Controlling with external fields the quantum-mechanical core-hole manganese spin in III-V semiconductors

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For applications in quantum devices the control of spin-degree of freedom has been one the major goals in semiconductor physics in the past few years. In III-V semiconductors (e.g., in GaAs or InSb) this could be achieved with manganese impurities. Manganese forms a complex, where a J = 3/2 hole from the host aligns antiferromagnetically with the 5/2 spin of the 3d5 manganese core [1]. STM images with theoretical calculations showed the potential to characterize the spatial structure of a single manganese [2] and the exchange interaction between manganese pairs [3]. Classically treating the manganese core spin, its orientation would affect the spatial structure of the manganese complex [2]. In our work, based on previous ESR measurements [1], we show a new pathway to treat the manganese core fully quantum-mechanically and, using an analytical treatment to treat the hole part of the wavefunction, we suggest a coherent manipulation of spatial structure of a single manganese in bulk III-V semiconductors. We also investigate how a surface affects the spatial structure.

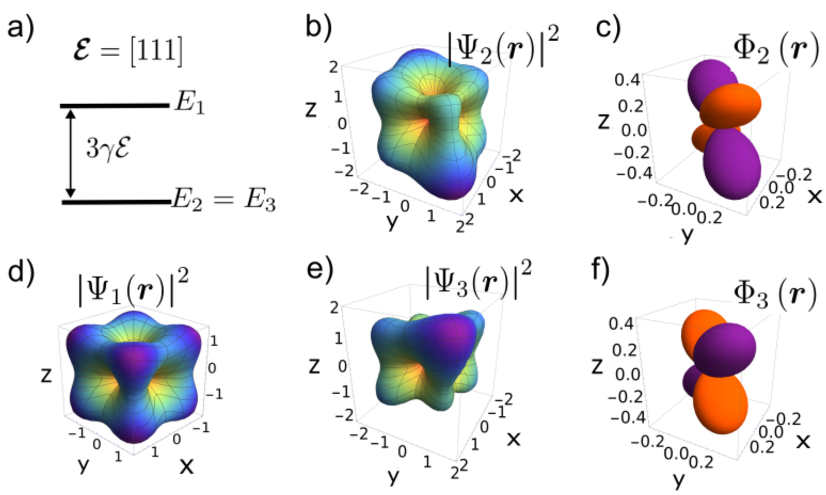

Figure 1 . An external electric field $\boldsymbol{\varepsilon}$ along the [111] direction splits the energy $E_{F=1}$ in a) leaving two states degenerate. b), d) and e) show how each state has a different spatial structure. The cubic shape changes due a non-zero spin texture in c) and f).

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Supplementary Information

With the quantum-mechanical treatment we have found that the probability density $|\Psi(\mathbf{r})|^2$ for the hole bound in the Mn-core has the following form

$$|\Psi(\mathbf{r})|^2 = \frac{2}{5}\langle\Psi|\boldsymbol{r}\rangle\,\widehat{\boldsymbol{S}}\;.\widehat{\boldsymbol{J}}\,\langle\boldsymbol{r}|\Psi\rangle + \Phi(\boldsymbol{r}). \quad (1)$$

In Eq.(1) $\widehat{\boldsymbol{S}}$ and $\widehat{\boldsymbol{J}}$ are the core and hole spin operators, respectively. While the first term in Eq.(1) has a cubic symmetry, which is the solution expected when treating the core-hole spin classically, the second term is a spin texture which depends on the direction of the core-hole spin. This second term shows up only because we are treating the core-hole spin fully quantum-mechanically.

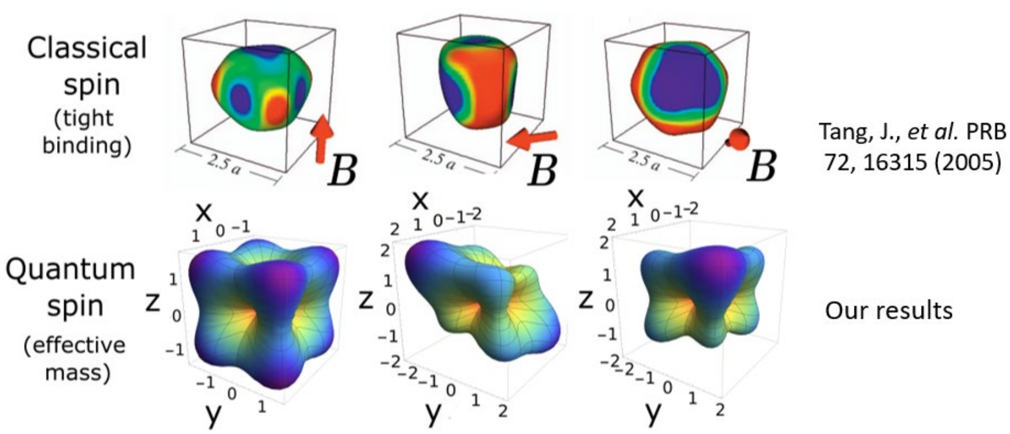

Figure 2 . Here we compare how our solution differs from the classical one when the core-hole manganese spin is under an external magnetic field $\boldsymbol{B}$, pointing to different directions.