Chiral spin textures in a frustrated kondo lattice model

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CHIRAL SPIN TEXTURES IN A FRUSTRATED KONDO LATTICE MODEL

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SCHOOL OF PHYSICAL AND MATHEMATICAL SCIENCES

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CHIRAL SPIN TEXTURES IN A FRUSTRATED KONDO LATTICE MODEL

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To my family and fiancée ...

Abstract

Strongly correlated electron systems in which there exists a subtle interplay between spin and charge degrees of freedom give rise to many novel and exotic phases. In these spin-charge coupled systems the itinerant electrons and localized moments affect each other in a self-consistent way. The magnetic interaction between the spins is mediated by the motion of electrons; on the other hand, the transport of these electrons is affected by the underlying spin textures. These systems when arranged on geometrically *frustrated* lattices stabilize topologically *non-trivial chiral* configurations of localized spins that drive unconventional transport phenomenon such as topological or geometrical Hall effect. The Shastry-Sutherland model with appropriate generalization is an excellent framework to study the interplay between charge and spin degrees of freedom on a *frustrated* geometry. Furthermore, such a model is directly relevant in understanding the transport of rare earth tetraborides – a family of *metallic* quantum magnets with underlying magnetic Shastry-Sutherland lattice. We investigate Shastry-Sutherland Kondo lattice model (SS-KLM) extensively in different parameter regimes for the ground state phases with unique topological properties using a suite of numerical methods. To reduce finite-size effects we have implemented two

approximate methods truncated polynomial expansion method and traveling cluster approximation – the CPU time for both these methods scales *linearly* with the system size making it possible to explore larger lattice sizes. We present results for integer quantum Hall effect on Shastry-Sutherland lattice in the presence of longitudinal magnetic field. The strong frustration results in decreasing the width of *plateaus* in Hall conductivity while strong disorder leads to the disappearance of higher *plateaus*. The rise in temperature smooths out the steps in Hall conductivity making longitudinal conductivity non-zero over the whole range of Fermi energy. We establish the existence of several *non-coplanar* ground states in the phase diagram of SS-KLM using variational ansatz at $T = 0$. The previously unknown *canted-Flux* state is shown to be stabilized over wide range of parametric space in the presence of Dzyaloshinskii-Moriya interaction. Using unbiased Monte Carlo method we show that this complex ground state can be generated dynamically starting from random spin configurations even at non-zero but a finite value of temperature at half filling of itinerant electrons. Moreover, the non-coplanarity of such topologically *non-trivial* spin textures can be tuned using magnetic field. We also demonstrate that *non-coplanar* ground states are stabilized for $n_e = 1/4$ and $3/4$ against thermal fluctuations. Tuning the strength of frustration is shown to drive the system from *canted-Flux* state through different intermediate topologically *non-trivial* states to topologically trivial anti-ferromagnetic ground state. We show that the ground states with different topological character can be stabilized with the help of magnetic field. Our results are crucial in understanding the emergence of complex spin textures in *metallic* magnets and will be important in explaining the magnetic and electronic properties of the rare earth tetraboride family of *frustrated metallic* magnets.

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Table of Contents

Abstract	iii
Acknowledgement	v
List of Figures	xi
List of Tables	xix
1 Background and Motivations	1
1.1 Introduction	1
1.2 Geometric Frustrations	3
1.3 Shastry-Sutherland Model	4
1.3.1 $\text{SrCu}_2(\text{BO}_3)_2$	6
1.3.2 Rare Earth Tetraborides RB_4	7
1.3.3 Magnetization <i>Plateaus</i>	8
1.4 Topological Hall Effect	10
1.4.1 Berry Phase and Scalar Spin Chirality	12

TABLE OF CONTENTS	ix
1.5 Filling Factor for Itinerant Electrons	19
1.6 Purpose and Organization of this Thesis	20
2 Model and Numerical Methods	22
2.1 Introduction	22
2.2 Model Hamiltonian	23
2.3 Numerical Methods	25
2.3.1 Exact Diagonalization	27
2.3.2 Polynomial Expansion Method (PEM)	28
2.3.3 Truncated Polynomial Expansion Method (TPEM)	30
2.3.4 Traveling Cluster Approximation (TCA)	34
2.4 <i>Simulated Annealing Method</i>	36
2.5 Variational Calculation Method (VCM)	37
2.6 Observables	37
3 IQHE on Shastry-Sutherland Lattice	40
3.1 Model Hamiltonian	42
3.2 Method	42
3.3 Results	44
3.3.1 Role of Frustration	45
3.3.2 Role of Disorder	47
3.3.3 Role of Temperature	50
3.4 Summary	51
4 Phase Diagram of SS-KLM: A variational Calculation Study	53

