Dominant Kitaev Interaction and Field-induced Quantum Disordered Phase in the Cobaltate Na2Co2TeO6

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The identification of quantum spin liquid phases in Kitaev candidate materials remains a major experimental challenge. Since most Kitaev candidates develop antiferromagnetic (AFM) order at low temperatures, currently there are great interest on the field-induced magnetic disordered phase in these compounds, that are distinct from (partially) polarized states. Recently, a cobaltate $Na_2Co_2TeO_6$ has emerged as a promising Kitaev candidate with high-spin $t^5_{2g}e^2_g$ configuration and spin-orbit entangled J_{eff} = 1/2 honeycomb lattice system. There are intensive studies on field-induced magnetic states and phase transitions under in-plane magnetic fields. In this study, we identify an intermediate disordered phase induced by an out-of-plane field along the *c*-axis, through high-field magnetization and magnetocaloric effect measurements.

To explain the high-field behavior of $Na_2Co_2TeO_6$, we develop an effective *K*-*J*-Gamma-Gamma' spin model featuring a dominant AFM Kitaev interaction. This framework uncovers an intermediate quantum spin liquid phase, establishing the material as a unique platform for exploring Kitaev physics and field-induced quantum-disordered states.

Anisotropic Magnetic Phase Diagram of Multipole Order in the 4f2 Face-Centered Cubic Compound PrCdNi4

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In a face-centered cubic (fcc) Pr lattice with a non-Kramers Γ_3 doublet ground state, anisotropic quadrupole interactions could give rise to additional ordered states, such as the triple-q quadrupole order [1,2]. We report a multipolar phase transition and the anisotropic magnetic field versus temperature phase diagram in the $4f^2$ fcc lattice compound $PrCdNi_4$. This compound crystallizes in the cubic $MgSnCu_4$-type structure, where the point group of the Pr site is cubic -43m (T_d). Previous studies using polycrystalline samples have revealed that the crystalline electric field ground state is the Γ_3 doublet, and a multipolar transition occurs at T_c = 1 K [3].

In this work, we have synthesized single crystals of $PrCdNi_4$, and they were characterized by the electron-probe microanalysis to be nearly the stoichiometric atomic ratio of $Pr_{1.02(1)}Cd_{1.02(1)}Ni_{3.96(1)}$. We measured the electrical resistivity $\rho(T)$, magnetoresistance $\rho(B)$, specific heat $C(T)$, and magnetization $M(T, B)$ in magnetic fields of B // [100], [110], and [111]. The specific heat $C(T)$ data exhibit a sharp peak at T_c = 1.14 K due to the multipolar phase transition. A broad anomaly appears near 5 K, which is consistent with the Schottky-type contribution from the thermal excitation between the ground doublet and an excited triplet lying at 12 K. The magnetic entropy increases from 0.4 K to 1.14 K, whose change is approximately 1/2 of Rln2. Moreover, specific heat measurements in B = 4 T along the [100], [110], and [111] axes reveal pronounced anisotropy; for **B** // [100], T_c shifts downward to 0.96 K, whereas T_c increases to 1.24 K at 4 T for **B** // [110] and 1.19 K at 4 T for **B** // [111]. We will elaborate on the sample characterization, magnetic field versus temperature phase diagrams, magnetoresistance, and the possible order parameters of the multipole order.

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Implementing advanced trial wave functions in fermion quantum Monte Carlo via stochastic sampling

