

Anharmonic lattice dynamics and superconductivity in β -pyrochlore KOs_2O_6

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Anharmonic lattice dynamics and superconductivity mediated by these excitations in β -pyrochlore oxide KOs_2O_6 are theoretically investigated. K ions are confined in oversized $\text{Os}_{12}\text{O}_{18}$ cages and subject to shallow crystalline field potential with large anharmonicity. Unusual behaviors are observed in many properties, such as resistivity, specific heat, and NMR $1/T_1$, as well as strong coupling superconductivity [1]. It is believed that they are related to anharmonic lattice dynamics of K-ions, called rattling motion.

We first investigated low-temperature thermodynamics of rattling motion [2]. We studied a toy model of K-ion quantum dynamics, considering local symmetry, and analyzed it by a mean-field theory and exact diagonalization. With lowering temperature, a first-order phase transition occurs and the width of K-ion wavefunction abruptly shrinks. This may explain the mysterious first-order transition at $T_p=7.5$ [K] in KOs_2O_6 , where no symmetry breaking is reported [1].

We then studied the superconductivity driven by this rattling ion motion. In particular, we focused on the relation of the anharmonicity of ion dynamics and superconducting transition temperature [3]. With increasing the third-order anharmonic term, b , of the effective ion potential, the first excited ion eigenenergy shows a large reduction at a crossover value, b^* . The superconducting transition temperature is strongly enhanced in a narrow region around b^* . Details will be reported in the presentation.

[1] Z. Hiroi, S. Yonezawa, and Y. Muraoka, J. Phys. Soc. Jpn. **73**, 1651 (2004); Z. Hiroi *et al.*, J. Phys. Soc. Jpn. **74**, 1682 (2005); Z. Hiroi *et al.*, Phys. Rev. B **76**, 014523 (2007).

[2] K. Hattori and H. Tsunetsugu, J. Phys. Soc. Jpn. **78**, 013603 (2009).

[3] K. Hattori and H. Tsunetsugu, unpublished.