Usage Report for Fiscal Year 2016

Project Title:

Spin interference in quantum networks

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Background and purpose of research

The research project belongs to the field of computational condensed matter physics. We specifically focus on spin phenomena in low-dimensional mesoscopic semiconductor systems. Phase coherence length in semiconductor systems is of the order of a few micrometers which allows studies interference phenomena in mesoscopic systems. Especially Nitta group in Sendai university has years of experience in realizing these systems with various types of spin interference phenomena that allow studies of topological effects as well as geometric and dynamic quantum phases. Numerous achievements have been obtained in their group that illustrate quantum wave nature of electrons.

This project specifically investigates spin-related effects in mesoscopic semiconductor systems in regimes where phase coherence allows studies of spin interference phenomena with topological effects and studies of spin-orbit coupling effects that have their origin in special relativity. Diverse physical phenomena in these mesoscopic systems are complex and simulations are needed to either predict them or extract signatures of them from experimental data.

The quantum geometric phases emerge naturally in these studies. These include Berry phases in the adiabatic limit as well as Aharonov-Anandan phase in the nonadiabatic case as well as other emergent geometric phases such as effective geometric phase studied by the PI of this project and his coworkers [H. Saarikoski, J. E. Vazquez-Lozano, J. P. Baltanas, F. Nagasawa, J. Nitta, and D. Frustaglia, Phys. Rev. B 91, 241406(R) (2015)]. It was shown in this work that topological transitions of the geometric phase gives rise to characteristic interference pattern in conductance through the loop-interferometer. However, realization of these signals in experiments is still challenging and further simulations are needed to search for a regime where unambiguous signals of these phenomena are clearly identified. This helps experimentalists also to choose an appropriate transport regime and geometric configuration of the system. Eventual detection of a topological transition in experiments paves way for robust control of phase of electron spin in spin interferometers.

This research project has been performed in collaboration with a research group at University of Seville by prof. Diego Frustaglia, prof. Jose-Pablo Baltanas and PhD student J. Enrique Vazquez (now holding a PhD student position at Nanophotonics research center at University of Valencia, Spain). Their role in the project has been calculations of spin transport in 1D semiclassical ballistic systems. The PI of this project on the other hand performed complex 2D simulations of spin dynamics in realistic multi-mode quantum interferometers. Experimental aspects of this work was discussed with prof. Junsaku Nitta and Dr. Fumiya Nagasawa at Tohoku University.

Supercomputer usage at ACCC

The calculations in the supercomputer system were performed using Kwant code (www.kwant-project.org) that is a python-based software package developed to solve transport and structural properties of quantum systems. Modeling of disorder using the Ando-model of lattice disorder requires averaging over different random disorder potential configurations. This consumes lots of computing time. Simulations of large systems with high precision is also needed and therefore the multi-core calculations in Hokusai has been employed with up to 3 cores per each configuration.

As of 14th of February 2016 the project had consumed 7.2 million core hours at Massively Parallel Computer (Hokusai). This is 100% of the maximum number of core hours allocated for the project. Extension of the project with 360,000 additional core-hours was requested and granted to perform additional computations during the last 6 weeks of the Fiscal Year 2016.

Results

The Hokusai supercomputer system has been used extensively to calculate spin transport in realistic spin interference devices with disorder added in the system as well 2D effects resulting in multiple transport modes and finite thickness of the wire where electrons move. These calculations have been very successful in predicting expected experimental outcomes in the search for topological phenomena in spin interference. Many of the central theoretical findings are still waiting for experimental confirmation and simulations of realistic systems are essential in the research work.

Recent experimental measurements show anisotropy of magnetoresistance as a function of in-plane field strength. This is tentatively caused by complex spin-orbit fields consisting of Rashba and Dresselhaus spin-orbit terms. The effective field caused by the spin-orbit interaction competes with the Zeeman term and causes anisotropy. Recent simulations at Hokusai supercomputer has shown emergence of this phenomenon in simulations (see Figure 1). The results show also oscillations of anisotropy as a function of in-plane field strength (see Figure 2).

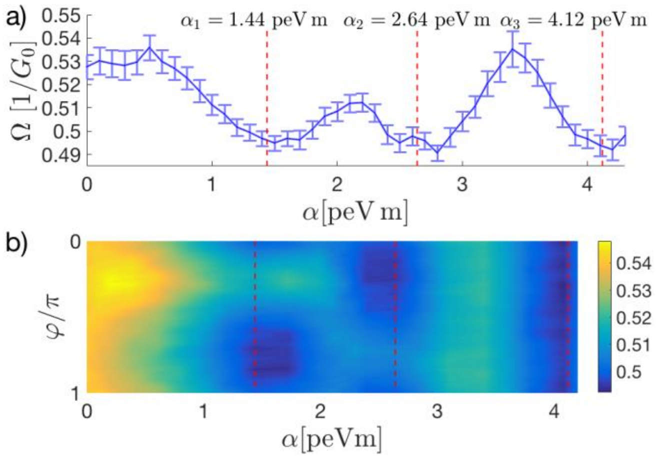

Figure 1 a) Altshuler-Aronov-Spivak resistance oscillations in a mesoscopic ring device. b) Resistance as a function of in-plane magnetic field and in-plane angle show anisotropy. The results are calculated using the Hokusai supercomputer.

These results could be checked by applying a strong in-plane magnetic field to the system. A publication of these results is under writing process right now.