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We introduce an efficient approach to implement correlated many-body trial wave functions in auxiliary-field quantum Monte Carlo (AFQMC). To control the sign/phase problem in AFQMC, a constraint is derived from an exact gauge condition but is typically imposed approximately through a trial wave function or trial density matrix, whose quality can affect the accuracy of the method. Furthermore, the trial wave function can also affect the efficiency through importance sampling. The most natural form of the trial wave function has been single Slater determinants or their linear combinations. More sophisticated forms, for example, with the inclusion of a Jastrow factor or other explicit correlations, have been challenging to use and their implementation is often assumed to require a quantum computer. In this work, we demonstrate that a large class of correlated wave functions, written in the general form of multi-dimensional integrals over hidden or auxiliary variables times Slater determinants, can be implemented as trial wave function by coupling the random walkers to a generalized Metropolis sampling. We discuss the fidelity of AFQMC with stochastically sampled trial wave functions, which are relevant to both quantum and classical algorithms. We illustrate the method and show that an efficient implementation can be achieved which preserves the low-polynomial computational scaling of AFQMC. We test our method in molecules under bond stretching and in transition metal diatomics. Significant improvements are seen in both accuracy and efficiency over typical trial wave functions, and the method yields total ground-state energies systematically within chemical accuracy. The method can be useful for incorporating other advanced wave functions, for example, neural quantum state wave functions optimized from machine learning techniques, or for other forms of fermion quantum Monte Carlo.

Dominant apical-oxygen electron-phonon coupling in a high-Tc cuprate revealed by orbital-selective excitation

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How electron-phonon interactions influence high-temperature superconductivity in cuprates remains contested, and their role outside the CuO_2 planes has been largely overlooked. Here we use oxygen K-edge resonant inelastic X-ray scattering (RIXS) to probe the trilayer cuprate $HgBa_2Ca_2Cu_3O_{8+}x$ (Hg1223). When both incident photon energy and polarization are tuned to the apical-oxygen 1s to 2p transition, the RIXS spectra exhibit a ladder of at least ten phonon overtones, evenly spaced by 70 meV, whose intensities follow a Franck-Condon envelope, signaling exceptionally strong electron-phonon coupling. Quantitative modelling that incorporates core-hole lifetime evaluation yields an apical-phonon coupling energy that is significantly larger than that of the planar stretching mode. Such a coupling strength offers a strong contender for explaining the universal 70-meV kink observed by photoemission and suggests that the dominant electron-phonon channel resides outside the CuO_2 planes. By elevating inter-layer lattice dynamics from a peripheral factor to a central actor, our results provide a fresh starting point for theories seeking to reconcile strong correlations, lattice dynamics and high-temperature superconductivity.

Quantum tunneling effects on hydrogen transport in lanthanum trihydrides

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Ionic conductivity in solids is a topic of great interest in the fields of physics, materials science, and energy applications. Previous studies have primarily focused on the activation energy of ion transport based on classical transition state theory, lacking considerations from the perspective of nuclear quantum effects. Herein, by considering the effects of zero-point energy and quantum tunneling, we examine the quantum behaviors of hydrogen migration in lanthanum trihydrides (LaH_3), through the two dominant pathways—concerted migration and single-ion migration. Our first-principles calculations based on instanton rate theory indicate that the quantum rate constants diverge significantly from their classical counterparts at low temperatures. We predict that quantum tunneling becomes dominant over thermal diffusion for concerted hydrogen migration at liquid nitrogen temperature, and emerges even at room temperature when concerted transport is suppressed. We also demonstrate the tuning of migration rates by strain, as the quantum tunneling rate is highly sensitive to the width of the energy barrier. Our findings depict a complete quantum picture of hydrogen transport in lanthanide hydrides and provide a new perspective on ionic conductivity of solid materials.

Cd substitution effect on the structural and magnetic properties of a cage compound PrRu2Zn20

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The cage compounds PrT_2X_{20} (T: transition metal; X = Al, Zn) with the cubic $CeCr_2Al_{20}$-type structure, have attracted much attention due to their fascinating properties, such as non-Fermi-liquid behavior and coexistence of multipolar ordering and superconductivity. These behaviors are thought to arise from the multipolar degrees of freedom of the non-Kramers doublet ground state of Pr^{3+} ions. On the other hand, the isostructural compound $PrRu_2Zn_{20}$ undergoes a structural transition at T_S = 138 K, which lowers the point symmetry at the Pr site. Due to the symmetry lowering, the multipolar degrees of freedom of the doublet ground state are quenched below T_S. Previous studies suggest that the structural transition is driven by low-energy vibrations of Zn atoms at the 16c site.

