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Microscopic theory of multipole ordering in NpO_2

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In recent years, multipole ordering in f-electron systems has been studied extensively. Among them, possibility of octupole ordering is discussed for NpO_2 [1,2] and phase IV of $Ce_xLa_{1-x}B_6$ [3–6]. Several experimental observations on these materials have been found to be reconciled by assuming octupole ordering.

To understand the origin of the octupole ordering in NpO_2, we investigate an f-electron model on an fcc lattice based on a j-j coupling scheme [7]. First, we derive an effective multipole-interaction model in the strong-coupling limit. Figure 1 shows correlation functions in the ground state of the effective model on an 8-site cluster. Large values of correlation functions are obtained for Γ_{4u}, Γ_{5u}, and Γ_{5g} moments at $\boldsymbol{q} = (0, 0, 1)$. We note that the effective model does not include a term which stabilizes Γ_{5g} quadrupole order at $\boldsymbol{q} = (0, 0, 1)$. The enhancement of this correlation function indicates an induced quadrupole moment in Γ_{4u} or Γ_{5u} moment ordered states. Therefore, the interactions which stabilize Γ_{4u} and Γ_{5u} order at $\boldsymbol{q} = (0, 0, 1)$ are relevant to the ground state.

Then, we apply mean field theory to the simplified model including only these interactions, and find that the longitudinal triple-$\boldsymbol{q}$ Γ_{5u} octupole order is realized in our model by the combined effects of multipole interactions and anisotropy of the Γ_{5u} moment. We will discuss a possible relation between the present results and experimental observations for NpO_2.

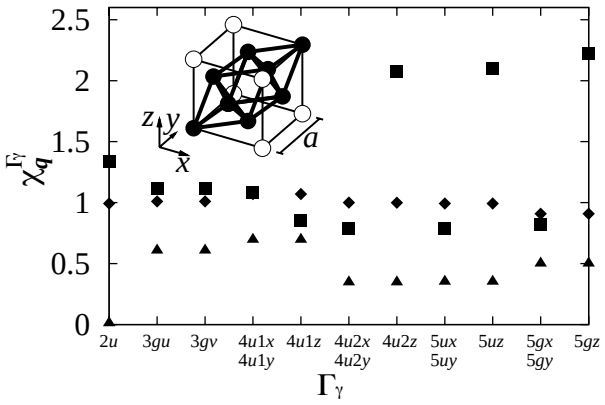

Figure 1: Correlation functions $\chi^{\Gamma\gamma}_{\boldsymbol{q}} = (1/N)\sum_{\boldsymbol{r},\boldsymbol{r}'} e^{i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\langle X^{\Gamma\gamma}_{\boldsymbol{r}} X^{\Gamma\gamma}_{\boldsymbol{r}'}\rangle$ ($N = 8$) for $\boldsymbol{q} = (0, 0, 0)$ (triangles), $\boldsymbol{q} = (0, 0, 1)$ (squares), and $\boldsymbol{q} = (1/2, 1/2, 1/2)$ (diamonds) in units of $2\pi/a$. The inset shows the fcc cluster (solid spheres) taken in the calculation.

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