Spintronics in MoS$_2$ monolayer quantum wires

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We study analytically and numerically spin effects in MoS$_2$ monolayer armchair quantum wires and quantum dots. The interplay between intrinsic and Rashba spin orbit interactions induced by an electric field leads to helical modes, giving rise to spin filtering in time-reversal invariant systems. The Rashba spin orbit interaction can also be generated by spatially varying magnetic fields. In this case, the system can be in a helical regime with nearly perfect spin polarization. If such a quantum wire is brought into proximity to an s-wave superconductor, the system can be tuned into a topological phase, resulting in midgap Majorana fermions localized at the wire ends.

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Introduction. Atomic monolayers such as graphene sheet have attracted much attention over the years. However, the small spin orbit interaction (SOI) in graphene makes spin effects negligibly small. In contrast, transition-metal dichalcogenide semiconductors in particular MoS$_2$, possess giant values of SOI. Combined with a direct band gap this SOI makes these materials attractive for optical effects. However, previous work emphasized valleytronics in MoS$_2$ while the spin degrees of freedom have received much less attention, despite the fact that these materials can be expected to display interesting spintronics effects, such as helical states in quantum wires, Majorana fermions, spin qubits in quantum dots, electrical control of spin, etc. This gap of understanding has motivated the present work where we will propose and analyze spin effects specifically for quantum confined structures in MoS$_2$ monolayers.

One of our main findings is that the intrinsic SOI needs to be complemented by Rashba-like SOI to obtain interesting spin effects in the conduction band. In particular, we will focus on suitably defined quantum wires of armchair type and show that they allow for helical modes, with and without time-reversal symmetry. The Rashba-like interaction can be generated by breaking structure inversion symmetry with gates or adatoms or, alternatively, by nanomagnets with alternating magnetization direction. Helical modes serve as basis for spin filters but also as platform for exotic quantum states such as Majorana fermions or fractionally charged fermions. We finally discuss quantum dots with well-defined Kramers doublets that can serve as spin qubits.

Bandstructure. A molybdenum disulphide (MoS$_2$) monolayer consists of two layers of S atoms stacked over each other forming an effective trigonal lattice and of Mo atoms located in the center of the sulphur lattice, see Fig. 1a. The Brillouin zone consists of a hexagon with two nonequivalent corners (valleys) at $K$ ($\tau_z = 1$) and $-K$ ($\tau_z = -1$) (see Fig. 1b) that determine the low energy spectrum of the monolayer. This part of the spectrum is dominated by three $d$ orbitals of Mo: the conduction band by $|\psi_c \rangle = |d_{xz}\rangle$ and the valence band by $|\psi_v \rangle = (|d_{x^2-y^2}\rangle + i\tau_z |d_{xy}\rangle)/\sqrt{2}$. The effective Hamiltonian is given by

$$H_0 = \hbar v_F (k_x \tau_z \sigma_1 + k_y \sigma_2) + \Delta \sigma_3,$$

where the Pauli matrices $\sigma_i$ act on the $d$ orbital space. The momenta $k_x$ and $k_y$ are calculated from the corresponding valley characterized by $\tau_z$. Here, $v_F \approx 0.53 \times 10^6$ m/s is the Fermi velocity and the mass term, $\Delta \approx 830$ meV, arising from broken inversion symmetry, has been extracted from DFT calculations. The spectrum of $H_0$ is given by $E_{\sigma,\nu} = \pm \sqrt{\left(\hbar v_F k_x^2 + k_y^2 + \Delta^2\right)}$. The large gap $2\Delta$ between the valence and conduction bands makes the monolayer attractive for optical effects. The wavefunctions at fixed energy $E$ and momentum $k_y$ are written in the basis $(\psi_c, \psi_v)$ as

$$\psi_{\tau_z,\nu}(x) = e^{i(\tau_z K + p k_x) x + i k_y y} \left( b_{\tau_z,\nu} \frac{1}{\sqrt{2}} \right),$$

where $b_{\tau_z,\nu} = \hbar v_F (\tau_z k_x - i k_y)/(E - \Delta)$, $k_x > 0$, and the index $\nu$ labels right- and left- movers in $x$ direction.

