Kwansei Gakuin University
Report of Research Outcome

2021/03/29

To President

Department : Science and Technology
Position : Postdoctoral fellow
Name : Moumita Patra

I report the outcome of the research as follows.

Name of the Fund/Program	□Sabbatical leave with grant □Sabbatical leave with no grant □KGU Joint Research □Individual Special Research ⊠Postdoctoral fellow ※Please report by designated form as for "International Research Collaboration".
Research Theme	Theoretical Aspects of spin orbit interaction on electronic properties of matter
Research Site/Venue	India (May - November,2020) & Kwansei-Gakuin University, Kobe Sanda Campus (December,2020 - March,2021)
Research period	2020/05/01 ～ 2021/03/31 （11 months）

◆ **Summary of the research outcome** （**approx. 2,500 words**）
Please write down the outcomes in detail regarding the research theme above.

[1] Topological aspects of Aubry-André-Harper model in the presence of spin-orbit interaction:

Topological insulators have a bulk band gap like an ordinary insulator but have gapless conducting edges or surface states such that the electrons can propagate only along the edge or surface of the material. These states are topologically protected against local perturbations such as surface roughness or impurity scattering. This makes it a promising candidate for quantum computing or ultra-low power consumption electronic devices. The bulk gaps of the topological insulators are characterized by a global order parameter, called topological invariant. These topological invariants are integers, and cannot be smoothly deformed, within the same symmetry class of the Hamiltonian, to another phase with a different value of the topological invariant. Therefore, topological phase transitions are always accompanied by the closing and reopening of the bulk energy gap. These phases are classified by their symmetries such as time-reversal, particle- hole, chiral symmetry and so on.

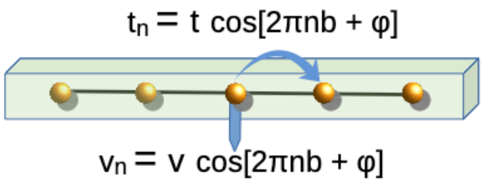

Figure 1:1D AAH System with modulation in onsite-potential and hopping integral

The Aubry-André-Harper (AAH) model with incommensurate on-site modulations, has been extensively studied for its metal to insulator transition due to its self-dual nature. On the other hand, this model shows topological behavior. For example, 1D diagonal AAH model can be exactly mapped to the 2D Hofstadter model, i.e., 2D electron systems on square lattice under a magnetic field. It exhibits topological boundary states enabled by their nontrivial topology in virtual dimensions and this makes it possible to study higher dimensional topological properties considering lower dimensional AAH systems. The non-zero topological edge modes of 1D diagonal AAH model are characterized by first Chern number. For off-diagonal chiral symmetry protected AAH system, the zero-energy edges appear in the energy bands, which are characterized by another topological invariant, the winding number. In 2D AAH model, the zero-energy state is protected by a quantized quadrupole moment and the nonzero-energy corner localized states is protected by the second Chern number. Here we study the effect of spin-orbit coupling (SOC) on the topological states of one and higher dimensional AAH quasi-periodic systems.

AAH system has cosine term in the form cos $[2\pi nb+\phi]$ in on-site energy term, or in hopping, or in both as shown in Fig.1. where (a) and (b) represent off-diagonal and diagonal AAH systems, respectively. n is the site-index. AAH-phase ϕ acts as the momentum in another spatial dimension. Recent experiments have realized the quasiperiodic 1D and 2D AAH model in optical lattices and observed the signature of a localization transition in agreement with theory.

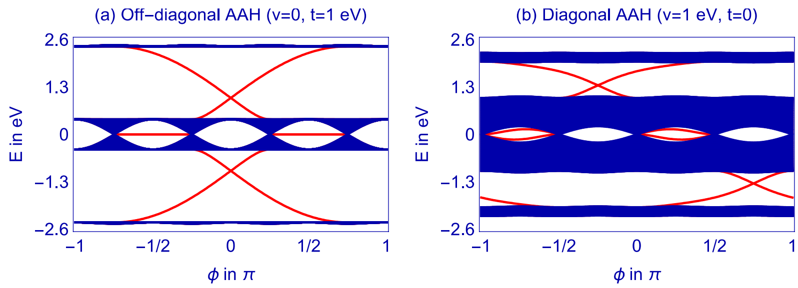

Figure 2: Energy spectra with AAH-phase (virtual momentum) for 1D AAH systems.

