of sublattices. We first note that the Kohn-Sham solutions $\psi_{i\mathbf{k}}(\mathbf{r})$ are expanded in terms of LAPW basis set functions $\chi_{\mathbf{k}+\mathbf{K}}(\mathbf{r})$ in the following way

$$\psi_{i\mathbf{k}}(\mathbf{r}) = \sum A^{\mathbf{k}}_{i\mathbf{K}} \chi_{\mathbf{k}-\mathbf{K}}(\mathbf{r}) \tag{12}$$

where $A^{\mathbf{k}}_{\mathbf{k}-\mathbf{K}}$ are eigenvectors, written in *case.vector*. Since the LAPW basis functions transform under shift in the same way as plane waves, we have

$$G(\mathbf{r}_1+\delta_1,\mathbf{r}_2+\delta_2) = \sum_{ij\mathbf{k},\mathbf{K},\mathbf{K}'} A^{\mathbf{k}}_{i\mathbf{K}} e^{i(\mathbf{k}-\mathbf{K})\delta_1} \chi_{\mathbf{k}-\mathbf{K}}(\mathbf{r}_1) g_{\mathbf{k}ij} \chi^*_{\mathbf{k}-\mathbf{K}'}(\mathbf{r}_2) e^{-i(\mathbf{k}-\mathbf{K}')\delta_2} A^{\mathbf{k}*}_{j\mathbf{K}'} \tag{13}$$

The generalized expression for G in the non-magnetic unit cell, in terms of the four components of the Green's function, is

$$G_{\mathbf{k}} = \int d\mathbf{r} \left[G(\mathbf{r},\mathbf{r}) + G(\mathbf{r},\mathbf{r}+\delta)e^{i\mathbf{k}\delta} + G(\mathbf{r}+\delta,\mathbf{r})e^{-i\mathbf{k}\delta} + G(\mathbf{r}+\delta,\mathbf{r}+\delta) \right] \tag{14}$$

Using the above expression for $G(\mathbf{r}_1+\delta 1,\mathbf{r}_2+\delta_2)$, we have

$$G_{\mathbf{k}} = \sum_{ij\mathbf{K},\mathbf{K}'} A^{\mathbf{k}}_{i\mathbf{K}} O^{\mathbf{k}}_{\mathbf{K}\mathbf{K}'} A^{\mathbf{k}*}_{j\mathbf{K}'} g_{\mathbf{k}ij} (1 + e^{i\mathbf{K}'\delta} + e^{-i\mathbf{K}\delta} + e^{i(\mathbf{K}'-\mathbf{K})\delta}) \tag{15}$$

where overlap is

$$O^{\mathbf{k}}_{\mathbf{K}\mathbf{K}'} = \langle \chi_{\mathbf{k}-\mathbf{K}'} | \chi_{\mathbf{k}-\mathbf{K}} \rangle. \tag{16}$$

It is clear that $e^{i\mathbf{K}\delta}$ is unity for the reciprocal vectors of the non-magnetic unit cell, and it is -1 for the new reciprocal vectors, which are not part of the non-magnetic unit cell. Hence, if one of the $\mathbf{K}$ in the above expression is the "new" reciprocal vector, and one is "old" (part of the non-magnetic reciprocal set), the sum of the exponents in the bracket vanishes. The same is true when both $\mathbf{K}$ and $\mathbf{K}'$ are "new" vectors, because $\mathbf{K}'-\mathbf{K}$ is now the "old" vector, and hence $e^{i(\mathbf{K}'-vK)\delta} = 1$. We see that only the terms which include the original non-magnetic reciprocal vectors survive in the above expression. Hence the expression is equivalent to the expression in the previous chapter, but it is more convenient for implementation. To compute it, we only need Kohn-Sham eigenvectors $A^{\mathbf{k}}_{i\mathbf{K}}$, since the overlap can also be expressed in terms of the overlap. The eigenvalue problem demands $AOA^\dagger = 1$, hence

$$\sum_{\mathbf{K}\mathbf{K}'} A^{\mathbf{k}}_{i\mathbf{K}} O^{\mathbf{k}}_{\mathbf{K}\mathbf{K}'} A^{\mathbf{k}}_{j\mathbf{K}'} = \delta_{ij} \tag{17}$$

We use SVD decomposition to invert eigenvectors (because they are not quadratic matrice). The SVD is

$$A = UZV \tag{18}$$

where U and V are unitary matrices, and Z are singular values. We then have

$$O = V^\dagger \frac{1}{Z} U^\dagger U \frac{1}{Z} V. \tag{19}$$

We would like to write the final expression in a more compact way. We define the "coherence"-like factors

$$C^{\mathbf{k}}_{ji} = \sum_{\mathbf{K}\mathbf{K}'} A^{\mathbf{k}}_{i\mathbf{K}} O^{\mathbf{k}}_{\mathbf{K}\mathbf{K}'} A^{\mathbf{k}*}_{j\mathbf{K}'} (1 + e^{i\mathbf{K}'\delta} + e^{-i\mathbf{K}\delta} + e^{i(\mathbf{K}'-\mathbf{K})\delta}) \tag{20}$$

and note that G is then simply given by

$$G_{\mathbf{k}} = \sum_{ij} C^{\mathbf{k}}_{ji}\, g_{\mathbf{k}ij}. \tag{21}$$

Finally, it is convenient to express the Green's function in terms of the LDA+DMFT eigenvalues and LDA+DMFT eigenvectors. We note that the LDA+DMFT green's function expressed in Kohn-Sham basis is

$$g_{\mathbf{k}ij} = A^{R}_{\mathbf{k}\omega,il} \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}l\omega}} A^{L}_{\mathbf{k}\omega,lj} \tag{22}$$

Hence, we can define the LDA+DMFT frequency dependent "coherence" factors

$$\widetilde{C}^{\mathbf{k}}_{l\omega} = \sum_{ij} A^{L}_{\mathbf{k}\omega,lj} C^{\mathbf{k}}_{ji} A^{R}_{\mathbf{k}\omega,il} \tag{23}$$

In terms of these "coherence" factors we finally have

$$G_{\mathbf{k}} = \sum_{l} \frac{\widetilde{C}^{\mathbf{k}}_{l\omega}}{\omega + \mu - \varepsilon_{\mathbf{k}\omega l}} \tag{24}$$