We focus now on the quasi-one-dimensional limit where the system forms a quantum wire. Similarly to...
carbon-based materials, this quantum regime can be achieved in two ways: either by growing a nanoribbon of MoS$_2$ with particular boundaries or by electrostatically confining the electrons into a quantum wire by placing metallic gates on a MoS$_2$ monolayer flake (with unspecified boundaries), see Fig. 3. In both cases we consider the armchair regime where the direction of propagation is perpendicular to a lattice translation vector. The details of the boundaries are not essential provided that they do not suppress the transport. In addition, we assume for both cases hard-wall type boundary conditions. A most characteristic feature of such armchair quantum wires is that the two valleys $[\pm \mathbf{K} = (\pm 4\pi/3a, 0)]$, projected onto the propagation direction along the $y$ axis, coincide at $k = 0$. The valleys easily hybridize (lifting their degeneracy), for instance, by impurities, irregular boundaries or, in particular, by our hard-wall boundaries.

We determine now the spectrum for a quantum wire of width $W = N a$, where $a$ is the lattice constant and $N$ the number of unit cells in the $x$ direction. To find the quantization conditions on $k_x$, we virtually extend our quantum wire by two sides, $W' = (N + 2)a$, and impose the boundary conditions at these virtual sites on the total wavefunction $\psi(x) = \sum_{\mathbf{r},\mu} a_{\mathbf{r},\mu} \psi_{\mathbf{r},\mu}(x) \equiv \sum_j \psi_j(x)$, where $\psi_j(x)$ is the probability amplitude to find the electron in one of the orthogonal states $j = d_{z^2}, d_{x^2-y^2}, d_{xy}$. This gives us six conditions (three at each edge) for four fundamental solutions [see Eq. (2)]. To solve this overconstrained boundary value problem we use mixed boundary conditions. On the orbitals $d_{z^2}$ and $d_{x^2-y^2}$ we impose Dirichlet boundary conditions, $\psi_{d_{z^2}}(x=0,W') = 0$, while on the orbital $d_{xy}$ we impose von Neumann boundary conditions, $\partial_x \psi_{d_{xy}}(x=0,W') = 0$.

These boundary conditions can be fulfilled only for those values of $k_x = |\kappa_m|$ that satisfy $(K + \kappa_m)W' = \pi m$, where $m$ is an integer. If $W = (3M + 1)a$, where $M$ is a positive integer, this leads to $\kappa_m = \pi m/W'$. We note that in this case all energy levels except the lowest one in the conduction band and the highest one in the valence band are two-fold degenerate. If $W = (3M + 2)a$ [$W = 3Ma$], this leads to $\kappa_m = (\pi m + 2\pi/3)/W'$ [$\kappa_m = (\pi m - 2\pi/3)/W'$]. In this case, the energy levels are non-degenerate. The conduction band spectrum for small momenta is quadratic,

$$E_{c,w} = \sqrt{(\hbar v_F \kappa_m)^2 + (\hbar v_F k_y)^2 + \Delta^2} \approx \Delta_m + \frac{(\hbar v_F k_y)^2}{2\Delta_m},$$

where we define the minimum energy for the $m$th subband as $\Delta_m = \sqrt{(\hbar v_F \kappa_m)^2 + \Delta^2}$, see Fig. 2a. We note that the slope of the spectrum branches at small momenta is decreasing with increasing $m$, resulting in crossings of different subbands, see Fig. 2c. The corresponding wavefunction is given by

$$\psi_m(x) = \psi_{1,p}(x) - \psi_{-1,-p}(x),$$

where $p = \text{sgn}\kappa_m$. Again, we note that for $W = (3M + 1)a$ the subbands $m$ and $-m$ have the same energy.

To confirm our analytical results numerically, we develop a tight-binding model for a honeycomb lattice composed of two kinds of atoms, $A$ (representing $d_{z^2}$ orbitals) and $B$ (representing $d_{x^2-y^2} + it_z d_{xy}$ orbitals). The effective Hamiltonian $H_0$ consists of an on-site energy term and a term describing hopping between nearest neighbours, respectively,

$$H_0 = \sum_i \varepsilon_i c^\dagger_i c_i + \sum_{ij > 0} t_{ij} c^\dagger_{ij} c_{ij}.$$  

where $c^\dagger_i$ creates an electron with spin $\mu$ at site $i$. The on-site energy $\varepsilon_i$ is equal to $\Delta (\pm \Delta)$ on $A$ ($B$) sublattice. The hopping matrix element $t_{ij}$ is assumed to be uniform, $t_{ij} \equiv t = 2\hbar v_F/\sqrt{3}a$. The Hamiltonians $H_0$ and $\tilde{H}_0$ are equivalent for momenta close to $\pm \mathbf{K}$ and result in the same low energy spectrum, see Fig. 2a.

