

A Theoretical Study of Influence of Lattice Structure on Multi Pole of f-electron Systems

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ABSTRACT

Using the theoretical formalism of K Kubo, *et al.*⁷ and R Yamamura *et al.*,⁸, we have theoretically studied the influence of lattice structure on multi pole interaction in f-electron systems. We have applied second order perturbation theory with respect to intersite hopping.

The derivation of multi pole interactions was performed for different lattice interactions. One obtains quadrupole interaction for SC lattice, octupole interaction for bcc lattice and for fcc lattice both interactions were observed.

It appears that lattice structure plays essential role in the multi pole ordering. The general tendencies of the multi pole interactions were discussed and the results were compared with those of the Γ_8 quartet systems of f^1 ions. We have also mentioned the effective f-f hopping. The important point is that the symmetry of f-orbitals restrict the form of hopping for the both cases of lattice structure. The work will be quite helpful for those who will be interested to understand the influence of lattice structure and also to know the multi pole interactions.

Keywords: multi pole interaction, Second order perturbation theory, Dipole, quadrupole and octupole interaction, Multi pole fluctuations, f-f hopping, Anisotropic magnetization, CEF ground state, Kramers theorem.

INTRODUCTION

In the field of the f-electron systems, the phenomena which originate from the multi pole degrees of freedom have been widely studied. Such degrees of freedom, in addition to the dipole are expected to become source of exotic ordering and physical properties. The quadrupole moments couples to lattice and its influence can be detected by ultrasonic measurements¹. In recent years, even the effects of the octupole moment have been studied. One of the most representative phenomena discovered in multi pole physics is the quadrupole and octupole ordering. Resonant X-ray scattering, NMR, anisotropic magnetization and neutron scattering have confirmed the octupole order²⁻⁶. In these compounds, the crystalline electric field(CEF) ground state is Γ_8 quartet. This has sufficient degrees of freedom to possess quadrupole, octupole and even dipole moments. Therefore Γ_8 quartet has been regarded as an ideal system for multi pole physics.

The anisotropy in the multi pole moment are closely tied to the real space direction and the multi pole interactions are intrinsically anisotropic. It is the sharp contrast to the isotopic spin-spin interaction in a system without spin-orbit coupling. Thus, the nature of the multi pole interactions in a system can depend drastically on lattice structure.

MATHEMATICAL FORMULAE USED IN THE STUDY

The model Hamiltonian is given by

$$H=H_{kin} +H_{loc} \quad (1)$$

Here H_{kin} is the kinetic energy term. H_{loc} is the local part of the Hamiltonian. The local part of the Hamiltonian is given by

$$H_{loc} = \Delta \sum_r (n_{r8} - n_{r7}) + J_{78} \sum_r s_{r7}^{\rightarrow} \cdot s_{r8}^{\rightarrow} \quad (2)$$

$$\text{Here, } n_{r7} = \sum_{\sigma} c_{r7\sigma}^{\dagger} c_{r7\sigma} \quad (3a)$$

$$n_{r8} = \sum_{\tau\sigma} c_{r\tau\sigma}^{\dagger} c_{r\tau\sigma} \quad (3b)$$

$$s_{r7}^{\rightarrow} = \frac{1}{2} \sum_{\sigma\sigma'} c_{r7\sigma}^{\dagger} \sigma_{\sigma\sigma'}^{\rightarrow} c_{r7\sigma'} \quad (3c)$$

$$s_{r8}^{\rightarrow} = \frac{1}{2} \sum_{\tau\sigma\sigma'} c_{r\tau\sigma}^{\dagger} \sigma_{\sigma\sigma'}^{\rightarrow} c_{r\tau\sigma'} \quad (3d)$$

Here, $\tau = \alpha$ or β and σ are the Pauli matrices. Δ denotes the CEF level splitting and J_{78} denotes the coupling constant of the anti-ferromagnetic interactions between the Γ_7 and Γ_8 orbitals.