The spin interference and its associated topological transition has a close analogies in classical systems of a rotating micromagnet. The geometric phase obtains just different value of the effective geometric

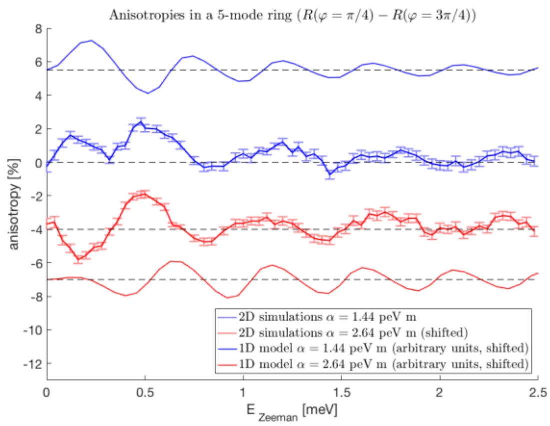

Figure 2 Oscillations in anisotropy in a mesoscopic ring system as a function of in-plane field strength. 2D simulation performed at Hokusai supercomputer are compared to a 1D model.

phase being 2π in the adiabatic limit which is in contrast to Berry phase π in the quantum case. We studied this in a recent paper H. Saarikoski et al., J. Phys. Cond, Mat. 28, 166002 (2016) (open access, see list of publications). Systems at ACCC were used to calculate results in this work.

Future work and prospects

The additional computations to be performed during the last 6 weeks of the fiscal year are necessary to investigate surprising and interesting new features that appeared during the primary phase of the project. These features included appearance of Zeeman oscillations in a mesoscopic ring system at low spin-orbit coupling. These should be much weaker than expected and disappear in the limit of high disorder. The additional calculations aim to investigate whether these arise from the Aharonov-Casher effect of direct interference paths through the ring or whether they are caused by the backscattered wave at the ring intersection point that interferes with the waves going around the ring. Future plans for the next fiscal year include changing geometry of the system towards polygonal structures instead of circular shapes. This may yield higher effective spin-orbit field effect as well as may give rise to new physical phenomena.

Anisotropy calculations are also planned to be extended to compute the whole phase diagram as a function of Rashba spin-orbit field. The 1D method shows that anisotropy contains signs of the topological transition as a phase shift of the anisotropy oscillations (see Figure 3). Calculation of this phase diagram within the 2D method is expected to show similar pattern in anisotropy. Anisotropy is expected to be more robust quantity than direct magnetoresistance due to natural cancellation of the background signal at each point in the phase diagram. However, anisotropy involves small changes in the magnetoresistance signal as a function of in-plane field angle and therefore it is computationally much more demanding. The 2D calculation is going to be very heavy because high degree of accuracy is needed. If 2D calculations confirm signs of the topological transition experiments may be carried out to confirm existence of the signal. This would be a major result and an experimental confirmation of the emergent effective geometric phases in spin systems.

Large-scale quantum networks are also under consideration. They would consist of several interconnected ring systems. Interference phenomena in such systems are expected to be complex and very challenging to study. This would, however, consume a lot of computing resources. Currently a plan is being devised to perform simulations of quantum networks of moderate size in the supercomputing system in the next fiscal year.

Conclusions

The results provide very fascinating insights into spin interference phenomena in mesoscopic structures. with topological properties and the calculations indicate that the phenomena are observable in experiments. Furthermore the results are promising for future developments in the field towards simulations of large-scale quantum networks.

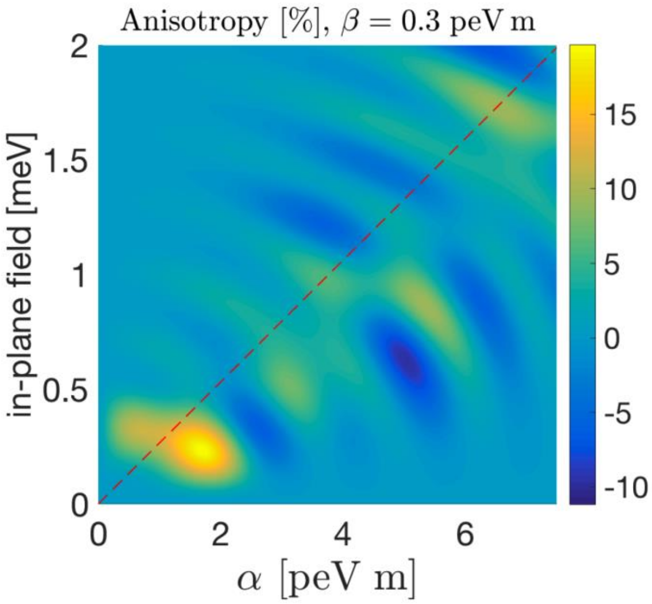

Figure 3 Anisotropy calculated within the 1D method shows signs of the topological phase shift around the critical line (dashed line).

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Fiscal Year 2016 List of Publications Resulting from the Use of the supercomputer

Peer reviewed publication：

H. Saarikoski, José Pablo Baltánas, J. Enrique Vázquez-Lozano, Junsaku Nitta, and Diego Frustaglia, *Effective geometric phases and topological transitions in SO(3) and SU(2) rotations*, Journal of Physics: Condensed Matter **28**, 166002 (2016). (ACCC acknowledged in this publication)

Manuscript "Spin-interference in complex spin-orbit fields in mesoscopic rings" by H. Saarikoski, F. Nagasawa, M. Wang, and J. Nitta is under preparation and will be submitted shortly within this Fiscal Year.

[Oral presentation at an international symposium]

8/2016 "Topological effects in spin interference", PASPS9 conference (9th International Conference on Physics and Applications of Spin-related Phenomena in Solids), Kobe, Japan (contributed talk)

3/2016 "Effective geometric phases and topological transitions in SO(3) and SU(2) rotations", German Physical Society (DPG) Spring Meeting 2016, Regensburg (contributed talk)

3/2016 "Topological transitions in spin interferometers", Japanese Physical Society (JPS) Spring Meeting 2015 (contributed talk)