Intrinsic spin orbit interaction. The intrinsic spin orbit interaction in MoS$_2$ monolayer is much larger than in other monolayers, for example, in graphene, arising from $d$ orbitals of the heavier atom. Symmetry arguments confirmed by DFT calculations lead to the intrinsic SOI Hamiltonian of the form:

$$H_{so} = \alpha \tau_z s_z (1 - \sigma_3),$$
where Pauli matrices $s_i$ act on spin space, and $\alpha = 38$ meV is the SOI strength.

**Rashba spin orbit interaction.** Breaking of structure inversion symmetry by an electric field $E$ along the $z$ axis perpendicular to the monolayer leads to a Rashba term of the form \[ H_R = H_{Rx} + H_{Ry}, \]

\[ H_{Rx} = -\alpha_R s_y \sigma_2, \quad H_{Ry} = \alpha_R \tau_z s_y \sigma_1, \]  \(7\)

where the Rashba SOI strength, in general, is proportional to the electric field strength. Such an electric field could be produced by gates\(^{22}\) or by doping with adatoms\(^{37,38}\). For both cases, $\alpha_R$ is best determined by ab initio calculations or experimentally.

An alternative way to generate Rashba SOI is to apply a spatially varying magnetic field\(^{39}\) produced, for instance, by a magnetic field $B_n$ rotating in the plane of a quantum wire produces the Zeeman term

\[ H^2_Z = \Delta_Z[s_x \cos(k_n y) + s_y \sin(k_n y)], \]  \(8\)

where $\Delta_Z = g \mu_B B_n / 2$, and the period of the rotating field is $\lambda_n = 2\pi / k_n$. The unitary spin-dependent transformation $U_n = \exp(-i k_n y s_z / 2)$ allows us to gauge away the coordinate dependent term $H^2_Z$ in the Hamiltonian $H = H_0 + H_{so} + H^2_Z$. This results in $H_n = U_n^\dagger H U_n$,

\[ H_n = H_0 + H_{so} - \alpha_{Rn} s_z \sigma_2 + \Delta_Z s_x, \]  \(9\)

where $\alpha_{Rn} = hv/F k_n / 2$, so the strength of the induced Rashba SOI depends only on the rotation period $\lambda_n$ but not on the magnetic field strength $B_n$. We note that the induced Rashba SOI described by $H_{Rn} = -\alpha_{Rn} s_z \sigma_2$ reaches $\alpha_{Rn} \approx 11$ meV for the nanomagnets placed with a period $\lambda_n = 100$ nm. Here we note that for a quantum wire created by gates, we can estimate that the misalignment angle should be less than $a / \lambda_n$ (i.e. $\lesssim 1^\circ$)\(^{22}\). If one works with a nanoribbon, then the propagation in the armchair or zigzag direction should be favoured by the growth process\(^{\text{[22]}}\). We note that also a Zeeman term $H_Z = \Delta_Z s_x$, which breaks the time-reversal invariance of the system, inevitably arises.

To account for the Rashba SOI of Eq. \((7)\) in the tight-binding model, we allow for spin-flip hoppings\(^{22,35}\)

\[ \tilde{H}_R = \frac{3i\alpha_R}{4} \sum_{<ij>, \mu, \mu'} c^\dagger_{i\mu}(e_{ij} \times e_z) \cdot s_{\mu\mu'} c_{j\mu'}, \]  \(10\)

where $s = (s_x, s_y, s_z)$, and where the unit vectors $e_z$ points along $z$ and $e_{ij}$ along the bond connecting sites $i$ and $j$. The intrinsics SOI, see Eq. \((4)\), can be modeled by

\[ \tilde{H}_{so} = \frac{2i\alpha}{3\sqrt{3}} \sum_{<ij>, \mu, \mu'} \nu_{ij} c^\dagger_{i\mu} s_z \cdot s_{\mu\mu'} c_{j\mu'}, \]  \(11\)