For a sufficiently large J_{78} the f^2 ground states are spin singlets composed of the Γ_7 and Γ_8 orbitals.

$$|\tau(r^{\rightarrow})\rangle = B_{\sigma\sigma'} c_{r\tau\sigma}^{\dagger} c_{r\tau\sigma'}^{\dagger} |0\rangle \quad (4)$$

These states constitute a basis of the Γ_3 representation of cubic symmetry. The present model is one of the simplest model to realize the Γ_3 ground state. Now one considers the exchange process between nearest neighbor sites with the Γ_3 ground state. Among the intermediate f^1 - f^2 states, one considers only the lowest energy states. If the f^3 site has zero or two Γ_7 electrons, it cannot gain the energy from the anti-ferromagnetic interaction. The intermediate f^1 states are the Γ_7 states.

$$|\sigma(r^{\rightarrow})\rangle = c_{r\sigma}^{\dagger} |0\rangle \quad (5)$$

One calculates the matrix elements of the annihilation operator of the Γ_8 electron between the f^1 and the Γ_3 states. The effect of the annihilation operator on the Γ_3 state is written as

$$c_{r\tau\sigma} |\tau'(r^{\rightarrow})\rangle = B_{\tau\sigma,\sigma'}^{\tau'} |\sigma'(r^{\rightarrow})\rangle \quad (6)$$

The hopping process are described by the kinetic energy term of the Hamiltonian for the Γ_8 orbitals.

$$H_{kin} = \sum_{r,\mu,\tau,\sigma,\tau',\sigma'} c_{r+\mu\tau\sigma}^{\dagger} t_{\tau\sigma,\tau'\sigma'}^{\mu} c_{\tau\tau'\sigma'} \quad (7)$$

μ connects nearest neighbor sites. One introduces $\nu = (\tau, \sigma)$, Since H_{kin} is Hermitian $t_{\nu\nu'}^{\mu} = t_{\nu\nu'}^{-\mu}$.

MULTI POLE INTERACTION

By applying the second order perturbation theory with respect to H_{kin} , one derives the effective Hamiltonian

$$H^{(eff)} = \sum_{a,b,u} \sum_{m \neq 0} |0,a\rangle \langle 0,a| H_{kin} \frac{|m,u\rangle \langle m,u|}{E_0 - E_n} H_{kin} |0,b\rangle \langle 0,b| \quad (8)$$

Here, $|0,a\rangle$ is a ground state without H_{kin} , with the energy E_0 and $|m,u\rangle$ is the m -th excited state with the energy E_{kin} . Now, one considers only the first excited states which are described by a pair of nearest neighboring f^1 and f^3 sites

Now, one can show the effective Hamiltonian for SC lattice, bcc lattice and fcc lattice for both quadrupole and octupole interactions.

SC lattice

For the SC lattice, one obtains only the following quadrupole interaction,

$$H^{eff} = \frac{3}{2} \sum_q [\cos q_x O_{2q}^0 O_{2-q}^0 + \cos q_x \frac{1}{4} (\sqrt{3} O_{2q}^2 - O_{2q}^0) (\sqrt{3} O_{2-q}^2 - O_{2-q}^0)]$$

$$+ \cos q_y \frac{1}{4} (\sqrt{3}O_{2q}^2 + O_{2q}^0)(\sqrt{3}O_{2-q}^2 + O_{2-q}^0)] \quad (9)$$

In the unit of $t^2 / \Delta E$. One can understand why this interaction is dominant since the z direction is congenial to $3z^2-r^2$ symmetry.

Bcc lattice

For the bcc lattice, one obtains only the following octupole interaction,

$$H^{eff} = 6 \sum_q \cos(q_x / 2) \cos(q_y / 2) \cos(q_z / 2) x T_{xyzq} T_{xyz-q} \quad (10)$$

In the unit of $t^2 / \Delta E$. The ground state of the effective model is the staggered ordered state of the octupole moments. By ordering of this type of octupole moments occurs, one will observe an anomaly in the specific heat as in an ordinary phase transition. The determination of the order parameter will be challenging since neither the dipole nor quadrupole moments will be induced in contrast to the octupole order.

