# 1 Title of the research project

Quantum spin Hall effect in semiconductor quantum wells.

# 2 Applicant

Alina Mariana Hriscu

# 3 FOM research group

FOM-G-13

# 4 Summary of the research proposal

Quantum spin-Hall effect is the equivalent of the quantum Hall effect for spin systems. It has been theoretically proven and experimentally confirmed that in two-dimensional electron and hole gases, a charge current can induce a perpendicular spin current in the absence of magnetic field. Open questions to be answered include the exact definition of the spin current and the corresponding spin-resistivity. Quantum wells of zero-gap semiconductors are natural systems where the effect arises. To find new materials which can host the quatum spin-Hall effect is one of the quests of the intended research.

# 5 Host institution

Zernike Institute for Advanced Materials University of Groningen Nijenborgh 4, NL-9747 AG, Groningen

# 6 Personnel

| Name | Main task |
|---:|---|
| Prof. Dr. Jasper Knoester | Promoter |
| Dr. Maxim Mostovoy | Supervision |
| MSc. Alina Hriscu | Calculations |

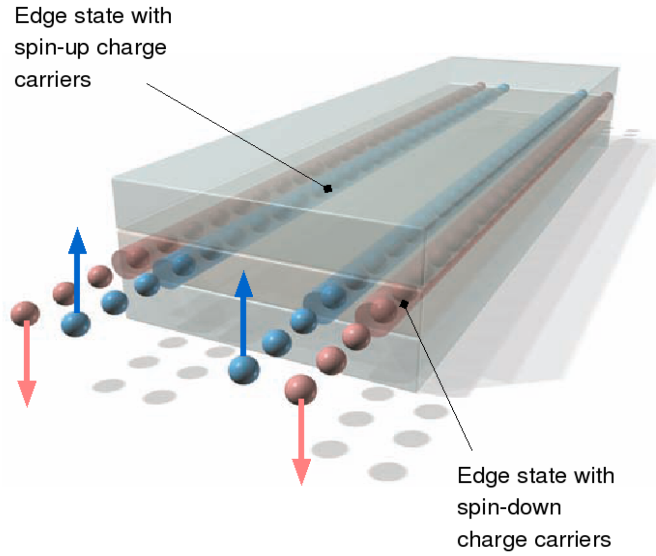


Figure 1: Schematic of the spin-polarized edge channels in a quantum spin Hall insulator. (from [1])

# 7 Cost estimates

| **Costs** (in K€) | 2008 Sept.-Dec. | 2009 | 2010 | 2011 | 2012 Jan.-Aug. | **Total** |
|---|---|---|---|---|---|---|
| Applicant[1] | 13 | 41 | 43 | 45 | 31 | 176 |
| Consumables | 2 | 2 | 1 | 2 | 2 | 9 |
| Travel | | 3 | 4 | 4 | 2 | 13 |
| **Total** | 15 | 46 | 48 | 51 | 35 | 199 |

1. The estimates for salary costs are based in the salary tables of the CAO Nederlandse Universiteiten (www.vsnu.nl).

# 8 Brief desription of the research proposal

## 8.1 Introduction

The possibility to manipulate the spin degree of freedom of electron (spintronics) has raised a lot of interest in the scientific world for the past 20 years. Apart from many potential applications in information technology it also posses many interesting and challenging fundamental questions.

In the electronic circuits, on which our present technology is based, dissipation of the charge currents induces an intrinsic limitation. On the other hand, in two-dimensional semiconductors showing quantum Hall effect (QHE), the electrical current is flowing without dissipation. Unfortunately, the experimental conditions necessary to reach the quantum Hall effect (magnetic fields of order of 10 T and extremely low temperatures) make these systems impractical.

Similarly, the dissipationless transport of charge in superconductors only becomes possible at rather low temperatures.

The (quantum) spin Hall effect may help to overcome these limitations. It is the generalization of the quantum Hall effect for spin systems. The spin Hall effect occurs in a paramagnets with strong spin-orbit coupling. A spin current perpendicular to a charge current is generated in the absence of magnetic field. This leads to a spin accumulation on the edges of the sample. While the charge current necessary to separate spins is dissipative, the spin current is dissipationless and has a universal (quantized) conductance.