The topological phases appear depending on the choice of b(=1/q). For example, for 1D diagonal case, topological non-zero edge states appear when q is greater than 2. On the other hand, for an off-diagonal zero-zero energy appear for q greater than 1 as shown by red color in Fig.2 where we choose a 100-site chain with q=4. By examining the wave functions associated with these non-zero and zero-energy band crossing states, we find that they are actually boundary states localized around the two edges of the system. These are the topological edge modes. For an odd number of sites off-diagonal system, there exists a single zero energy mode, which is always localized on either one of the edges except for the Dirac points. This is an even-odd effect due to the chiral symmetry in the off-diagonal AAH model.

The electron localization properties in a low-dimensional conductor can be significantly modified with spin–orbit interaction (SOI). We consider Rashba spin-orbit coupling in the system. It appears as a result of a local symmetry breaking in the crystal potential in the perpendicular direction of the plane where the electrons are confined. The asymmetrical potential produces the precession of electron spins, which is responsible for spin-flip scattering between neighboring sites in the system which eventually gives rise to a spin-polarized current. Consideration of the SOI can be useful in spintronics, e.g., as spin–orbit qubits, spin pumps, or basic elements of spin transistors. The spin-orbit coupling strength can be experimentally tuned by external gates and can lead to oscillatory behavior of the ballistic spin conductance.

We focus on the topological properties of 1D, 2D, and 3D AAH systems considering the spin-orbit scattering. In an 1D system, the with the SOI, the zero-energy, edge modes disappear. The corresponding wave function is now spreaded through-over the crystal. The non-zero edge modes are found to be very robust against SOI, although the energies are shifted away from their initial values.

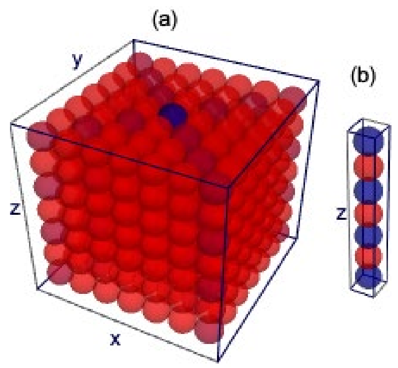

Figure 3: (a) Wave-function amplitudes over a perfect crystal where the blue color represents maximum probability amplitude and lightest Color represents the minima. (b) The central region of parallel to (a).

We further consider 3D systems. We mainly concentrate on two system sizes viz., 7×7×7 (odd) and 8×8×8 (even). Highly degenerate zero-energy-modes (ZEM) appear for odd and even cases without spin-orbit interaction (SOI). The corresponding wave-functions are distributed over the whole system. With the introduction of SOI, the number of degeneracies of the zero-energy-modes reduce to two for odd number of system sizes and to zero for even number of cubic system sizes and this remains unchanged in the presence of AAH modulation. The distribution of amplitudes of the ZEM wave-functions for a 7×7×7 crystal in the presence of SOI is shown in Fig. 3(a). The maximum localizations occur through the central line parallel to the Z-axis for up and down spins in similar as shown in Fig.3(b). As the Rashba spin-orbit interaction is a two-dimensional phenomenon, we consider it in the XY- planes. Each plane parallel to the XY, have identical SOI variation. As in this case the localization appears parallel to Z-axis, therefore if we consider SOI in other planes, viz., YZ or ZX, the corresponding localizations will appear to the central line parallel to the X and Y, respectively. With SOI, corner, surface, and hinge modes appear. Below we summarize the results.

- AAH off-diagonal modulation only along the X direction in 3D crystal:

(a) Highly degenerate flat bands appear for odd system size throughout the AAH - phase window without SOI along with two Dirac points at AAH-phase $\varphi_x = \pi/2$ and $3\pi/2$.
(b) With SOI the degeneracies are reduced to two for all φ_x.
(c) For even system size, zero-energy modes appear only at $\varphi_x = \pi/2$ and $3\pi/2$ without SOI, which are topologically trivial. Therefore SOI, there are no zero-energy modes appear with even number of system size.