4.1	Model	54
4.2	Method	55
4.3	Results and Discussions	58
4.4	Summary	62
5	Field-tuned Chiral Phase Transition in SS-KLM at half filling	63
5.1	Model	64
5.2	Method	64
5.3	Physical Observables	65
5.4	Results and Discussions	65
5.5	Summary	72
6	Chiral Phase Transitions driven by Temperature, Geometrical Frustration and Magnetic Field in SS-KLM at $n_e = 1/4$ and $n_e = 3/4$	73
6.1	Model	74
6.2	Methods	75
6.3	Physical Observables	75
6.4	Results and Discussions	75
6.5	Summary	90
7	Conclusions and Outlook	92
7.1	Conclusions	93
7.2	Future Work	96
	Appendices	98

TABLE OF CONTENTS	xi
A Kubo Formalism for Transverse Conductivity	98
B Chebyshev Polynomials	103
References	112

List of Figures

1.1	The geometry of Shastry-Sutherland lattice where the strength of exchange interaction on axial bonds is J while on diagonal bonds it is J' . We have chosen z -axis as our reference direction and longitudinal magnetic field means external magnetic field applied along z -axis.	5
1.2	The magnetic lattice of $\text{SrCu}_2(\text{BO}_3)_2$ in which (a) Cu^{2+} ions are arranged on a lattice which can be topologically transformed to (b) SSL.	6
1.3	Crystal structure of RB_4 the big red spheres denote the R^{4+} ions that are arranged on a lattice which can be topologically transformed to SSL, figure reproduced from reference [1].	8
1.4	The magnetization <i>plateaus</i> observed experimentally in (a) $\text{SrCu}_2(\text{BO}_3)_2$ compound (b) TmB_4 [2].	9
1.5	Parallel transport of a vector on a sphere. Here it is just shown for one-quarter of a sphere and the change in angle of the vector after it returns to the initial position is $\Omega = \pi/2$	13

- 1.6 The figure to illustrate the extra phase $\phi = \Omega/2$ gained by an itinerant electron while traversing the closed path with a finite chirality ' χ ', figure reproduced from reference [3]. 18
- 1.7 Energy spectrum plotted as a function of momentum along symmetric points in the 1st Brillouin Zone (BZ) including Kondo-like interaction term with triple-q order stabilized at $\mathbf{q} = (\pi, 0)$, $(0, \pi)$ and $(0, 0)$. (a) when $t = t' = 1.0$ and $J_K = 3.0$ (b) when $t = 1.0$, $t' = 0.25$ and $J_K = 8.0$. . 19
- 2.1 The snapshot that illustrate the propagation of vector-matrix product elements. The vertical axis indicates the number of multiplication steps while the circles on horizontal axis represent sites. The darkness of these circles shows the amplitude of non-zero elements of vector-matrix products on that site. The initial site is represented by index k while the hatched circle at site l indicates the position where Hamiltonian matrix element is updated. The figure is reproduced from reference [4]. 32
- 3.1 Energy spectrum for 20×20 SSL when $t = 1.0$ and $\phi = 0.1$ (a) for $t' = 0.0$ (b) for $t' = 0.1$ (c) for $t' = 0.25$ and (d) for $t' = 0.5$ 46
- 3.2 Transverse conductivity as a function of Fermi energy for different values of t' at $T = 0.01$ and $w = 0$. The calculations are done on 30×30 SSL when $t = 1.0$ and $\phi = 0.1$ 47
- 3.3 The plots illustrating the energy spectrum for 20×20 SSL when $t = 1.0$, $\phi = 0.1$, $t' = 0$ and (a) $w = 0$ (b) $w = 1.0$ (c) $w = 2.0$. It is clear from the diagrams that with the increase of disorder strength the broadening of energy levels increases. 48

