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 $Os_{12}O_{18}$ 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.

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[3] K. Hattori and H. Tsunetsugu, unpublished.