It is worth noting another special property of the spin current, namely the time-reversal symmetry. While the charge current changes sign under time-reversal, the spin current remains unvariant [2]. The spin current in the $i^{th}$ direction with the spins polarized in the $j^{th}$ direction, produced by an electric field applied in the $k^{th}$ direction is expressed as:

$$j_j^i = \sigma_s \varepsilon^{ijk} E_k, \tag{1}$$

where $\varepsilon^{ijk}$ is the Levi-Civita totally antisymmetric tensor. Equation (1) shows that the spin current is disipationless because it is time-even. Since both parts of the Eq.(1) are time-even, no dissipation is necessary. On the other hand, in the Ohm's law the charge current is time-odd, while the electric field is time-even, which is why the conductivity must be inverse proportional to the relaxation time. One can also conclude from this that by breaking the time-reversal symmetry the effect is destroyed. Thus, the spin-Hall effect cannot occur in a magnetic field .

The effect has been predicted [3] three decades ago by invoking the earlier theories for the anomalous Hall effect in ferromagnets, which originates from spin-dependent scattering off magnetic impurities. Recently the possibility of an intrinsic spin Hall effect has been put forward, which originates from the modification of the band structure of semiconductors due to spin-orbit coupling rather than from scattering from impurities [3]. Furthermore, the interest in the intrinsic spin-Hall effect has been enhanced by the possibility that such a spin current is quantized.

There are several theoretical models used to calculate the spin currents and the corresponding resistivity. The main difference between them is the phenomenological form of the spin-orbit coupling. Murakami et al. [2] predicted the effect in p-doped semiconductors with Luttinger type of spin-orbit, while Sinova et al.[4] used Rashba spin-orbit coupling in n-doped semiconductors.

Remarkably, recent experiments provide a strong evidence for the existance of the quantum spin Hall effect [1]. Effort is still being made by some groups to test the remaining theoretical predictions.

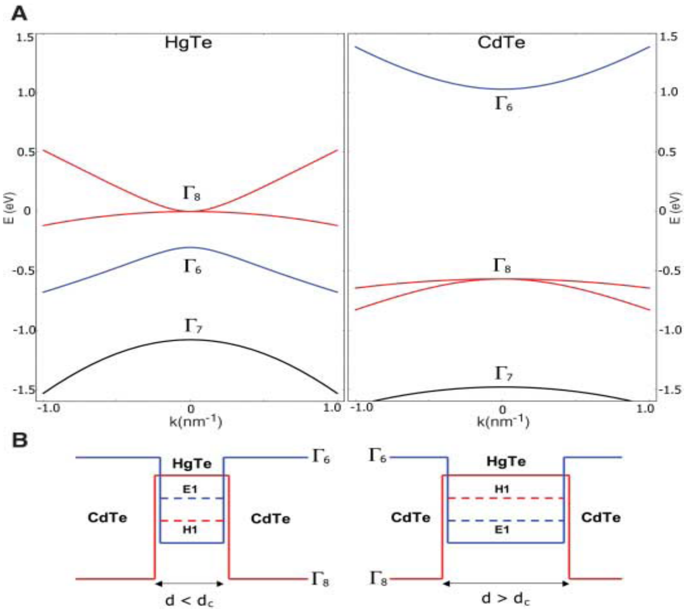


Figure 2: (A) Bulk energy bands of HgTe and CdTe near the Γ point. (B) The CdTe-HgTe-CdTe quantum well in the normal regime $E1 > H1$ with $d < dc$ and in the inverted regime $H1 > E1$ with $d > dc$. In this and other figures, $\Gamma8/H1$ symmetry is indicated in red and $\Gamma6/E1$ symmetry is indicated in blue.(from [5])

## 8.2 Research questions

The simplest and the most intuitive model which naturally gives rise to a spin current in the Hall regime has been proposed by Sinova et al. [4]. The model Hamiltonian includes the Rashba spin-orbit coupling and reads $H = \hbar^2 k^2/(2m) + \lambda(\sigma_x k_y - \sigma_y k_x)$. The spin-Hall conductivity of this model has an universal value of $e/8\pi$. It has been the subject of a long debate whether the first order vertex correction due to disorder-induced scattering exactly cancels this conductivity, leading to zero net conductivity [6]. This cancellation of the spin-conductivity might also be due to spin-dynamics within the particular model [7]. One of the purposes of the intended research is to investigate this model as well as related models where the spin-orbit coupling is non-linear in the carrier momentum.

