Numerical Calculation of the Transverse Modes in 1T' MoS_2 Nanoribbons

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Recently it has been found that MoS_2 in the 1T' phase is a topological insulator [1]. Ab-initio calculations predict an inverted band structure. Adopting the parabolic band approximation for the band extrema and taking spin-orbit interaction into account yields the following effective Hamiltonian [2]

$$\mathbf{H}(k_x, k_y) = \begin{pmatrix} \delta - c_1 k_x^2 - c_2 k_y^2 & c_6 k_y - \alpha E_z + i c_5 k_x \\ c_6 k_y - \alpha E_z - i c_5 k_x & -\delta + c_3 k_x^2 + c_4 k_y^2 \end{pmatrix} \tag{1}$$

with the coefficients

$$c_1 = \frac{\hbar^2}{2m_x^p}, \quad c_2 = \frac{\hbar^2}{2m_y^p}, \quad c_3 = \frac{\hbar^2}{2m_x^d}, \quad c_4 = \frac{\hbar^2}{2m_y^d}, \quad c_5 = \hbar v_1, \quad c_6 = \hbar v_2 \,.$$

Here, the x-coordinate represents the longitudinal direction, the y-coordinate the transverse direction, and the z-coordinate the direction perpendicular to the nanoribbon.
The characteristic polynomial $p(k_x, k_y, E) = \mathrm{Det}\,(E\mathbf{I} - \mathbf{H})$ is of fourth degree in k_y. For given energy E and longitudinal momentum k_x there exist four roots designated as k_y^j. We adopt a mode space approach with wavefunctions $\psi(x, y) = \exp(ik_x x)\,\varphi(y)$ where $\varphi(y)$ is the transverse mode.

$$\varphi(y) = \sum_{j=1}^{4} A_j \begin{pmatrix} a \\ b \end{pmatrix} \exp(i\, k_y^j\, y) \tag{2}$$

The spinor $(a, b)^T$ is an eigenvector of (1). Setting the wave function to zero at both edges of the nanoribbon yields a homogeneous equation system for the coefficients A_j. The resulting matrix $\mathbf{M} = (\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3, \mathbf{m}_4)$ is composed of the column vectors $\mathbf{m}_j$ defined as

$$\mathbf{m}_j = \big(a,\, b,\, a\exp(i\, k_y^j\, d),\, b\exp(i\, k_y^j\, d)\big)^T, \qquad j = 1, 2, 3, 4\,. \tag{3}$$

For the simultaneous solution of the characteristic equation, $p(k_x, k_y, E) = 0$, and the quantization condition, $\mathrm{Det}\,(\mathbf{M}) = 0$, we propose a modified Newton scheme. We choose the unknown vector as $\mathbf{x} = (k_y^1, k_y^2, k_y^3, k_y^4, E)^T$ and treat k_x as an input parameter. Since the k_y^j satisfy Vieta's formulae, we use the latter as the defining equations. Adding the quantization condition, $\mathrm{Det}\,(\mathbf{M}) = 0$, gives a nonlinear equation system of the form $\mathbf{F}(\mathbf{x}) = \mathbf{0}$. The update vector is multiplied by a damping factor $\alpha < 1$ so as to keep the updates of the energy and of the wavenumbers below predefined limits. In the course of the Newton

ISBN 978-89-89453-30-7

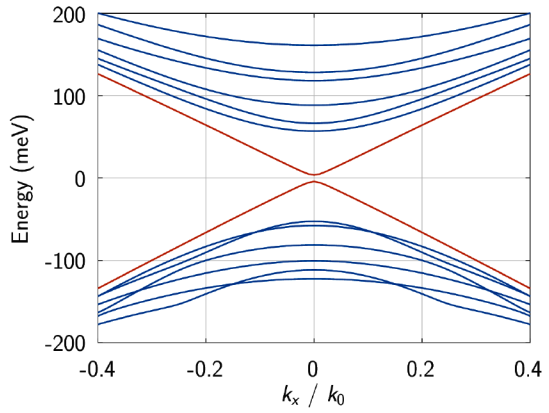

Figure 1: Subbands in a nanoribbon of the width $d = 40/k_0$ at $E_z = 0$. The almost linear dispersion corresponds to topologically protected edge states.

