Improved effective equation for the Rashba spin-orbit coupling in semiconductor nanowires

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1. Outline

Semiconductor Rashba nanowires are quasi-one dimensional materials that have large spin-orbit coupling (SOC) arising from a broken crystal potential symmetry due to an external electric field. There exist parametrized multiband models that can describe accurately this effect. However, simplified single band models are highly desirable to study geometries of recent experimental interest, since they may allow to incorporate the effect of the electrostatic environment of the nanowires at a reduced computational cost. **We demonstrate here that an effective equation for the linear Rashba SOC of the semiconductor conduction band can reproduce the behaviour of more sophisticated eight-band k·p model**, what is achieved by adjusting a single effective parameter that depends on the nanowire crystal structure and its chemical composition. **We further compare our approach with the Rashba coupling extracted from several magneto-conductance experiments finding an excellent agreement.**

2. Effective Rashba SOC

We solve self-consistently the Schrödinger-Posson equation to compute the eigenspectrum of *realistic* nanowires.. The conduction-band (CB) can be effectively described as

$$\hat{H}_{\rm CB} = \frac{\hbar^2\hat{\vec{k}}^2}{2m_{\rm eff}} + E_F - e\phi(\vec{r}) + \hat{\vec{\alpha}}_{\rm eff}(\vec{r})\cdot(\hat{\vec{k}}\times\vec{\sigma}),$$

where $\alpha_{\rm eff}$ is the SOC, that we describe using the following *heuristic* expression

$$\hat{\vec{\alpha}}^{(j)}_{\rm eff}(\vec{r}) = \frac{P^2_{\rm eff}}{3}\vec{\nabla}\left\{\frac{1}{\Delta_g + e\phi(\vec{r}) + E^{(j)}} - \frac{1}{\Delta_g + \Delta_{\rm SOff} + e\phi(\vec{r}) + E^{(j)}}\right\}$$

where $P_{\rm eff}$ is an effective parameter which depends on the crystal structure and chemical composition of the wire, Δ_g and $\Delta_{\rm SOff}$ are the (tabulated) semiconducting and split-off band gaps, and $E^{(j)}$ is the energy of the transverse sub-band *j*.

In previous works, a similar (but *oversimplified*) expression has been used to describe the SOC

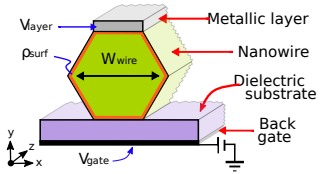
$$\hat{\vec{\alpha}}_{\rm os}(\vec{r}) \simeq -\frac{P^2}{3}\left[\frac{1}{\Delta_g^2} - \frac{1}{(\Delta_g + \Delta_{\rm SOff})^2}\right]\vec{\nabla}(e\phi(\vec{r}))$$

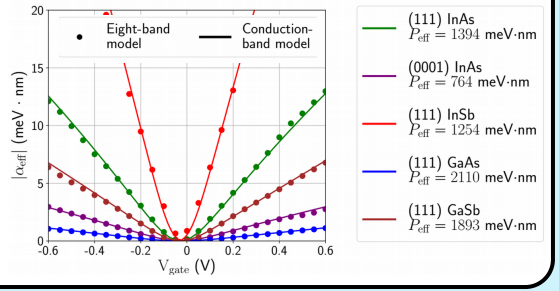
Which ignores the energy-dependency with the transverse sub-band, and the precise crystal structure, since *P* only depends on the chemical composition.

3. $P_{\rm eff}$ for different materials

It is possible to extract $P_{\rm eff}$ from fitting $\alpha_{\rm eff}$ to eight-band k·p model calculations, which are known to correctly predict the SO effects in some semiconductor materials.

We do this for different crystals and materials. To this end, we simulate an arbitrary electrostatic environment.





4. Comparison to experiments

To test the validity of our approach, we compare it with several experimental works of magneto-conductance. We find an excellent agreement. We also compare it with the oversimplified SOC equation, which is worse predicting the SOC.