Theory on Dispersion and Spectral Shape of Neutron Excitation of Paramagnetic Pr-ion Systems with Degenerate Crystal-Field Levels and Multipolar Type Exchange Interactions.

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The spectral line shape of inelastic neutron excitation in the paramagnetic state was theoretically studied for Pr ion systems with the crystal-field splitting and the inter-site exchange interactions. It was assumed that the ground level is the doublet E (Γ_3) and the excited level is the triplet T1 (Γ_4) of the cubic point group. The excitation spectra are given by a superposition of two components: One has larger dispersion, and is relatively sharp and strong; The other has small dispersion and broad width. Similar features were recently observed in PrMg₃ and were explained by the calculation. The former component is ascribed to the usual E \rightarrow T1 excitation with the dispersion due to the dipole type exchange interaction, and the latter to a transition accompanied by the simultaneous excitation of fluctuation in the manifold of the ground level. Multipolar type exchange interactions increase the intensity of the latter. The theory was developed based on Mori's memory function formalism, and a symmetrized form of a standard operator was introduced to treat the multipolar interaction systematically.

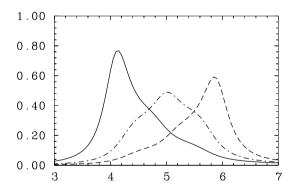


Figure 1: Neutron excitation spectra of a dipole and a T2a octupolar type exchange interaction model. The horizontal axis is the excitation energy in meV. It is assumed that the ground crystal-field level is E state, and the first excited level is T_4 located at 5 meV above. Solid, dashed, and dot-dashed lines are spectra calculated for wave number vectors at the minimum, the center and the maximum points of dispersion. The magnitude of the exchange constant of T2a type is assumed to be 0.65 of the dipole type one. Peaks of spectra are ascribed to the usual $E \to T_4$ excitation with the dispersion due to the dipole type exchange interaction. The shoulder structures of the solid and the dashed lines around 5 meV are due to the transition accompanied by the simultaneous excitation of fluctuation in the manifold of the ground level. The latters form the component with the broad width and the weak dispersion.