3.4	The plots of (a) <i>transverse</i> conductivity (b) longitudinal conductivity for different values of disorder potential. The conductivities are calculated on 30×30 SSL keeping $t = 1.0$, $t' = 0.1$, $\phi = 0.1$ and $T = 0.01$	49
3.5	(a) Transverse conductivity (b) longitudinal conductivity as a function of Fermi energy for three different values of T keeping $t' = 0.1$ and $w = 1.0$. The calculations are done on 30×30 SSL when $t = 1.0$ and $\phi = 0.1$	51
4.1	DMI defined on the unit cell of SSL where direction of arrow from site i to j indicates the direction of cross product $\mathbf{S}_i \times \mathbf{S}_j$. The red arrows represent the in-plane components of $\mathbf{D}$ while $\otimes$ and $\odot$ represent into and out-of-plane components of $\mathbf{D}$. Blue arrows indicate the in-plane components of $\mathbf{D}'$ on the diagonal bonds. The directions of x , y and z -axes are also mentioned.	55
4.2	Different ordered configurations used in the variational calculations (a) AFM state (b) FM state (c) coplanar Flux state (d) stripe state (e) 3:1 collinear state (f) all-out state (g) 2-in 2-out (h) 3-in 1-out state (i) <i>canted-Flux</i> state (here this ground state is shown on an 8×8 lattice). From a-e are coplanar arrangements of localized spins while f-i are <i>non-coplanar</i> configurations.	57

- 4.3 The phase diagrams at $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$ (a) $|\mathbf{D}| = |\mathbf{D}'| = 0$ (b) $D_{\parallel} = -0.1$, $D_{\perp} = 0.1$ and $D' = -0.12$. The calculations are done on 8×8 lattice and the regions marked with a-i indicates the portions where ordered states in Fig. 4.2 are stabilized. PS describes a phase separation region. 59
- 4.4 The Phase diagrams at $t = 1.0$, $t' = 2.2$, $J = 0.1$, $J' = 0.22$ (a) $|\mathbf{D}| = |\mathbf{D}'| = 0$ (b) $D_{\parallel} = -0.1$, $D_{\perp} = 0.15$ and $D' = -0.22$. The calculation are done on 8×8 lattice and the regions marked with a-i indicates the portions where ordered states in Fig. 4.2 are stabilized. PS describes a phase separation region. 61
- 5.1 Plots of (a) static spin structure along q_x and q_y indicating the peaks appearing at $\mathbf{q} = (0, 0)$, $(0, \pi)$ and $(\pi, 0)$ for 12×12 lattice (b) The magnitudes of peaks at $\mathbf{q} = (0, 0)$, and $(\pi, 0)$ for 8×8 and 12×12 lattices at $h^z = 0$. The other interaction parameters used in calculations are $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$, $J_K = 3.0$, $D_{\parallel} = -0.1$, $D_{\perp} = 0.1$ and $D' = -0.12$ 66
- 5.2 (a) Magnetization per unit site as a function of magnetic field for 12×12 at three different values of $D_{\parallel}$ while keeping $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$, $J_K = 3.0$, $D_{\perp} = 0.1$ and $D' = -0.12$. (b) The total chirality as a function of longitudinal magnetic field. The different interaction parameters used are $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$, $J_K = 3.0$, $D_{\parallel} = -0.1$, $D_{\perp} = 0.1$ and $D' = -0.12$ 67

- 5.3 The real space configurations of local spins for 8×8 lattice shown at different values of magnetic field (a) $h^z = 0.0$ (b) $h^z = 0.8$, just prior to a phase transition (c) $h^z = 1.2$, after the phase transition point and (d) $h^z = 1.6$, when local spins are almost becoming polarized with magnetic field. The color bar besides each plot indicates the out-of-plane component of the spin vector. The different interaction parameters used are $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$, $J_K = 3.0$, $D_{\parallel} = -0.1$, $D_{\perp} = 0.1$ and $D' = -0.12$ 69
- 5.4 Snapshot depicting the circulation of flux, clockwise or anticlockwise, on each plaquette of 8×8 lattice for different values of magnetic field (a) $h^z = 0.0$, (b) $h^z = 0.8$, just before the phase transition (c) $h^z = 1.2$, just after phase transition (d) $h^z = 1.6$, when almost all spins become parallel with h -field. The other interaction parameters used are the same as for Fig. 5.3. 71
- 6.1 (a) Geometry of SSL, where there are diagonal bonds on alternate plaquette in addition to axial bonds along x and y -axes. (b) 1st BZ of SSL lattice with high symmetric points mentioned. 74
- 6.2 Plots of (a) magnetization per unit site and (b) chirality as a function of temperature T at $n_e \simeq 1/4$. The calculations are done on $L = 8 - 16$ lattice sizes keeping $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$ 76