- AAH off-diagonal modulation along two directions in 3D crystal:

(a) The degeneracies of the zero-energy modes remain same as previous case.
(b) For odd system size, localized edges appear without SOI. With SOI, similar to the previous case, there are two energy levels in the flat band. The localization occurs at the one edge of the system which is parallel to the Z-axis for these zero-energy wave-functions except $\varphi_x = \pi/2$ and $3\pi/2$. As in this case we get a localized edge parallel to Z-axis, therefore if we consider SOI in other planes, viz., in YZ the localization will occur to the edge parallel to X-axis. So, changing the direction of the SOI, we can manipulate the localization directions in edges.

(c) For even system size the results are similar to the previous case.

We shall further extend our studies by considering 2D AAH system to study second order topological insulator and characterize the edge and corner modes in the presence of spin-orbit interaction for various AAH systems, i.e., the commensurate, incommensurate cases with odd and even system sizes.

[2] Effect of Spin-orbit interaction on circular spin currents:

While most of the studies involving transport properties of an quantum conduction junctions have focused on the overall conduction properties of the junction geometry and electronic structure, some attention has been given to current distribution within the junction. When the bridging conductor contains a loop structure, there is a possibility to induce circular currents.

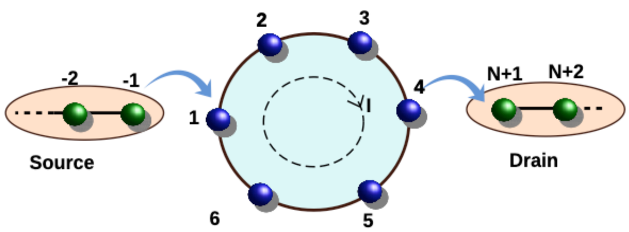

Figure 4: Schematic-representation of the Tight-Binding quantum ring, attached with two semi-infinite electrodes, namely source and drain.

The circular currents in quantum loops have been discussed in several different context. In the early 80’s Buttiker et al. [1] first proposed theoretically that a small conducting ring carries a net circulating charge current in presence of magnetic field. Using phase locked infra-red laser pulses Pershin and Piermarocchi [2] have shown that circular current can be established in an isolated quantum ring. Several theoretical works have indicated the possibility to excite such currents by using external radiation [3], shaped photon pulses [4,5], circularly polarized light, and twisted light. Loop currents can be also induced in rings driven by an external voltage and/or temperature bias. For example, S. Nakanishi and M. Tsukada [6] have predicted the existence of a quantum internal current through the C_{60} molecular bridge. Large loop currents circulating around the zigzag and chiral carbon nanotubes has been observed by N. Tsuji et.al. [7]. Theses circular currents due to different driving forces are closely related in nature.

The regulation of the bias-induced circular current is much easier specially than the persistent current due to magnetic field as confining magnetic field in a nano-ring is a challenging issue. Though the idea of bias-induced circular current is so far limited to theoretical computations, the results involve various important factors in the context of quantum transport, such as it gives the measurement of current through the individual section of a complicated quantum loop system consist of multiple pathways. Depending on the voltage bias, the circular current may rise to a very high value compared to the transport current in the outgoing leads ($\sim 10^3$ times). This circular current induces a large magnetic field (in some cases it may even reach to few millitesla or even tesla) at the center of the ring, which very important in the context of local spin regulation and several other electronic and spintronic applications like storage of data, logic functions, spin switching, spin-selective electron transmission, spin-based quantum computations, etc.

In one of our recent work, we have calculated the spin circular current, where the spin components have been defined by the conservation law between the bond currents and transport currents in a one-dimensional quantum chain. With this formulation, here we make an in-depth analysis of the effect of Rashba spin-orbit interaction on circular current. We choose Rashba spin-orbit coupling, so that we can manipulate the current externally by tuning the Rashba SO. As we only concentrate on circular current (i.e., not transport current), we call it only 'current' for the sack of simplicity.

Based on a tight-binding (TB) framework we compute circular current using waveguide formalism. With this approach, one can find current carried by each section of the ring. We have examined the characteristic features of current densities, branch currents, total circular currents. Circular current may decrease with voltage (showing negative differential resistance, NMR) contrary to the transport current which increases with voltage.