Recently, we found a new non-Kramers doublet system $PrRu_2Sn_2Zn_{18}$ in which Zn atoms at the 16c site in $PrRu_2Zn_{20}$ are selectively substituted with Sn. The Sn substitution into the 16c site suppresses the structural transition; therefore the multipolar degrees of freedom are not quenched even at low temperatures. In this study, we investigated the effect of Cd substitution on the magnetic and structural properties of $PrRu_2Zn_{20}$ to develop a new non-Kramers doublet system. The single crystal of Cd-substituted $PrRu_2Zn_{20}$ was grown by the self-flux method, and its structural and magnetic properties were investigated by a single-crystal X-ray diffraction analysis and measurements of electrical resistivity, magnetization and specific heat.

The single-crystal X-ray diffraction analysis revealed that the Cd ions are preferentially substituted into the 16c site. The electrical resistivity monotonically decreases with decreasing temperature, suggesting the suppression of the structural transition. Below 10 K, Van-Vleck paramagnetism was observed in the magnetization measurements. The specific heat shows a Schottky anomaly at around 12 K, and the anomaly can be reproduced by assuming a doublet CEF ground state. These results suggest that the ground state of Pr^{3+} ions is a non-Kramers doublet.

Magnetocaloric effect of Gd5Ru2

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Magnetic refrigeration is a refrigeration technology using the magnetocaloric effect (MCE) of magnetic materials. Owing to the high efficiency of magnetic refrigeration, it is expected to be applied in household appliances such as air conditioners and refrigerators. In addition, it is recently proposed that magnetic refrigeration can be applied to hydrogen liquefaction. For this reason, many magnetic refrigeration materials that exhibit a large MCE above hydrogen boiling temperature have been developed. In this study, we focus on a Gd-based compound Gd_5Ru_2, which crystallizes with a monoclinic Mn_5C_2-type structure. Considering the high concentration of Gd ions in Gd_5Ru_2, it is possible that this compound exhibits a large MCE if a ferromagnetic transition occurs. To investigate the magnetic and magnetocaloric properties of Gd_5Ru_2, we synthesized polycrystalline samples of Gd_5Ru_2 by arc melting and measured its magnetization and specific heat.

Figure 1 shows the X-ray diffraction pattern of the obtained sample. The diffraction pattern can be explained by the Mn_5C_2-type structure. Figure 2 shows temperature dependence of the magnetization divided by magnetic field, M/B, measured under zero field cool condition at B = 0.02 T. M/B exhibits a cusp at T_N = 55 K, suggesting a magnetic transition. In addition, at T_{SR} = 40 K, a ferromagnetic behavior is observed. In the presentation, we will discuss the MCE of Gd_5Ru_2 estimated from the isothermal magnetization curves and specific heat.

Investigation of Elastic Properties in Approximant Crystals RCd6 (R = Y, Gd) via Ultrasonic Measurements

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RCd_6 (R = rare earth; space group $Im3^-$) is a Cd-based approximant crystal structurally related to the icosahedral quasicrystals $YbCd_{5.7}$ and $CaCd_{5.7}$. Its structure features a periodic body-centered cubic (bcc) arrangement of Tsai-type clusters, composed of concentric polyhedral shells. Previous studies based on electrical resistivity measurements have demonstrated that certain RCd_6 approximants undergo a structural order-disorder transition near 160 K. Notably, the nature and magnitude of elastic anomalies observed around the transition temperature are strongly dependent on the specific rare-earth ion. To explore the elastic properties and gain insight into the underlying electronic states of RCd_6, we conducted ultrasonic measurements on samples with R = Y and Gd. The temperature dependence of the principal elastic constants was systematically examined. Figure 1 depicts the temperature dependence of the longitudinal elastic constant C_{11}, the tetragonal shear constant $C_E = (C_{11} - C_{12})/2$, and the transverse elastic constant C_{44} for YCd_6 under zero magnetic field. Pronounced elastic anomalies were observed in the vicinity of 160 - 170 K, indicative of a structural phase transition. In this talk, we report the temperature-dependent elastic behavior of RCd_6 (R = Y, and Gd), with particular emphasis on the elastic anomalies associated with the structural phase transition and discuss their implications for the electronic and structural characteristics of these approximant systems.