Asuming that we deal with a non-vanishing spin conductivity, the accumulation of spin on the edges produces a homogeneous in-plane spin polarization in the two-dimensional electron(or hole) gas ( 2DE(H)G ). The spin-Hall insulators have a non-zero moment of magnetization which is a prerequisite of magnetoelectric effect. We therefore propose to investigate the magnetoelectric effect in the spin-polarized 2DEG.

The quantum spin-Hall is the cousin of quantum anomalous Hall effect, which is the charge Hall effect produced by internal magnetization rather than by external magnetic field. Consequentely, extension of the model for the anomalous quantum Hall effect provided good grounds for the study of quantum spin-Hall effect [8, 9].

Inverted band-gap semiconductors are most likely realizations of a system showing the quantum spin-Hall effect and therefore a great deal of theoretical work has been focused on materials like graphene and HgTe. It turned out that graphene is not a good candidate, since the gap opened the spin-orbit coupling is too small. The aim of the proposed research is to find suitable materials in which quantum spin-Hall effect can be realised.

Some other issues that the intended research will adress are

1. The effect of scattering on the induced spin-currents and spin-coherence in a strongly spin-orbit coupled system (in general and in the specific models mentioned above).

2. Mechanism of spin-relaxation and the relation to scattering. How does spin relax near the boundaries?

3. Considering other spin-current definitions which give a clearer picture and can be readily connected to spin-accumulation.

## 8.3 Approach

To test if the spin conductivity in the Rashba model vanishes, we will consider non-linear spin-momentum model. In these premises we will use the

Kubo formula to calculate the spin-current conductivity, as well as the first order vector corrections due to disorder-induced scattering.

We will study the effects of a magnetic field in the Rashba model, as well as in the related models. The time succesion of the applied pulsed electric and magnetic field plays an important role in our approach. To get the spin accumulation at the edges we apply the in-plane electric field (no magnetic field!). Subsequently, we remove the electric field and apply the magnetic field to the two-dimensional electron gas. We calculate the electrical polarization produced by the magnetic field.

For zero-gap semiconductors, such as HgTe and CdTe, the important bands near the Fermi level are close to the $\Gamma$ point in the Brillouin zone, and they are s-type band (with $\Gamma_6$ symmetry) and p-type band which is split into a $J = 3/2$-band ($\Gamma_8$) and a $J = 1/2$-band by spin-orbit coupling. HgTe as a bulk material has a negative energy gap, which indicates that the $\Gamma_8$ band, which usually forms the the valence band, is above the $\Gamma_6$ band (see Fig. 8.1). The light-hole bulk subband of the $\Gamma_8$ band becomes the conduction band, the heavy-hole bulk subband becomes the first valence band, and the s-type band ($\Gamma_6$) is pushed below the Fermi level. Based on this unusual sequence of states, such a band structure is called inverted.

Quantum wells of the type III semiconductors provide a natural realisation of the band-inversion [5]: the barrier material (e.g., CdTe) has a normal band progression, with the s-type band that has $\Gamma_6$ symmetry lying above the p-type band that has $\Gamma_8$ symmetry, and the well material (e.g., HgTe) having an inverted gap progression, as explained above. By tuning the quantum well thickness we can continously pass from a normal band progression to a inverted band progression regime in the well material. In this “inverted” regime, which happens above a certain thickness $d_c$, it has been shown that the quantum spin-hall state can be realized [5]. The level crossing which takes place at $d_c$ is similar to the case of graphene, and furthermore, the electronic states near the $\Gamma$ point are described by a relativistic Dirac equation in 2+1 dimensions.