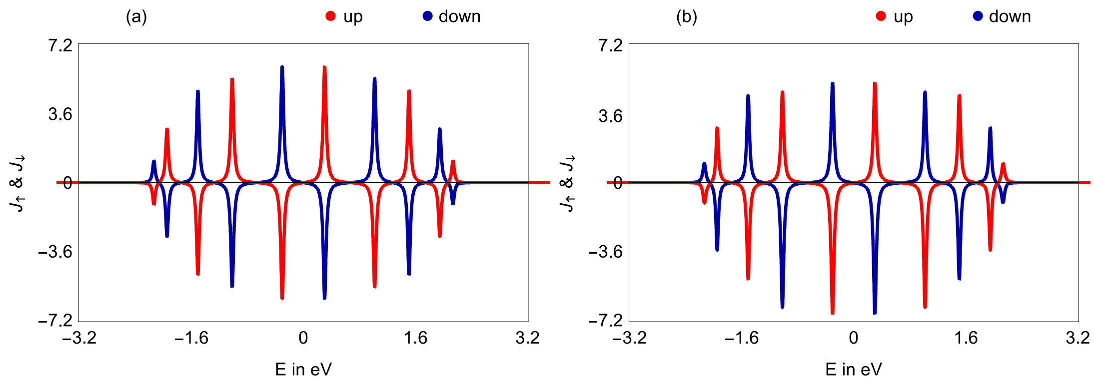

Figure 5: Current densities with energy for symmetric (a) and most asymmetric (b) configurations.

We come across several symmetry relations between the different spin components of the current. In Fig.5 we plot the up and down spin current densities with energy. Here we consider a 10-site ring, connected to the electrodes in two different configurations. In each of these cases, there is a total of 10 peaks and dips for $J_\uparrow$ as well as for $J_\downarrow$ at different energies correspond to the energy eigenvalues of the system. Careful observation reveals that the up (or down) current density at positive energy is exactly equal to the down (or up) current density at negative energy or vice-versa, i.e., $J_\uparrow(E) = J_\downarrow(-E)$ and $J_\downarrow(E) = J_\uparrow(-E)$. Whereas for symmetric bias (Fig.5 (a)), we find another equality relation as: $J_\uparrow(E) = -J_\uparrow(-E)$ and $J_\downarrow(E) = -J_\downarrow(-E)$. These relations eventually lead to the conclusion that under symmetric bias i.e., when the leads are connected to the ring symmetrically, the charge current (which is the integration of the sum of $J_\uparrow$ and $J_\downarrow$ over energy) is always zero, but the spin current (that is the integration of the ($J_\uparrow - J_\downarrow$) over energy) is non-zero. So a pure spin current is generated which means the transfer of spin angular momentum without any charge transport. This is very important as the energy dissipation due to Joule heating, the major source of power dissipation in conventional electronics can be completely suppressed in this case. In an asymmetric junction, if we set the Fermi energy at zero, the spin current vanishes, resulting in a pure charge current. We find that spin current is robust against different asymmetric ring-to-lead configurations, unlike the charge current. For the generation of spin-based quantum computers, proper spin regulation is highly important. Tunning the strength of SOI, we propose a suitable way to control the current externally.

Rectification is one of the fundamental operations in electronic circuits. But we are only familiar with transport current rectification, where the current is always positive in positive bias and opposite in negative bias. Therefore, it will be interesting to study the rectification in circular current as it may has any sign in both the bias conditions as the sign of the current depends on the direction of its circular motion. This is our future plan in this direction.

References:

[1] M. Buttiker, Y. Imry, R. Landauer, Phys. Lett. A **96**, 365 (1983).
[2] Yu. V. Pershin and C. Piermarocchi, Phys. Rev. B **72,** 245331 (2005).
[3] O. Entin-Wohlman, Y. Imry, A. Aharony, Phys. ReV. Lett., **91**, 046802, (2003).
[4] A. Matos-Abiague and J. Berakdar, Phys. ReV. Lett. **94**, 166801 (2005).
[5] S. S. Gylfadottir, M. Nita, V. Gudmundsson, A. Manolescu, Phys. E **27**, 278 (2005).
[6] S. Nakanishi and M. Tsukada, Phys. ReV. Lett **87,** 126801 (2001).
[7] N. Tsuji, S. Takajo, and H. Aoki, Phys. Rev. B **75**, 153406 (2007).

Deadline : Within two months after finishing the research period.
Sabbatical leave with grant: Submit this report to President with confirmation by the dean of school you belong to.
※Postdoctoral fellow is required to submit this report with confirmation by the dean of graduate school before the end of employment period.
Where to submit : Organization for Research and Development and Outreach (NUC)
◆We put this report on the web of KGU. If there is any problem about it because of difficulties on your research, please let us know.