Multiband theory of hyperfine interactions in quantum dots

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We derive a theoretical description of hyperfine coupling for a carrier confined in a self-assembled semiconductor QD based on the multi-band wave function obtained from the $\boldsymbol{k}\cdot\boldsymbol{p}$ theory in the envelope function approximation, taking into account a component of the valence-band Bloch functions originating from atomic d shells. In this way, we provide a model of the hyperfine interaction compatible with the standard $\boldsymbol{k}\cdot\boldsymbol{p}$ modeling of carrier states, which opens the way towards combining the effects of hyperfine coupling with reliable modeling of other characteristics of the QD system.

As an application of the formalism, we calculate the rms fluctuations of the longitudinal and transverse Overhauser field in InGaAs/GaAs QDs and compare the contributions to the transverse field fluctuations from band mixing and d-wave admixture to valence band states. We find, in agreement with previous estimates, that the transverse Overhauser field is of the same order of magnitude as the longitudinal one and is dominated by the d-shell admixture to atomic states with only a minor correction from band mixing in all the cases. In consequence, the $\boldsymbol{k}\cdot\boldsymbol{p}$ results are well reproduced by a simple box model with the effective number of ions determined by the wave function participation number, as long as the hole is confined in the compositionally uniform volume of the dot, which holds in a wide range of parameters, excluding very flat dots.