- 6.3 Real space configurations of localized spins obtained from MC calculations on 8×8 lattice (a) when $T = 0.03$, after the phase transition and (b) when $T = 0.06$, prior to phase transition. The data is obtained for $n_e \simeq 1/4$ case when $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$ 77
- 6.4 The momentum dependence of spin structure factor for (a) $T = 0.02$, where the sharp peaks appears at $\mathbf{q} = (0, \pi)$, $(\pi, 0)$ and a small peak at $(0, 0)$ (b) $T = 0.06$, where there is just one peak at $\mathbf{q} = (0, 0)$. The results are obtained using parameters $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$ for 12×12 lattice at $n_e \simeq 1/4$ 78
- 6.5 The MC results for (a) magnetization per site (b) chirality as a function of T for $n_e \simeq 3/4$. The data is obtained while keeping $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$ 79
- 6.6 Energy bands plotted along symmetric points in the 1st BZ with triple- Q order stabilized at $\mathbf{q} = (\pi, 0)$, $(0, \pi)$ and $(0, 0)$. The values of interaction parameters used are $t = 1.0$, $t' = 0.25$ and $J_K = 8.0$ 80
- 6.7 The diagrams illustrating the frustration dependence of (a) magnetization per site and (b) chirality at $n_e \simeq 1/4$. The calculations are done keeping the values of parameters $t = 1.0$, $J = 0.1$, $J' = 0.025$, $h^z = 0$, $J_K = 8.0$ and $T = 0.02$ 81

- 6.8 The snapshots of real space configurations of localized spins obtained from MC calculations on 12×12 lattice (a) when $t'/t = 0.2$, before 1st phase transition and (b) when $t'/t = 0.8$, just after the 1st phase transition (c) when $t'/t = 1.0$, just before the 2nd phase transition and (d) when $t'/t = 1.3$, just after the 2nd phase transition. The data is obtained for $n_e \simeq 1/4$ case when $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$ at $T = 0.02$ 82
- 6.9 The plots for $n_e \simeq 1/4$ case of magnitude of peaks appearing in spin structure factor at $\mathbf{q} = (\pi, 0)$, $(0, 0)$ and (π, π) as a function of frustration. The MC results are obtained when $J = 0.1$, $J' = 0.025$, $h^z = 0$, $J_K = 8.0$ and $T = 0.02$ 84
- 6.10 (a) Magnetization per site (b) chirality for $n_e \simeq 3/4$ case while varying the degree of frustration. The MC results are obtained when $J = 0.1$, $J' = 0.025$, $h^z = 0$, $J_K = 8.0$ and $T = 0.02$ 85
- 6.11 The equilibrium real space spin configurations obtained from MC calculations on 8×8 lattice (a) when $t'/t = 0.2$, before 1st phase transition and (b) when $t'/t = 0.8$, after 1st phase transition (c) when $t'/t = 1.0$, just before 2nd phase transition and (d) when $t'/t = 2.2$, after the 2nd phase transition. The data is obtained for $n_e \simeq 3/4$ case when $J = 0.1$, $J' = 0.025$, $h^z = 0.0$ and $J_K = 8.0$ at $T = 0.02$. See text for more details about these two phase transitions. 86

- 6.12 The plots for $n_e \simeq 3/4$ case of magnitude of peaks appearing in spin structure factor at $\mathbf{q} = (\pi, 0)$, $(0, 0)$ and (π, π) as a function of frustration. The MC results are obtained when $J = 0.1$, $J' = 0.025$, $h^z = 0$, $J_K = 8.0$ and $T = 0.02$ 87
- 6.13 The magnetic field dependence of (a) magnetization per site (b) chirality for $n_e \simeq 1/4$ case. The calculations are done at $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $J_K = 8.0$ and $T = 0.02$ 87
- 6.14 The magnitude of peaks in spin structure factor at $\mathbf{q} = (\pi, 0)$ and $(0, 0)$ while changing magnetic field for $n_e \simeq 1/4$ case. The MC results are obtained when $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $J_K = 8.0$ and $T = 0.02$ 88
- 6.15 The plots depicting the behavior of (a) magnetization per site (b) chirality as a function of external magnetic field for $n_e \simeq 3/4$ case. The calculations are done at $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $J_K = 8.0$ and $T = 0.02$ 89
- 6.16 The magnetic field dependence of magnitude of peaks appearing in spin structure factor at $\mathbf{q} = (\pi, 0)$ and $(0, 0)$ for $n_e \simeq 3/4$ case. The MC results are obtained keeping parameters values at $t = 1.0$, $J = 0.1$, $J' = 0.025$, $J_K = 8.0$ and $T = 0.02$ 90