Fcc lattice

For the fcc lattice, one obtains both quadrupole and octupole interactions

$$\begin{aligned} H^{eff} = & \frac{3}{49} \sum_q [\cos(q_x / 2) \cos(q_y / 2) O_{2q}^0 O_{2-q}^0 + \cos(q_y / 2) \cos(q_z / 2) x \frac{1}{4} (\sqrt{3}O_{2q}^2 - O_{2q}^0)(\sqrt{3}O_{2-q}^2 - O_{2-q}^0) \\ & + \cos(q_z / 2) \cos(q_x / 2) x (1/4) (\sqrt{3}O_{2q}^2 + O_{2q}^0)(\sqrt{3}O_{2-q}^2 + O_{2-q}^0)] \\ & (144 / 49) \sum_q [\cos(q_x / 2) \cos(q_y / 2) + \\ & \cos(q_y / 2) \cos(q_z / 2) + \cos(q_z / 2) \cos(q_x / 2)] T_{xyzq} T_{xuz-q} \end{aligned} \quad (11)$$

$t^2 / \Delta E$. For the fcc lattice its characteristic is between simple cubic and body centered cubic. Due to this reason, one has calculated both quadrupole and octupole interaction.

DISCUSSION OF RESULTS

Using the theoretical formalism of K Kubo, *et al.*⁷ and R Yamamura *et al.*⁸, we have studied the influence of lattice structure on multi pole interactions in f-electron systems. The study has been made by investigating the multi pole interactions using the second order perturbation theory by a simple model. In this model the f^2 ions with Γ_3 non kramers doublet ground state under CEF. The lattice structure plays a very crucial role in multi pole ordering in f-electron system. One has obtained the Γ_{3g} quadrupole interaction for SC lattice and the Γ_{2v} quadrupole interaction for the bcc lattice. For fcc lattice both types of interactions are obtained. These characteristics are the same as those for the $f^1 - \Gamma_8$ model. Thus, one expects that such tendencies or correspondences between the dominant multi pole interactions and the lattice structures are common as long as the ground CEF state has these multi pole degree of freedom.

It was observed that several kinds of multi pole order are possible to occur in general. But Γ_{2v} octupole order is particularly fascinating because it will induce neither the dipole nor the quadrupole moments, even though the specific heat will show an anomaly at the transition point as in an ordinary phase transition. In this regard, it would be interesting to search bcc lattice and diamond structure for the Γ_{2v} order⁹. Since, one has obtained a strong interactions for this kind of moments in the $f^2-\Gamma_8$ and $f^1-\Gamma_8$ modes.

In this paper the general forms of the multi pole interactions have been derived. This shows that another form of quadrupole interaction is possible for SC lattice in general. One expects such type of components appear when one introduces hopping integrals other than $(f, f\sigma)$. This indicates that the applicability of the present results are limited to the cases where the effective hopping processes¹⁰ are mainly described by $f, f\sigma$.

CONCLUSION

From the above theoretical investigation and analysis, we have come across the following conclusions

- (1) We have theoretically studied the influence of lattice structure on multi pole interactions in f-electron systems. We have applied second order perturbation theory with respect to intersite hopping.
- (2) The derivation of multi pole interactions were performed for different lattice interactions. One obtains quadrupole interaction for SC lattice, octupole interaction for bcc lattice and for fcc lattice both interactions were observed
- (3) It appears that lattice structure plays essential role in the multi pole ordering. The general tendencies of the multi pole interactions were discussed and the results were compared with those of the Γ_8 quartet systems of f^1 ions. We have also mentioned the effective f-f hopping. The important point is that the symmetry of f-orbitals restrict the form of hopping for the both cases of lattice structure. The work will be quite helpful for those who will be interested to understand the influence of lattice structure and also to know the multi pole interactions.

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