Possible form of multi-polar interaction in cubic lattice

Osamu Sakai [a,1], Ryousuke Shiina [a], Hiroyuki Shiba [b]

[a] *Department of Physics, Tokyo Metropolitan University, Tokyo 192-0397, Japan*
[b] *Department of Physics, Kobe University, Kobe 657-8501, Japan*

Abstract

The invariant form of interaction between multi-poles, including the octupole, is studied for the simple cubic(*s.c*), body centered(*b.c.c.*) and face centered (*f.c.c*) cubic lattices. The coupling terms can be arranged in a way similar to that of the hopping matrix between the LCAO's. A table for *s.c.* by Shiina et. al. (J. Phys. Soc. Jpn. **66** (1997) 1741) is generalized for the general wave number case of the three types of lattice. Recent experimental result of TmTe is thereby analyzed. The development of the ferromagnetic moment below the anti-ferromagnetic transition under the anti-ferro quadrupolar order phase is discussed in this connection.

Key words: anti-ferro quadrupolar ordering, multi-polar interaction in solid, neutron diffraction, TmTe

1. Introduction

The identification of the anti-ferro quadrupolar ordering (AFQ) is intensively being tried in various methods[1]. The application of the magnetic field in the AFQ state usually induces the anti-ferro magnetic moment (AFM).The symmetry analysis of the AFQ order parameter of AFQ using the induced AFM seems to be a promising method. In fact, such approach has been extensively applied to CeB_6 [2–4], and recently to TmTe[5–7]. The product of AFQ moment and the magnetic field has symmetry of the octupole moment.

Shiina et. al. presented a table which gives grouping of concurrent induced AFM and AFQ order parameters in *s.c.* based on the symmetry argument[3]. It was successfully applied to determine the AFQ order parameter of TmTe by Mignot et. al[6,7]. In general, however, the grouping should be made based on the small group of the wave number of the ordering. Therefore cares are needed to apply the table of *s.c.* for TmTe of *f.c.c.*, because they have different point symmetry at the L-point, $\mathbf{Q} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

The grouping of order parameter based on the small group for various wave vectors is rather a formidable work. If one can derive the expression of the invariant interaction between multipoles for general $\mathbf{q}$, the grouping can be carried out without the symmetry argument only by setting $\mathbf{q} = \mathbf{Q}$.

As an example, let us consider the interaction between the quadrupolar moments of Γ_5^+ at a site (say, 0-site) and the quadrupolar moments of Γ_3^+ type on the 12 nearest neighbor sites (*n.n.* shell). ¿From 24 operators on the *n.n.* shell, we can make a combination of operators, $-O(u,110)+O(u,1\bar{1}0)+O(u,\bar{1}10)-O(u,\bar{1}\bar{1}0)$, which has the xy symmetry around the 0-site. Here we have used notation: $O_2^0 = O(u)$ and $O_2^2 = O(v)$. This expression has the same form to that of the LCAO on *n.n.* shell, and other combinations which have the yz and zx symmetry are also prepared. The invariant form is made by the product between these symmetrized operators and the operators on the 0-site.

Next we make the Fourier transformation $O(\gamma, \mathbf{R}_\ell) = \sum_{\mathrm{q}} O(\gamma, \mathbf{q}) \mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{R}_\ell}$, where $\mathbf{R}_\ell$ denotes the site, and γ denotes the symmetry of multipolar operator. The interaction between the nearest neighbor pairs of quadrupolar moments are given as follows.

$$H_{even}^{fcc} = a_1 [O_{u,-\mathbf{q}} O_{u,-\mathbf{q}} c_x c_y$$

[1] Corresponding author. Department of Physics, Tokyo Metropolitan University, Tokyo 192-0397, Japan E-mail: sakai@phys.metro-u.ac.jp