List of Tables

2.1 Computational complexity for each method 36

Background and Motivations

1.1 Introduction

Metallic frustrated magnets have attracted heightened interest in the recent past. The interplay between geometric frustration and strong interaction between itinerant electrons and localized moments in these systems results in novel quantum phases and phenomena that are not observed in their non-frustrated or insulating counterparts [5, 6, 7, 8, 9, 10, 11, 12]. The study of competing interactions between itinerant electrons and local moments in correlated metals is of course, neither new nor restricted to *metallic* magnets. The Kondo lattice model has long served as a paradigm to understand the behavior of *f*-electron systems, such as the heavy fermions materials. In this model, antiferromagnetic (AFM) coupling between the local moments and the spin of the itinerant electrons drives a Kondo singlet phase which can destroy long-range magnetic order [13, 14, 15, 16, 17]. On the other hand, the double exchange model (DEM) considers a ferromagnetic (FM) interaction between the classical local moments and itinerant electrons arising from Hund's coupling is instrumental in un-

derstanding giant magnetoresistance in d -electron systems [18, 19, 20, 21].

Geometric frustration adds greatly to the richness of these systems. *Frustrated* interactions between the local moments, in addition to crystal electric field effects and coupling to the itinerant electrons, often stabilize *non-coplanar* ordering of these moments [5, 22, 23, 24, 25, 9, 26, 27, 28, 29, 30]. When an electron moves through such background spin textures, it picks up a Berry phase which underlies many interesting transport phenomena such as the topological (or geometric) Hall effect (where a transverse Hall current is observed even in the absence of any magnetic field – driven solely by the cumulative Berry phase acquired by the electrons), and unconventional magnetoresistive properties [31, 32, 33, 34]. The interest in these systems is driven both by the desire to understand the underlying mechanism driving the novel phenomena as well as control, their emergence by external tuning fields in order to harness their unique functionalities for practical applications. Many of these systems are comprised of rare-earth elements with large magnetic moments that can be treated as classical moments. This, in turn, renders the theoretical modeling of such systems more tractable. In the limit of classical moments, the Kondo Lattice and DEM can be mapped onto one another. The Shastry-Sutherland Kondo lattice model (SS-KLM) has previously been studied with $S = 1/2$ local moments [35, 36, 37, 38] where quantum fluctuations of the local moments play a crucial role in determining the character of the ground state. The current model is motivated by the desire to understand completely the magnetic (and subsequently, transport) properties of rare-earth tetraborides (RB_4 , $\text{R}=\text{Tm, Er, Ho, Dy}$) – a family of quasi-two-dimensional *metallic* magnets where the magnetic moment-carrying rare earth ions are arranged in a Shastry-Sutherland lattice (SSL) in the layers. Due to strong spin-orbit coupling, the rare-earth ions in these

compounds carry large magnetic moments and consequently, can be treated as classical spins. They act as effective local fields that interact *strongly* with the electron spin. In this Chapter, we will cover the basic introduction of geometrical frustration, SSL and topological Hall effect (THE).

1.2 Geometric Frustrations

Frustrations occur due to the competing forces which can not be satisfied simultaneously. A system is said to be spin *frustrated* when one can not find a spin configuration in which all the interactions between each pair of spins is satisfied and thus the ground state does not correspond to the minimum energy due to all bonds or interactions within the system [39, 40, 41]. For example when we have AFM Ising model on a triangle, in this case, the spins on neighboring sites try to align anti-parallel to each other to minimize energy. But there is no ground state in which spins on all three bonds are anti-parallel there is always one unsatisfied or so-called *frustrated* bond. The ground state is $2n_s$ fold degenerate where n_s is the number of sites. When frustration spans the whole lattice then the situation becomes very complicated. There is an intensive competition between different orders of the systems and the possibilities are

- a uniform phase in which a single order exist in the system.
- inhomogeneous co-existence of two or more orders (e.g. stripe phases).
- homogeneous co-existence of two or more phases (e.g. supersolid).

