EQUILIBRIUM AND DYNAMIC BEHAVIORS OF CUBIC Ce$^{3+}$ SYSTEMS WITH
ANISOTROPIC COQBLIN–SCHRIEFFER AND CRYSTAL FIELD INTERACTIONS

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INTRODUCTION

The cerium and light actinide monopnictides and monochalcogenides show many similar and striking ordering and phase transition properties. The occurrence of the series of modulated magnetic structures in CeBi$^2$ and CeSb$^3$, in UAs$^4,5$ and possibly in USb$^5$, including the noncolinear structures observed$^5$ in uranium monopnictides, points to the existence of a strongly anisotropic exchange interaction which dominates the behavior of these systems.

One mechanism which yields an anisotropic exchange interaction is that of Coqblin and Schrieffer. They showed that the mixing of Ce$^{3+}$ ions with conduction electrons can be represented as the combined spin and orbital exchange scattering of conduction electrons by the localized ions. This leads to a Rudermann–Kittel type interaction between neighboring Ce$^{3+}$ ions:

$$H_{ij} = \sum_{MM'} f(R_{ij}) G(M'M')(L_{iM'M}^i - \frac{1}{6} \delta_{MM'M'}^i L_{MM'M}^i - \frac{1}{6} \delta_{MM'M'}^i L_{MM'M}^i)$$

$i,j$ label sites, $M, M'$ label the quantum states of the cerium ions, with quantum axis taken along the bonding axis. The operator $L_{iM'M}^i = |M'><M|$ projects an ion at site $i$ from state $M$ to $M'$, and $L_{i}^i$ is the identity operator at site $i$. As shown by Siemann and Cooper$^7$, the only nonvanishing $G(M,M')$ are the spin-only interaction, i.e. $M, M' = \pm \frac{1}{2}$, with $G(M,M')$ the same for $M, M' = \pm \frac{1}{2}$. In other words, the coupling comes dominantly from the $f$ orbital states with $m=0$ which pile up the charge along the bonding axis, giving the highly anisotropic Coqblin-Schrieffer (CS) interaction. This bonding axis anisotropy directly leads to the otherwise anomalous magnetic
ordering properties of cerium and light actinide monopnictides and monochalcogenides.

Upon transforming to the fcc crystalline coordinate system, this anisotropic CS exchange takes the form:

\[
H_{ij} = -E_{ij} \sum_{\mu \nu \sigma} e^{i(\mu-\nu+\sigma)} \psi_{\mu \nu \sigma}(\theta) \mathbf{L}_{\mu \nu}^i \mathbf{L}_{\nu \sigma}^j
\]

(2)

\[
\psi_{\mu \nu \sigma}(\theta) = \sum_{\mu M} (d_{\mu M}^0 d_{\nu M}^0 - \frac{1}{6} \delta_{\mu M}^0 \delta_{\nu M}^0)(d_{\sigma M}^0 d_{\sigma M}^0 - \frac{1}{6} \delta_{\sigma M}^0 \delta_{\sigma M}^0)
\]

(3)

where \( \theta \) and \( \psi \) are the angular coordinates of the bonding axis, \( \mathbf{R}_{ij} \), with respect to the crystal axes system. The Greek letters label the states with quantum axis taken along the \( <001> \) axis, \( d_{\mu \nu}^{0 \sigma}(\theta) \) is the rotational transformation matrix as conventionally defined \( \psi \) (J=5/2). As pointed out by Siemann and Cooper, as a simple consequence of the interaction being strongest when charge is piled up along the bonding axis, the CS interaction, for ions pairs with saturation moments, is strong in the \( <001> \) plane and weak between neighboring \( <001> \) planes. This effect, for the fcc lattice of \( Ce^{3+} \) ions with nearly equal nearest neighbor (nn) and next-nearest neighbor (nnn)CS interactions, is sufficient to stabilize the colinear orderings observed in the cerium monopnictides.

We have extended the investigation further to include the occurrence of noncolinear structures, and the dynamical behavior of the CS systems. The selection between colinear and noncolinear structures depends critically on the range of the CS interaction. In the dominately nn-only CS interaction system, the nn interaction can no longer stabilize the near saturation colinear ordering. The geometrical arrangement (of spins) which gives the best angular distribution of moments of each nn pair and optimizes the free energy, can be noncolinear. In the system with nn-only CS interaction the ground state is a ferromagnet with moments along \( <110> \). In the presence of a small antiferromagnetic Heisenberg exchange, we find the noncolinear canted ferromagnetic or antiferromagnetic \( 2k \) structures. With the addition of a cubic crystal field term, the Kouvel-Kasper noncolinear \( 3k \) antiferromagnetic ordering, with moments pointing along the cubic diagonal directions, can be stabilized. The excitation spectra observed in systems with CS interaction reflect the exchange interaction as seen by the ions in their ground states. In the systems with \( <001> \) or \( <110> \) ordering we observe anisotropic dispersion, reflecting the anisotropic CS interaction, while for systems with \( <111> \) alignment, the anisotropy is greatly diminished, leaving rather isotropic spectra.

**HAMILTONIAN OF SYSTEMS WITH COQUILLON-SCHRIEFFER INTERACTION**

We consider an fcc lattice of \( Ce^{3+} \) ions interacting with the