$$
\begin{aligned}
&+\frac{1}{2}(O_{u,-\mathbf{q}}-\sqrt{3}O_{v,-\mathbf{q}})\frac{1}{2}(O_{u,\mathbf{q}}-\sqrt{3}O_{v,\mathbf{q}})c_yc_z \\
&+\frac{1}{2}(O_{u,-\mathbf{q}}+\sqrt{3}O_{v,-\mathbf{q}})\frac{1}{2}(O_{u,\mathbf{q}}+\sqrt{3}O_{v,\mathbf{q}})c_zc_x] \\
&+a_2[O_{v,-\mathbf{q}}O_{v,-\mathbf{q}}c_xc_y \\
&+\frac{1}{2}(\sqrt{3}O_{u,-\mathbf{q}}+O_{v,-\mathbf{q}})\frac{1}{2}(\sqrt{3}O_{u,\mathbf{q}}+O_{v,\mathbf{q}})c_yc_z \\
&+\frac{1}{2}(\sqrt{3}O_{u,-\mathbf{q}}-O_{v,-\mathbf{q}})\frac{1}{2}(\sqrt{3}O_{u,\mathbf{q}}-O_{v,\mathbf{q}})c_zc_x] \\
&+a_3[O_{xy,-\mathbf{q}}O_{u,\mathbf{q}}s_xs_y \\
&+O_{yz,-\mathbf{q}}\frac{1}{2}(-O_{u,\mathbf{q}}+\sqrt{3}O_{v,\mathbf{q}})s_ys_z \\
&+O_{zx,-\mathbf{q}}\frac{1}{2}(-O_{u,\mathbf{q}}-\sqrt{3}O_{v,\mathbf{q}})s_zs_x] \\
&+a_4[O_{xy,-\mathbf{q}}O_{xy,\mathbf{q}}c_xc_y+\text{c.p.}] \\
&+a_5[O_{xy,-\mathbf{q}}O_{xy,\mathbf{q}}(c_yc_z+c_zc_x)+\text{c.p.}] \\
&+a_6[O_{xy,-\mathbf{q}}O_{yz,\mathbf{q}}s_zs_x+\text{c.p.}]. \qquad (1)
\end{aligned}
$$

Here $c_\nu(s_\nu)$ denotes $\cos\pi q_\nu(\sin\pi q_\nu)$, and c.p. means the cyclic permutation. The summation over $\mathbf{q}$ is assumed. The term having the factor a_3 corresponds to the interaction between Γ_5^+ and Γ_3^+ moments explained as the example.

The interaction between multipoles with odd power of the angular momentum are also given as,

$$
\begin{aligned}
H^{fcc}_{odd} = &\, b_1[J_{x,-\mathbf{q}}J_{x,\mathbf{q}}c_yc_z+\text{c.p.}] \\
&+b_2[J_{x,-\mathbf{q}}J_{x,\mathbf{q}}(c_zc_x+c_yc_x)+\text{c.p.}] \\
&+b_3[J_{x,-\mathbf{q}}J_{y,\mathbf{q}}s_xs_y+\text{c.p.}] \\
&+b_4[T_{xyz,-\mathbf{q}}(J_{x,\mathbf{q}}s_ys_z+\text{c.p.})] \\
&+b_5[J_{x,-\mathbf{q}}T^{\beta}_{x,\mathbf{q}}c_x(c_y-c_z)+\text{c.p.}] \\
&+b_6[J_{x,-\mathbf{q}}(T^{\beta}_{y,\mathbf{q}}s_xs_y-T^{\beta}_{z,\mathbf{q}}s_zs_x)+\text{c.p.}] \\
&+b_7[T^{\beta}_{x,-\mathbf{q}}T^{\beta}_{x,\mathbf{q}}c_yc_z+\text{c.p.}] \\
&+b_8[T^{\beta}_{x,-\mathbf{q}}T^{\beta}_{x,\mathbf{q}}(c_xc_y+c_zc_x)+\text{c.p.}] \\
&+b_9[T^{\beta}_{x,-\mathbf{q}}T^{\beta}_{y,-\mathbf{q}}s_xs_y+\text{c.p.}] \\
&+b_{10}[T_{xyz,-\mathbf{q}}T_{xyz,\mathbf{q}}(c_xc_y+\text{c.p.})]. \qquad (2)
\end{aligned}
$$

Terms in which J_ν are replaced by T^{α}_{ν} should be added.