where the sum runs over the next-nearest neighbour sites belonging to the $B$ sublattice. The spin dependent amplitude $\nu_{ij} = -\nu_{ji} = \pm 1$ depends on whether the electron takes a right or left turn by hopping from $i$ to $j$\(^{22}\). These two terms $\tilde{H}_{so}$ and $\tilde{H}_R$ are constructed in such a way that they are equivalent to $H_{so}$ and $H_R$ in the low-energy sector. We note that by taking only part of $\tilde{H}_R$ and changing $s_x$ to $s_z$, we can model $H_{Rn}$. The Zeeman term $H_z$ is given by

\[ \tilde{H}_Z = \Delta_Z \sum_{i, \mu, \mu'} c^\dagger_{i\mu} s_{x, \mu\mu'} c_{i\mu'} . \]  \(12\)

**Spectrum with SOI.** A part of the Rashba SOI, $H_{Rx}$ ($H_{Rn}$), can be easily included in $H_0$. The spin $s_x$ ($s_z$) is a good quantum number for the Hamiltonian $H_0 + H_{Rx}$ ($H_0 + H_{Rn}$). In this case, the SOI only results in the spin-dependent shift of the momentum, $k_y \rightarrow k_y - s_z \alpha_R / \hbar v_F$ ($k_y \rightarrow k_y - s_z \alpha_R / \hbar v_F$), see Fig. 2c. Next, we treat the remaining SOI terms, $H' = H_{so} + H_{Ry}$ ($H_{so}$), as a perturbation. We note that $H'$ ($H_{so}$) is proportional to $\tau_z$. At the same time, the wavefunctions $\psi_m(x)$ [see Eq. \((4)\)] are eigenstates of the Pauli matrix $\tau_1$, so the intrasubband matrix elements vanish\(^{34\text{[a]}}\) which is consistent with Kramers degeneracy at $k_y = 0$ for a time-reversal invariant Hamiltonian. The intersubband matrix elements $t_{mm'}$, however, are non-zero, but they contain a strong suppression factor arising from the sublattice degree of freedom as follows. At small momenta, the mass term $\Delta \delta_3$ dominates in the Hamiltonian, so the wavefunctions $\psi_m(x)$ are close to the eigenstate of $\sigma_3$. As a result, the sublattice terms in $H' (H_{so})$, $1 - \sigma_3$ and $\sigma_1$, lead to a suppression of SOI effects, where the intrinsic SOI is suppressed by a factor of $(E - \Delta) / \Delta < 1$ and the Rashba SOI by a factor $\sqrt{(E - \Delta) / \Delta}$. Thus, the corrections to the spectrum are small in the parameter $\omega_{mm'} / (\omega_{mm'}$), where $\omega_{mm'}$ denotes the subband splitting at given $k_y$. However, these terms lead to an anticoercing between two different subbands with opposite spin (with the same spin) along $x$ (along $z$), see Fig. 2d. We note here that in spite of having strong SOI, the spin degeneracy is not lifted in case of quantum wires.

**Helical modes via electric field.** The Rashba SOI induced by an electric field offers the possibility to generate helical modes in a time-reversal invariant system. As shown above, $H'$ results in subband anticrossings, see Fig. 2c. If in the low-energy sector, $t_{mm'} \ll \omega_{mm'}$, the subbands are spin-polarized by the Rashba SOI $H_{Rx}$ in the $x$ direction, see Fig. 3. However, passing through the anticrossing the spin polarization goes through zero $k_y$. All this suggests that if the Fermi level is tuned close to the anticrossing (see Fig. 2d) in such a way that there are four propagating modes (two left and two right), the system is in a quasi-helical regime. The lowest subband $n = 1$ is almost fully spin-polarized and transports opposite spins into opposite directions, whereas the next subband $n = 2$ is only partially polarized. This means that scattering due to impurities between subbands is allowed and helical modes are not protected from backscattering.