Due to all these possibilities, the phase diagram of *frustrated* spin systems is very rich that makes them very susceptible to small variation in any control parameter. A

small change in external potential can drive a system through multiple phase transitions. The motivation behind studying these systems is driven from both theoretical and technological point of view. Investigating and most importantly controlling the basic mechanism behind the occurrence of these exotic and complex phases is important theoretically. The degenerate manifold in these systems can be controlled with realistic external fields which offers a good potential for next generation of technology – the use of giant magnetoresistive materials in the high capacity memory devices is one example.

1.3 Shastry-Sutherland Model

The Shastry-Sutherland (SS) model is a paradigm to study the effects of frustration on magnetic and electronic properties. Shastry and Sutherland proposed this artificial model, that has an exactly solvable ground state, for 2D *frustrated* square lattice whose geometry is shown in Fig. 1.1.

In addition to usual axial bonds that we have for square lattice, there are diagonals bonds on alternate plaquette that are responsible for frustration in the SSL. They considered $S = 1/2$ Heisenberg model on this lattice described by the Hamiltonian,

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (1.1)$$

where $\langle \dots \rangle$ and $\langle\langle \dots \rangle\rangle$ denote the pair of sites on axial and diagonal bonds respectively. For $J' = 0$, the SSL changes to unfrustrated square lattice and in this case Heisenberg $S = 1/2$ model has a magnetic ground state with long-range Néel order. The Néel order exists even for the small and finite value of diagonal interaction J' . On the other

Figure 1.1: The geometry of Shastry-Sutherland lattice where the strength of exchange interaction on axial bonds is J while on diagonal bonds it is J' . We have chosen z -axis as our reference direction and longitudinal magnetic field means external magnetic field applied along z -axis.

hand, when $J = 0$ then the system is reduced to isolated dimers on the diagonal bonds. For these dimers, two spins connected by diagonal bond form a singlet state $|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, and ground state is direct product of these singlet states,

$$|\Psi\rangle_S = \Pi_a |S\rangle_a = \Pi_a \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle_a - |\downarrow\uparrow\rangle_a) \quad (1.2)$$

It is astonishing that above non-magnetic state is also an eigenstate of the model with finite value of J . Shastry and Sutherland found out that in the absence of an external magnetic field by varying the ratio of the interactions between the diagonal and axial bonds there is an interesting quantum phase transition between these two ground states [42]. Later on, with the help of mean field theories and different numerical techniques it is found that the dimer singlet state is stabilized when $J'/J \gtrsim 1.45$.

1.3.1 $\text{SrCu}_2(\text{BO}_3)_2$

The compound $\text{SrCu}_2(\text{BO}_3)_2$ was discovered by Smith and Keszler in 1991 [43] and it took almost one more decade when Miyahara and Ueda pointed out that the magnetic carrying layer in $\text{SrCu}_2(\text{BO}_3)_2$ can be mapped onto SSL [44]. In this compound there are weakly coupled layers – each magnetic layer consists of Cu^{2+} ions carrying $S = 1/2$ spins arranged on a lattice that is topologically equivalent to SSL as shown in Fig. 1.2.

Figure 1.2: The magnetic lattice of $\text{SrCu}_2(\text{BO}_3)_2$ in which (a) Cu^{2+} ions are arranged on a lattice which can be topologically transformed to (b) SSL.

For this compound fitting the experimental data for magnetic susceptibility as a function of temperature the ratio of the diagonal and axial coupling was found to be $J'/J \sim 1.7 - 1.8$ and ground state was confirmed to be non-magnetic with a spin gap. SS model has been used successfully to understand and describe the magnetic properties of this compound.