When we put $\mathbf{q}=\mathbf{Q}$, and make rearrangement of operators, the quadrupolar moments are grouped as $(O(u), 2O(xy)-O(yz)-O(zx))$, $(O(v), O(yz)-O(zx))$ and $(O(xy)+O(yz)+O(zx))$ which couple with each other in the same group. Here the suffix $\mathbf{Q}$ is dropped. The odd terms are also grouped as $(J_x+J_y+J_z, T_{xyz}, T^{\beta}_x+T^{\beta}_y+T^{\beta}_z)$, $(2J_z-J_x-J_y, T^{\beta}_x-T^{\beta}_y)$ and $(J_x-J_y, 2T^{\beta}_z-T^{\beta}_x-T^{\beta}_y)$. This grouping is equivalent to $H\parallel[111]$ case of *s.c.* Even when the field is not applied, the symmetry is lowered to D_{3d} in *f.c.c.* The *n.n.n.* pair interaction is obtained from the expression of *s.c.*, but the new grouping is not generated.

To classify the grouping under the magnetic field, the product between the AFQ moment and the field H_x, H_y, H_z are rearranged to have symmetrized combination of octupoles[9].

When the field $H\parallel[110]$ is applied, the products are classified by comparing with the the grouping of odd terms under the condition $H_x=H_y$. Then the operators are combined into two groups: $(O(u), \cdot\cdot, O(xy)+O(yz)+O(zx), J_x+J_y+J_z, \cdot\cdot, 2J_z-J_x-J_y, \cdot\cdot)$ and $(O(v), \cdot\cdot, J_x-J_y, \cdot\cdot)$. In the place of $(\cdot\cdot)$, terms should be added following the grouping of $H=0$. The AFM of J_x-J_y is observed in experiment, thus the AFQ of $O(v)$ type will be the candidate as concluded by Link et. al[6]. We note that the AFQ is necessarily mixed combination of $O(v)$ and $O(yz)-O(zx)$. If the AFQ had $O(u)$ character, the AFM would appear in the [110]-[001] plane.

When the field $H\parallel[001]$ is applied, we obtain the same grouping to that of the $H\parallel[110]$ case. Therefore we expect the AFM of J_x-J_y type in the $\mathbf{Q}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ domain. The AFM will not be expected if one uses the table for *s.c*[7]. A tilting of field into the [110] direction will be necessary to align the $\mathbf{Q}$ domains.

When the spontaneous AFM magnetization of J_x-J_y appears in the AFQ of $O(v)$ group, the ferromagnetic moment in the [110]-[001] plane will appear. This has been already expected in ref. [10] based on a microscopic model, and has been proved in experiment[7].

Acknowledgements

The authors would like to thank J.-M. Mignot for sending us preprints before publication, and stimulation. The numerical computation was partly performed in the Computer Center of Tohoku University and the Supercomputer Center of Institute for Solid State Physics (University of Tokyo).

References

[1] See for example, *Proceedings of the International Conference on Strongly Correlated Electrons with Orbital Degrees of Freedom* eds. K. Hirota, H. Aoki, Y. Kuramoto, J. Phys. Soc. Jpn. **71** (2002) Supplement.

[2] J. M. Effantin, et. al., J. Magn. Magn. Mater. **47&48** (1985) 145.

[3] R. Shiina, et. al. J. Phys. Soc. Jpn. **66** (1997) 1741.

[4] O. Sakai, et. al., J. Phys. Soc. Jpn. **66** (1997) 3005.

[5] T. Matsumura, et. al., J. Phys. Soc. Jpn. **67** (1998) 612.

[6] P. Link, et. al., Phys. Rev. Lett. **80** (1998) 4779

[7] J.-M. Mignot, et. al., J. Phys. Soc. Jpn. **71** (2002) Suppl. 39.

[8] R. Shiina,et. al., J. Phys. Soc. Jpn.**68** (1999) 2105.

[9] O. Sakai, et. al., to be submitted to J. Phys. Soc. Jpn.

[10] R. Shiina, et. al. J. Phys. Soc. Jpn. **68** (1999) 2390.