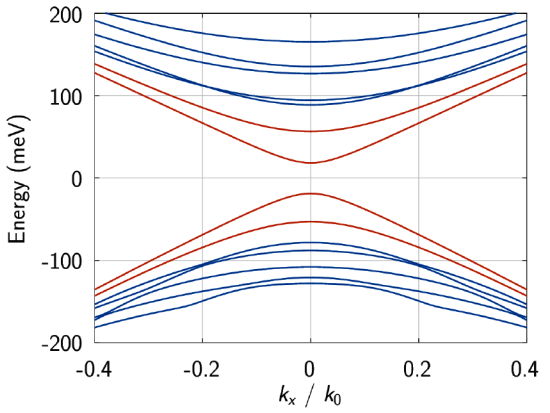

Figure 2: Subband energies at $\alpha E_z = v_2$. Red lines describe subbands with two real and two complex k_y, while blue subbands have four real k_y at small k_x.

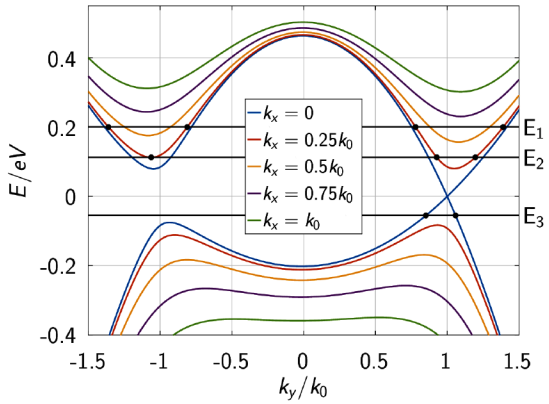

Figure 3: Contour lines of the bulk dispersion relation of 1T' MoS_2. At at a vertical field of $\alpha E_z = v_2$ the band gap closes in the point $(k_x, k_y) = (0, k_0)$.

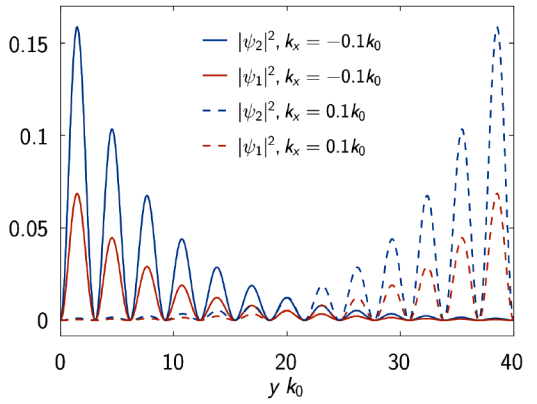

Figure 4: Wave functions squared of the topological edge states at $k_x = \pm 0.1k_0$ and $E_z = 0$. The related energy is 48.9 meV, see Fig. 1.

iteration, E can only assume real values, whereas the k_y^j are complex variables. The Newton scheme has been used to calculate the subbands shown in Fig. 1 and 2. In an extremum of a contour line ($E = E_2$ and $k_x = 0.25k_0$ in Fig. 3) a doubly degenerate solution k_y exists. Also in this case the system $\mathbf{MA} = \mathbf{0}$ has a nontrivial solution $\mathbf{A}$. However, with this coefficient vector the wavefunction (2) is identically zero. These spurious solutions which have to be disregarded have led to an incorrect interpretation of the subband structure in [3]. Fig. 4 shows that edge states with opposite signs of k_x are localized at opposite edges.

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