Bose-Einstein condensation of magnons in $Pb_2V_3O_9$ and $AgVOAsO_4$: insight from theory and experiment

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9.7 cm

We present a comprehensive microscopic study of quasi-one-dimensional spin-gap magnets $Pb_2V_3O_9$ and $AgVAsO_4$ that feature bond-alternating spin chains and show Bose-Einstein condensation (BEC) of magnons in high magnetic fields. Using density functional theory band structure calculations combined with quantum Monte-Carlo simulations, we obtain a remarkably accurate description of the experimental data on magnetic susceptibility, magnetization isotherm, and temperature–field BEC phase diagram of $Pb_2V_3O_9$. Our results challenge the former, purely one-dimensional scenario for this compound. Sizable ferromagnetic interchain couplings in $Pb_2V_3O_9$ arise from the peculiar arrangement of spin chains perpendicular to the structural chains. These couplings are a necessary prerequisite of the BEC.

A similar approach is applied to the novel compound $AgVOAsO_4$ where interchain couplings are frustrated. We will present recent experimental data on magnetic susceptibility and electron spin resonance, as well as magnetization and heat capacity measurements in high magnetic fields. These data suggest a quasi-one-dimensional magnetic behavior, a spin gap of about 13 K, and the saturation field of 48.5 T. Above the first critical field $H_{c1} \simeq 10$ T, the spin gap is closed, and the system undergoes two successive BEC transitions evidenced by heat capacity and low-temperature magnetization measurements. Possible reasons for this unconventional behavior will be discussed.

13.4 cm

Subject category :

2. Quantum and Classical Spin Systems

Presentation mode :

poster

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