Dynamical magnetic anisotropy in spin–1 molecular systems

DAVID RUIZ-TIJERINA, Ohio University, PABLO CORNAGLIA, CARLOS BALSEIRO, Centro Atomico Bariloche, e Instituto Balseiro, Argentina, SERGIO ULLOA, Ohio University — We study electronic transport through a deformable spin-1 molecular system in a break junction setup, under the influence of a local vibrational mode. Our study shows that the magnetic anisotropy, which arises due to stretching along the transport axis[Science 328 1370 (2010)], is renormalized by the interactions with vibrations. The coupling induces additional spin–asymmetric hybridizations that contribute to the net molecular anisotropy. We show that the low temperature physics of such device can be described by an anisotropic Kondo model ($J_\perp > J_\parallel$), with a magnetic anisotropy term, $A_{\text{Net}}S^2_z$, negative at zero stretching. A quantum phase transition (QPT) is explored by stretching the molecule, driving $A_{\text{Net}}$ into positive values, and changing the character of the device from a non–Fermi–liquid (NFL) to a Fermi liquid (FL) ground state. This transition can be directly observed through the zero–bias conductance, which we find to be finite for negative anisotropy, zero for positive anisotropy, and to reach the unitary limit at $A_{\text{Net}} \approx 0$. At that point, an underscreened spin-1 Kondo ground state appears due to the restitution of the spin-1 triplet degeneracy.

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