Skyrmion-Driven Elastic Anomalies in EuAl4 Probed via Ultrasonic Measurements

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$EuAl_4$ crystallizes in a body-centered tetragonal $BaAl_4$-type structure with space group $I4/mmm$, and undergoes a charge-density-wave (CDW) transition at T_{CDW} = 145.1 K under ambient pressure [1,2]. It also exhibits antiferromagnetic ordering at the Néel temperature T_{N1}=15.4 K, followed by successive transitions at T_{N2}=13.2 K, T_{N3}=12.2 K, and T_{N4}=10.0 K. In the antiferromagnetic state, a multi-step metamagnetic transition is observed when a magnetic field is applied along the [001] direction [3]. Recent studies have shown that the rhombic and tetragonal skyrmion lattice phases in $EuAl_4$ are accompanied by orthorhombic distortions of approximately 0.10 % and 0.03 %, respectively, within the ab-plane [4]. These findings highlight the crucial role of spin-lattice coupling in the structural instability of $EuAl_4$. In this context, ultrasonic measurements-owing to their high sensitivity to lattice elastic responses-offer a powerful approach for probing the skyrmion phase. In this study, we investigate the elastic properties associated with the skyrmion phase by measuring the shear elastic constant C_{66}, with shear displacement along [010] and wave propagation along [100], under a magnetic field applied along [001], where the skyrmion phase emerges. The magnetic field dependence of C_{66} at 4 K exhibits distinct elastic anomalies at the magnetic transition fields previously reported [3]. Moreover, pronounced anomalies are observed in phases II and III, which are likely attributed to lattice distortions induced by the skyrmion texture.

In this talk, we report on the elastic anomalies possibly associated with the skyrmion phase in $EuAl_4$, including detailed analyses of the temperature-field dependence of C_{66} and three-dimensional mapping of the elastic response.

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Sub-terahertz Collective Spin Resonance Modes and Field-adaptive Reservoir Computing in Chiral Helimagnet Cr1/3TaS2

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Monoaxial chiral helimagnets (CHMs) host rich helical spin textures, including chiral soliton lattices (CSLs) with tunable periods, arising from the delicate interplay between Dzyaloshinskii-Moriya interaction (DMI), ferromagnetic exchange coupling, uniaxial magnetic anisotropy, and Zeeman energy. However, existing CHMs exhibit spin resonance modes in the gigahertz frequency range, limiting their potential for high-speed signal processing. Here, with the combination of ferromagnetic resonance, electron spin resonance, and magneto-Raman techniques, we get access to uncover sub-THz CSL phonon modes in a typical CHM Cr1/3TaS2. Near the critical field, we identify nontrivial CSL phonon modes reaching 0.15 THz, while a uniform ferromagnetic resonance mode emerges at 0.375 THz in the forced ferromagnetic phase under 9 T. The CSL phonon frequency in Cr1/3TaS2 is 5-6 times higher than that of isostructural Cr1/3NbS2 due to larger spin-orbit coupling-induced DMI. Through micromagnetic simulations, we obtain the frequency spectrum and resolve the spatial distribution of amplitudes, phases, and precession trajectories of the CSL modes, providing deep insight into the characteristics of each resonance mode. Furthermore, we demonstrate that physical reservoir computing (RC), which exploits the nonlinear collective spin dynamics and field-controlled hysteresis of these nontrivial spin textures, achieves exceptional performance in time-series prediction tasks. Our findings not only elucidate the intricate dynamic properties of CSL phases but also pave the way for exploring the potential application of CHM materials for sub-THz signal processing and neuromorphic computing.