1.3.2 Rare Earth Tetraborides RB_4

Recently there is a new addition to SSL compounds – a whole family of rare earth tetraborides RB_4 where $\text{R}=\text{Tm}, \text{Tb}, \text{Dy}, \text{Ho}$ and Er [45]. These compounds consist of weakly coupled magnetic layers of R^{3+} ions arranged on a distorted square lattice topologically equivalent to SSL. As these systems are *metallic* unlike $\text{SrCu}_2(\text{BO}_3)_2$, so in addition to localized spins there are itinerant electrons and Shastry-Sutherland model needs to be generalized to include the interaction between localized spins and itinerant electron spins. Compounds belonging to this RB_4 family have a different magnetic ground state that varies from Ising-like AFM order in case of TmB_4 to XY-like AFM order for TbB_4 . In RB_4 most R^{3+} ions carry very large magnetic moment e.g. $J = 6$ for Tm^{3+} and $J = 7\frac{1}{2}$ for Er^{3+} . There is also a strong single-ion anisotropy along the c -axis due to crystal fields which splits the local Hilbert space into degenerate doublets. There is an energy gap $\sim D$ between these successive doublets. At low enough temperatures and high values of D , the excitation to higher levels are subdued and an effective $S = 1/2$ SS model can be used to study low-temperature properties.

The magnetic properties of these materials have been studied very extensively using a generalized SS model with additional long-range RKKY type interactions which are mediated by itinerant electrons. We are interested in studying both magnetic and transport properties in these systems that are relatively unexplored. In order to do that, we have considered additional terms in the Hamiltonian such as on-site Kondo-like interaction, between localized moments and itinerant electrons, and hopping term for itinerant electrons. In these compounds, the electrons in $4f$ orbitals have large magnetic moments, they stay close to Fermi level and contribute to low-temperature

Figure 1.3: Crystal structure of RB_4 the big red spheres denote the R^{4+} ions that are arranged on a lattice which can be topologically transformed to SSL, figure reproduced from reference [1].

behavior. These electrons are considered as localized moments which interact with the electron from $5d$ orbitals of R and $2p$ orbitals of B that form the conduction sea. In RB_4 the interaction between localized moments and itinerant electrons is AFM in nature detailed description of the Hamiltonian that we will use to study the magnetic and electronic properties is given in Chapter 2 where we cover the model Hamiltonian and numerical methods used in the thesis.

1.3.3 Magnetization Plateaus

The most remarkable and intriguing feature of these SS compounds is the appearance of *plateaus* in the magnetization plot. When these systems are subjected to an external magnetic field then some of the non-magnetic dimer singlets changes to the triplet ex-

Figure 1.4: The magnetization *plateaus* observed experimentally in (a) $\text{SrCu}_2(\text{BO}_3)_2$ compound (b) TmB_4 [2].

cited states. These triplet states are immobile due to frustration and there is a competition between the kinetic energy and the repulsive interaction energy of these triplet states. At certain magnetization values when these energies are comparable then there is the crystallization of the triplet excitations leading to magnetization *plateaus*. The magnetization remains constant over a range of field values and there is an energy gap between different *plateaus*. For $\text{SrCu}_2(\text{BO}_3)_2$ prominent fractional *plateaus* have been reported at $m/m_s = 1/8, 1/6, 1/4, 1/3$ and $1/2$ [46, 47, 48, 49, 50, 51]. In the case of RB_4 , the magnetic properties of TmB_4 compound have been explored extensively [52, 53, 54, 2, 55, 56, 57]. For this compound, a stable *plateau* is observed at $m/m_s = 1/2$ [54] while there is an additional fractional *plateau* at $m/m_s \approx 1/8$ that exhibits a unique magnetic hysteresis – the exact value of the magnetization changes

as the field is repeatedly ramped up and down, even though the critical field for the extent of the fractional *plateaus* remains unchanged [2].

1.4 Topological Hall Effect

During last half century, different types of Hall effects have appeared in literature these include spin Hall effect [58], integer quantum Hall effect [59], fractional quantum Hall effect [60], quantum spin Hall effect [61], and quantum *anomalous* Hall effect [62] to name a few. But it all started in the 19th century when Hall in 1879 observed that in an ordinary metal when a magnetic field B is applied perpendicular to the direction of the velocity of electrons then there is a Lorentz force acting on the electrons. This force gives rise to transverse or Hall voltage V_H [63]. This phenomenon is called ordinary Hall effect (OHE) and the transverse resistivity, in this case, can be calculated with Drude model that gives,

