Tight-binding theory with full spin-orbit effects

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The main qualitative consequence of the inclusion of relativistic effects in the computation of crystal properties is the appearance of spin. This leads to ferromagnetism and, even in paramagnets, to the presence of splitting in the bands due to the spin-orbit coupling. Spin-orbit interaction will cause a splitting at $\mathbf{k} = 0$ in a manner analogous to the fine structure atomic splittings, and can contribute an extra splitting at $\mathbf{k} \neq 0$ breaking the double degeneracy of the bands at a general $\mathbf{k}$ point in the Brillouin zone. Although the typical size of the latter spin splitting is only a few tens of meV, this energy scale determines the spin dynamics during relaxation and transport processes. Therefore, a good understanding of the intraband spin splittings is essential in any attempt to understand the operation of spintronic [1, 2] devices at a microscopic level. Also, the inclusion of spin-orbit effects is needed for the description of the bands of materials involving heavy elements, such as lead compounds, rare earths, etc.

Thus, it is important to have a systematic modeling tool which guarantees that all spin-related qualitative features in the band structures will be present. The empirical tight binding method as formulated by Slater and Koster [3] provides such a systematic way of generating all the symmetry-allowed terms that can appear in a Hamiltonian. It has been used extensively in the computation of bulk, heterostructure and surface properties, and today finds widespread use in the study of nanostructures involving thousands and even millions of atoms [4], or transport properties [5].

However, the original formulation by Slater and Koster was obtained through the use of single group symmetry operations, which prevented it from describing spin effects. Later, it has been supplemented with *ad hoc* extensions [6, 7] to describe the most important spin-orbit effects in zinc blendes, but that procedure does not guarantee *a priori* that all spin-orbit effects will be considered, and does not treat systematically other types of structures. The development presented in this poster allows us to address these issues precisely.

Stemming from the use of double group representations, we will present our results [8] for general symmetry-allowed tight binding expressions for the Hamiltonian of crystals including *all* spin-orbit effects. We have computed full-zone spin Hamiltonians for [001]-, [110]- and [111]-grown zinc blende heterostructures ($D_{2d}, C_{4v}, C_{2v}, C_{3v}$ point group symmetries), which are commonly used in spintronics, as well as bulk zinc blendes (T_d, see Fig. 1). We have performed small $\mathbf{k}$ expansions of those Hamiltonians about the zone center, yielding their $\mathbf{k} \cdot \mathbf{p}$ counterparts. The $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians thus obtained present spin-dependent terms that had not been previously described in the literature. In particular, we see that the Rashba Hamiltonian [9] can be supplemented with third order terms, which will need to be included in calculations where other sources of spin splitting are considered up to that order. We also generate additional, growth direction-dependent $\mathcal{O}(k^3)$ contributions to the Dresselhaus Hamiltonian [10, 11]. Thus, our work can serve as the basis for numerical studies of large scale nanostructures where spin effects are important, as well as an analytic tool for predicting spin properties in reduced-symmetry systems.

[1] G. A. Prinz, Phys. Today **48**, 58 (1995).

[2] S. A. Wolf, D. D. Awschalom, R. A. Buhrman, J. M. Daughton, S. von Molnár, M. L. Roukes, A. Y. Chtchelkanova, and D. M. Treger, Science **294**, 1488 (2001).

[3] J. C. Slater and G. F. Koster, Phys. Rev. **94**, 1498 (1954).

[4] F. Oyafuso, G. Klimeck, R. C. Bowen, T. Boykin, and P. von Allmen, Phys. Stat. Sol. C **4**, 1149 (2003).

[5] N. Hamada, S. Sawada, and A. Oshiyama, Phys. Rev. Lett. **68**, 1579 (1992).

[6] D. J. Chadi, Phys. Rev. B **16**, 790 (1977).

[7] T. B. Boykin, Phys. Rev. B **57**, 1620 (1998).

[8] X. Cartoixà, L.-W. Wang, D. Z.-Y. Ting, and Y.-C. Chang (2006), cond-mat/0511538 (submitted to Phys. Rev. B).

[9] Y. A. Bychkov and E. I. Rashba, J. Phys. C **17**, 6039 (1984).

[10] G. Dresselhaus, Phys. Rev. **100**, 580 (1955).

[11] M. I. D'yakonov and V. Y. Kachorovskiĭ, Fiz. Tekh. Poluprovodn. **20**, 178 (1986), [Sov. Phys. Semicond. **20**, 110 (1986)].

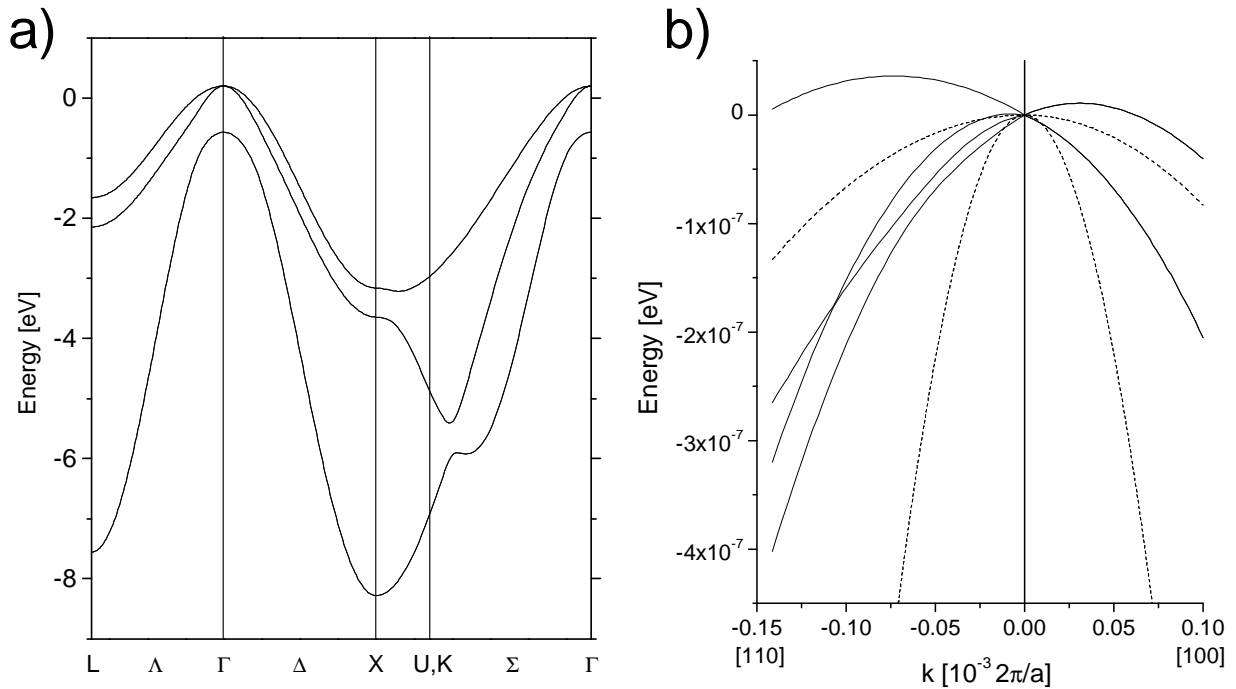[12] X. Cartoixà, D. Z.-Y. Ting, and T. C. McGill, Phys. Rev. B **68**, 235319 (2003).

FIG. 1: a) Full zone HH, LH and SO bands for GaSb. b) Bands very close to the zone center along [100] and [110] directions calculated with the present method (solid lines), featuring the linear valence band spin splitting [10], and calculated with the method of Ref. 12 (dashed lines).