In the models involving Luttinger-type of spin-orbit coupling there are topologically protected gapless bands of states localized at the edges of a semiconductor sample, as their energies lie in the gap of the bulk insulator. Once the spin-Hall effect is realized in the ground state, it is protected against thermal fluctuations by the bulk energy gap. These edge states have a distinct helical property: two states with opposite spin polarization counterpropagate at a given edge. [8, 5] (see picture 8.1). The origin of these chiral states is the Berry phase aquired by the holes moving in the momentum space, as we will briefly discuss in the next paragraph.

The starting point of the model is the two-band Luttinger effective

Hamiltonian [10], in two spatial dimensions.

$$H_{eff}(k_x, k_y) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(-k) \end{pmatrix}, H = \varepsilon(k) + d_i(\mathbf{k})\sigma_i, \tag{2}$$

where $\sigma_i$ are the Pauli matrices and $d_i(\mathbf{k})$ are functions of the in-plane momenta and some material-specific constants. They represent the spin-orbit coupling as a function of momentum. The spin-Hall conductivity using the Kubo formula ([9]), is given by

$$\sigma_x^y = -\frac{1}{4\pi^2} \int\int_{FBZ} dk_x dk_y \hat{\mathbf{d}} \cdot \partial_x \hat{\mathbf{d}} \times \partial_y \hat{\mathbf{d}}, \tag{3}$$

which is a topological invariant defined on the first Brillouin zone (FBZ), independent of the details of the band structure parameters. Considering $\hat{\mathbf{d}} : T^2 \to S^2$ as a mapping from the Brillouin zone to the unit sphere, the integrand is the Jacobian of this mapping. Thus the integration over it gives the total area of the image of the Brillouin zone on $S^2$, which is a topological winding number that is quantized. A schematic picture of a typical $\hat{\mathbf{d}}$ configuration (a half of Skyrmion, called also a meron) is shown in Fig. 8.3. Henceforth, the quantization of the conductivity in this system can be understood as a Berry phase in $\mathbf{k}$ space, similar to the quantum Hall effect, with the Skyrmion winding number related to the quantization of the current. The universal spin conductivity obtained in this system is $2e^2/h$.

In the attempt to find new materials and/or structures in which the quantum spin-Hall effect can be realised, we propose to study systems with simple band structures which can give rise to spin Hall effect. Starting with the Luttinger model, we will continue with Kane model [8] and verify the results within a tight-binding model. Furthermore, band structure calculations will give the final check.

Finally, we shall propose detailed experiments that can test our predictions.

## 8.4 Relevance for science

Either adding the spin degree of freedom to conventional charge-based electronic devices or using the spin alone has the potential advantages of non-volatility, increased data processing speed, decreased electric power consumption, and increased integration densities compared with conventional semiconductor devices. To successfully incorporate spins into existing semiconductor technology, one has to resolve technical issues such as efficient injection, transport, control and manipulation, and detection of spin polarization as well as spin-polarized currents [11]. There are numerous experimental challenges to overcome, as well as theoretical insight to be provided. But a spin-based electronics seems possible in the near future.

