Hole hyperfine interaction: valence band orbital composition and its effect on hole spin qubit dephasing

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Decoherence caused by nuclear field fluctuations is a fundamental obstacle to the realization of quantum information processing using single electron spins. Alternative proposals have been made to use spin qubits based on valence band holes having weaker hyperfine coupling. However, it was demonstrated recently both theoretically [1, 2] and experimentally [3, 4] that the hole hyperfine interaction is not negligible, although a consistent picture of the mechanism controlling the magnitude of the hole-nuclear coupling is still lacking. We address this problem by performing isotope selective measurement of the valence band hyperfine coupling in InGaAs/GaAs, InP/GaInP and GaAs/AlGaAs quantum dots [5], enabled by recent progress in nuclear magnetic resonance in nanostructures [6]. Contrary to existing models [1, 2] we find that the hole hyperfine constant along the growth direction of the structure (normalized by the electron hyperfine constant) has opposite signs for different isotopes and ranges from −15% to +15%. We attribute such changes in hole hyperfine constants to the competing positive contributions of *p*-symmetry atomic orbitals and the negative contributions of *d*-orbitals. Furthermore, we find that the *d*-symmetry contribution leads to a new mechanism for hole-nuclear spin flips which may play a major role in hole spin decoherence.

Material \ *C/A* (%)	In	Ga	As	P
InGaAs/GaAs	-15.0±3.5	-5.0±4.5	+9.0±2.0	-
GaAs/AlGaAs	-	-7.5±3.0	+16.0±3.5	-
InP/GaInP	-12.5±3.0	-		+18.0±8.0

The measured hole hyperfine constants (C) normalized by electron hyperfine constants (A) are shown in the Table for four different chemical elements (In, Ga, As, P) in three different quantum dot systems. The opposite signs of C for cations and anions cannot be explained by existing theories [1, 2]. Such discrepancy is due to inadequate description of the valence band states, which were assumed to be constructed of *p*-symmetry orbitals only. We show that this controversy can be resolved when the contribution of the cationic *d*-shells (*3d* for Ga and *4d* for In) into the valence band states is considered. Furthermore, previous conclusion that pure heavy holes are immune to hole-nuclear spin flips [1, 2] is shown to arise from the same oversimplified assumption about the orbital composition of the valence band.

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