**Helical modes via magnetic field.** If a Rashba SOI (along $x$) is generated by a spatially varying magnetic
field, the time-reversal invariance of the system is broken, giving rise to a Zeeman term $H_Z$. The corresponding magnetic field, pointing along $z$, is perpendicular to the spin quantization axis determined by the Rashba SOI. Thus, the spin degeneracy at $k_y = 0$ gets lifted, and a gap of size $2\Delta_Z$ is opened, see Fig. 4. The spin polarization along $z$ is given by

$$\langle s_z \rangle = \frac{\omega_{\uparrow\downarrow}}{\sqrt{\omega_{\uparrow\downarrow}^2 + 4\Delta_Z^2}}.$$  \hspace{1cm} (13)$$

where $\omega_{\uparrow\downarrow}$ is the energy difference between spin up and spin down states at given momentum $k_y$ for the unperturbed problem $H_0 + H_{Rn} + H_{so}$. If the chemical potential $\mu$, defining the Fermi momentum $k_y^{(n)}$ for the $n$th subband, is tuned close to the anticrossing (see Fig. 3), the total polarization $\langle s_z \rangle$ of a left (right) propagating electron is non-zero.

![FIG. 3. The spin polarization $\langle s_z \rangle$ along x direction as function of momentum $k_y$ for the nth level defined in Fig. 2. The spin projections onto the y and z directions vanish. Away from the anticrossings the spin is almost perfectly aligned along x. If the chemical potential $\mu$, defining the Fermi momentum $k_y^{(n)}$ for the nth subband, is tuned close to the anticrossing (see Fig. 3), the total polarization $\langle s_z \rangle$ of a left (right) propagating electron is non-zero.](image)

Quantum dots. In contrast to gapless graphene, quantum dots in MoS$_2$ can be created by gates. We note that the confining potential should be sharp enough to lift the valley degeneracy, as shown above for the quantum wires, and, in addition, to insure a non-equidistant spectrum, which is more suitable for optical experiments. If vanishing boundary conditions are imposed also along $y$, the momentum $k_y$ is quantized, $k_{y,m} = \pi n / (W_y + 2a/\sqrt{3})$, where $W_y$ is width in the $y$ direction, and $n$ is a positive integer. The dot spectrum then becomes $E_{n,m} = \sqrt{\hbar^2 v_F^2 (\kappa_{y,m}^2 + \kappa_{zm}^2) + \Delta^2}$. Each level is spin degenerate and the intrinsic SOI can neither lift this Kramers degeneracy, nor, due to its symmetry, change substantially splittings between levels [in the small parameter $\alpha(E - \Delta) / \Delta \ll \alpha$, see above]. The spin degeneracy can be lifted with a magnetic field, say, along $z$. Similar to nanotubes EDSR can then be achieved by applying an oscillatory electric field $E$ also along $z$, causing $\alpha_R$ to oscillate and thereby inducing spin rotations at a Rabi frequency $\sim |\alpha_R|$. Thus, we conclude that quantum dots in MoS$_2$ host well-defined Kramers doublets that can serve as platform for spin qubits.

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**Appendix A: Majorana Fermions**

We give here more details of the derivation of the Majorana fermions (MFs) introduced in the main text. Thereby we closely follow the derivation given in Ref. 43 which requires a few minor modifications for the present case. If the chemical potential $\mu$ is tuned inside the gap $2\Delta_Z$ opened by the magnetic field $B_n$ at $k_y = 0$, the two propagating modes are helical, see Fig. 4. The same helical states can be obtained by a Rashba SOI induced by an electric field in the presence of a uniform magnetic field giving rise to a Zeeman splitting $2\Delta_Z$. If such a
quantum wire is brought into tunnel contact with an s-wave superconductor, a superconducting proximity gap \( \Delta_{sc} \) is induced in the wire. Through the pairing mechanism coupling Kramers partners, the helical states get paired into a \( p \)-wave-like superconducting state.\(^{27,28}\)\(^{30}\)

There are no propagating modes inside the gap but there could exist bound states localized at the ends of the wire. If a certain topological criterion is satisfied, these states are MFs, particles that are their own antiparticles. To find this criterion, we describe the system by an effective linearized model for the exterior \( (\chi = e, \text{ states with momenta close to the Fermi momentum}, \ k_e = k_F) \) and the interior branches \( (\chi = i, \text{ states with momenta close to} \ k_i = 0)\).\(^{28}\) The electron operator is represented as \( \Psi(y) = \sum_{\rho=\pm 1, \chi=e,i} e^{i\rho k_y y} \rho \chi \), where the sum runs over the right \((R, \rho = 1)\) and left \((L, \rho = -1)\) movers and \( \rho \chi \) is an annihilation operator for the \((\rho, \chi)\) branch of the spectrum. The effective Hamiltonian becomes

\[
H = -i \hbar v \rho_3 \chi_3 \partial_y + \Delta_Z \eta_3 \rho_1 (1 + \chi_3)/2 + \Delta_{sc} \eta_2 \rho_2 (1 + \chi_3)/2 + \Delta_{sc} \eta_2 \rho_2 (1 - \chi_3)/2. \quad (A1)
\]

in the basis

\[
\tilde{\Psi} = (\Psi_{Re}, \Psi_{Le}, \psi^\dagger_{Re}, \Psi_{Li}, \Psi_{Ri}, \psi^\dagger_{Li}, \psi^\dagger_{Ri}),
\]

where the Pauli matrices \( \chi_i \) act in the interior-exterior branch (electron-hole) space.

