Implementing electric quadrupole transition in FPMS

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Muffin-tin approximation is commonly used for multiple scattering calculation, in this framework the electronic charge density and potential of each scattering sites are spherically averaged. However, when the anisotropy of them is not negligible, this spherical approximation is not appropriate. Hence we need to go beyond such treatment and use full-potential, that is to say, without using this spherical averaging but real potential as it is.

We have implemented Full-Potential Multiple-Scattering (FPMS) theory [1] and a code named FPMS based on the theory. The code calculates X-ray Absorption Spectroscopy (XAS) within electric dipole approximation. As is well known, we need a higher term of expansion of $exp[i(\boldsymbol{k}\cdot\boldsymbol{r})]$ in hard X-ray regime. In the absence of the magnetic field, the cross section is written [2]

$$\sigma(\omega) = 4\pi^2\alpha\hbar\omega\sum_{if}\left\{|\langle f|\hat{\boldsymbol{\varepsilon}}\cdot\boldsymbol{r}|i\rangle|^2 + \frac{1}{4}|\langle f|(\hat{\boldsymbol{\varepsilon}}\cdot\boldsymbol{r})(\boldsymbol{k}\cdot\boldsymbol{r})|i\rangle|^2\right\}\delta(E_f - E_i - \hbar\omega). \quad (1)$$

Here we used the fact that when the incident X-ray is linearly polarized, the matrix elements $|\langle f|\hat{\boldsymbol{\varepsilon}}\cdot\boldsymbol{r}|i\rangle|$ and $|\langle f|(\hat{\boldsymbol{\varepsilon}}\cdot\boldsymbol{r})(\boldsymbol{k}\cdot\boldsymbol{r})|i\rangle|$, which are the electric dipole and quadrupole transition amplitudes respectively, are real and do not interfere each other.[2] We implemented this electric quadrupole transition term within FPMS framework, so that the T-matrix and radial solutions of each site become matrices. (For the Muffin-tin case, they are vectors.) Therefore, the selection rules are modified from the Muffin-tin case and becomes more complicated forms. In this work, we present differences of the formulas between Muffin-tin and full-potential cases.

References

[1] K. Hatada, K. Hayakawa, M. Benfatto and C. R Natoli, *J. Phys.: Condens. Matter* **22**, 185501 (2010).

[2] C. Brouder *J. Phys.:Condens.Matter* **2**, 701-738 (1990).