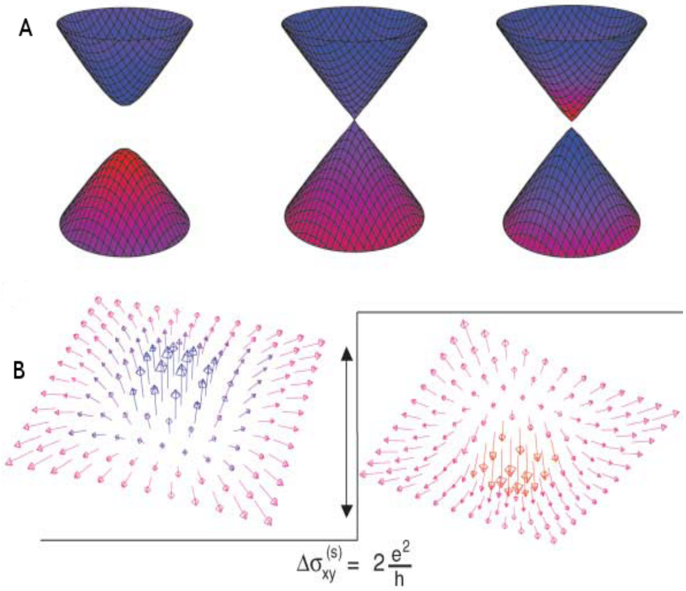


Figure 3: (A) Energy dispersion relations $E(k_x, k_y)$ of the E1 and H1 subbands at d = 40, 63.5, and 70  (from left to right). Colored shading indicates the symmetry type of the band at that k point. Places where the cones are more red indicate that the dominant state is H1 at that point; places where they are more blue indicate that the dominant state is E1. Purple shading is a region where the states are more evenly mixed. At 40 , the lower band is dominantly H1 and the upper band is dominantly E1. At 63.5 , the bands are evenly mixed near the band crossing and retain their d ¡ dc behavior moving farther out in k-space. At 70 , the regions near $k_{||} = 0$ have flipped their character but eventually revert back to the $d < dc$ farther out in k-space. Only this dispersion shows the meron structure (red and blue in the same band). (B) Schematic meron configurations representing the di(k) vector near the Γ point. The shading of the merons has the same meaning as the dispersion relations above. The change in meron number across the transition is exactly equal to 1, leading to a quantum jump of the spin Hall conductance $\sigma^s_{xy} = 2e^2/h$. We measure all Hall conductances in electrical units. (from [1])

Future devices based on quantum spin-Hall effect will have the advantage that there is no magnetic field required. The spin current can flow without dissipation in quantum spin-Hall systems, which will increases a lot the efficiency of the data storage and of the computational time in the spintronic-based computers.

Cheap, easy to produce and feasible new materials which can host the quantum spin-Hall effect are requirements in order to have a large-scale industry based on spintronics.

Interesting enough, a topic with numerous possible applications, also poses insightful fundamental questions. The quantum spin Hall state is a novel topological state of matter, in the same way as the quantum Hall effect is. A lot of work still needs to be done before we can completely understand the properties of these systems.

### 8.5 Plan of work

| Year | Research activities |
|---|---|
| 2008 | Magneto-electric coupling in Rashba-like 2DEG |
| 2009 | Analitic calculations for novel zero-band semiconductor systems |
| 2010 | Band structure calculations for novel zero-band semiconductor systems |
| 2011 | Writing the thesis |

## References


[1] Markus Konig, Steffen Wiedmann, Christoph Brune, Andreas Roth, Hartmut Buhmann, Laurens W. Molenkamp, Xiao-Liang Qi and Shou-Cheng Zhang. *Science*, **318**(5851):766–770, 2007.

[2] Shuichi Murakami, Naoto Nagaosa and Shou-Cheng Zhang. *Science*, **301**(5638):1348–1351, 2003.

[3] V.I. Perel M.I. Dyakonov. *Sov. Phys. JETP*, page 467, 1971.

[4] Jairo Sinova, Dimitrie Culcer, Q. Niu, N. A. Sinitsyn, T. Jungwirth and A. H. MacDonald. *Phys. Rev. Lett.*, **92**(12):126603, Mar 2004.

[5] Andrei Bernevig, Taylor L. Hughes and Shou-Cheng Zhang. *Science*, **314**, 2006.

[6] Jun-ichiro Inoue, Gerrit E. W. Bauer and Laurens W. Molenkamp. *Phys. Rev. B*, **70**(4):041303, Jul 2004.

[7] Jairo Sinova, Shuich Murakami, Shun-Qing Shen and Mahn-Soo Choi. *Solid State Communications*, **138**:214–217, 2006.

[8] C.L. Kane and E.J. Mele. *Phys. Rev. Lett*, **95**:226801, 2005.

[9] Xiao-Liang Qi, Yong-Shi Wu and Shou-Cheng Zhang. *Physical Review B (Condensed Matter and Materials Physics)*, **74**(8):085308, 2006.

[10] J. M. Luttinger. *Phys. Rev.*, **102**(4):1030–1041, May 1956.

[11] S. A. Wolf, D. D. Awschalom, R. A. Buhrman, J. M. Daughton, S. von Molnar, M. L. Roukes, A. Y. Chtchelkanova and D. M. Treger. *Science*, **294**(5546):1488–1495, 2001.