Here, \( \Delta_Z = g \mu_B B \pi / 2 \) is the Zeeman energy, and \( v = (\partial E / \partial h k_y)_{k_y = k_F} \) is the velocity at the Fermi level. In the limit of strong Rashba SOI \( (\alpha_Rn \gg \Delta_Z, \Delta_{sc}) \), the strength of the effective proximity induced superconductivity acting on the exterior branches \( \Delta_{sc} \) due to the nearly perfect spin polarization at the Fermi wavevector \( k_F \) is equal to \( \Delta_Z \). In the opposite limit of weak Rashba SOI \( (\alpha_Rn \ll \Delta_Z) \), \( \Delta_{sc} \) is getting suppressed by the magnetic field, \( \Delta_{sc} = \Delta_{sc} n / k_F \), where \( k_n = \pi / \lambda_n \) \( (\lambda_n = 2 \alpha_R / \hbar v_F) \) for Rashba SOI induced by rotating magnetic fields (by electric fields). Note that the Fermi wavevector \( k_F \) grows with magnetic field as \( k_F \propto \sqrt{\Delta_Z} \).

All this together leads us to the criterion for the topological phase given by

\[
\Delta_Z > \sqrt{\Delta_{sc}^2 + \mu^2}, \quad (A2)
\]

where the chemical potential \( \mu \) is now calculated from the middle of gap \( 2 \Delta_Z \).

Similarly, following Refs. \(^{28}\) and \(^{46}\) we can also obtain the localization length of the MFs. For example, in the strong SOI regime and for \( \mu = 0 \), the wavefunction of the left localized MF is written in the basis \( \tilde{\Psi} = (\psi^\dagger_{\uparrow}, \psi^\dagger_{\downarrow}, \psi^\dagger_{\sigma}, \psi^\dagger_{\sigma}) \) as

\[
\Phi_M(y) = \begin{pmatrix} i & 1 & 1 & 1 \\ 1 & -i & -1 & -i \\ -1 & i & -1 & i \\ -1 & -i & 1 & i \end{pmatrix} e^{-k_{\perp} y} - \begin{pmatrix} i e^{ik_F y} \\ e^{-ik_F y} \\ -i e^{-ik_F y} \\ e^{ik_F y} \end{pmatrix} e^{-k(y) y}, \quad (A3)
\]

where \( k_{\perp} = (\Delta_Z - \Delta_{sc}) / \hbar v \) and \( k(y) = \Delta_{sc} / \hbar \). The localization length is determined by the smallest gap in the system \( \xi = \max (1/k_{\perp}^2, 1/k(y)^2) \). Here, \( \Psi_{\sigma} = (\psi_{\sigma}) \) is a creation operator of the electron with spin up (down), where the spin quantization axis is determined by the Rashba SOI. In the weak SOI regime deeply in the topological phase, the left localized MF wavefunction is written as

\[
\Phi_M(y) = \begin{pmatrix} e^{-i\pi/4} \\ i e^{i\pi/4} \\ e^{i\pi/4} \\ -i e^{-i\pi/4} \end{pmatrix} \sin(k_F y) e^{-k(e) y}, \quad (A4)
\]

where \( k(e) = \Delta_{sc} / \hbar \). Note that both solutions explicitly satisfy the MF condition of being self-conjugate, \( \Phi_M \cdot \tilde{\Psi} = [\Phi_M \cdot \tilde{\Psi}]^\dagger \).

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More generally, the intersubband matrix element $t_{mm'}$ vanishes if $m - m' = 2l$, where $l$ is an integer.

We note that the spin polarization close to the anticrossing is also described by Eq. (13), where we make a change $\Delta Z \rightarrow t_{ij}$, see Fig. 3.