$$\rho_H = R_o B \quad (1.3)$$

where $R_o = -\frac{1}{ne}$ is ordinary Hall coefficient for the electrons. Surprisingly when Hall tried the same experiments on a magnetic conductor he reported that this effect is ten times greater than as compared to an ordinary non-magnetic conductor. This enhanced effect in ferromagnetic conductor got the name *anomalous* Hall effect (AHE) [64]. In case of magnetic metals, the conduction electrons scatter off localized spins and contributes an extra term in the transverse resistivity which is proportional to magnetization M ,

$$\rho_H = R_o B + R_S M \quad (1.4)$$

The *anomalous* Hall coefficient R_S is normally greater than ordinary Hall coefficient R_o by an order of magnitude. As in FM materials, the spontaneous magnetization is non-zero even after removing the magnetic field that means the AHE can be observed in the zero magnetic field. In 1954, Karplus and Luttinger suggested that when an electron moves in a conductor where there is an applied electric field E then its group velocity acquires an extra contribution [31]. This *anomalous velocity* will contribute to Hall conductivity in FM conductors.

The exact mechanism of AHE remained an *enigmatic* problem for almost a century. As AHE is proportional to M i.e. electron spin and transport properties are affected by this spin so spin-orbit coupling should be incorporated to understand this phenomenon. One group of people describes AHE in terms of external mechanisms like skew-scattering or side jump off the carriers from the localized impurity spins [65]. This scattering is different for spin-up and spin-down electrons and as a result electrons with different spins will be accumulated on two edges of the sample. In the case of FM materials the spin-up and spin-down electrons are unequal this leads to charge imbalance on the boundaries of the material creating a transverse potential that explains AHE. On the other hand, the *anomalous velocity* mechanism put forward by Karplus and Luttinger is of intrinsic nature as it depends upon the electronic energy band structure [66].

1.4.1 Berry Phase and Scalar Spin Chirality

The understanding of the AHE became much clearer after the discovery of Berry phase in 1984 [67]. The velocity which Karplus and Luttinger used to describe the AHE is related to the Berry curvature of the energy band. The concept of Berry phase can be obtained from the parallel transport where a vector is moved along a closed path on a curved surface with a condition to always lie on a local tangent. Then after returning to its starting point the direction of the vector is rotated by an angle known as Berry phase. The parallel transport of a vector on a sphere is depicted in Fig. 1.5 where a vector is moved over a closed path on a sphere. When this vector comes back to the point A from where it started the angle is changed by Ω . This effect is of purely geometrical nature and depends only on the curvature of the surface on which vector is moved. For example, if this vector is transported over the whole sphere then $\Omega = 2\pi$ and there will be no change in the direction of the vector. Moreover, this phase will be absent when the vector is moved over a plane or the surface of the cylinder. The same type of effect happens in quantum mechanics where a particle, which is transported adiabatically around a closed path in the space of external parameters – gains an extra phase that depends upon the geometry of the path [68]. A well-known example is that of Aharonov-Bohm effect in which the wavefunction of an electron acquires an extra Berry phase through interference with the magnetic potential while moving in a path where the magnetic field is negligible [69].

In order to derive Berry phase, we consider the adiabatic evolution of external parameters (on which Hamiltonian of the system depends) over a closed path $\mathcal{C}$ in a parametric space. The Hamiltonian for the system is $H(\mathbf{R})$ where $\mathbf{R}$ is a function

Figure 1.5: Parallel transport of a vector on a sphere. Here it is just shown for one-quarter of a sphere and the change in angle of the vector after it returns to the initial position is $\Omega = \pi/2$.

of time $\mathbf{R} = \mathbf{R}(t)$. Using Schrödinger equation we can find orthonormal eigenstates $|n(\mathbf{R})\rangle$ and eigenvalues $E_n(\mathbf{R})$,

$$H(\mathbf{R})|n(\mathbf{R})\rangle = E_n(\mathbf{R})|n(\mathbf{R})\rangle \quad (1.5)$$

We make a gauge choice such that the phase of the basis states changes smoothly and remains single valued along the path $\mathcal{C}$ in the parametric space. If we start with an initial state $|\psi_n(t=0)\rangle = |n[\mathbf{R}(t=0)]\rangle$ at $t=0$ then from quantum adiabatic theorem the system will remain in this state for a later time t with an extra dynamical phase.

$$|\psi_n(t)\rangle = e^{i\gamma_n(t)} \exp \left[-\frac{i}{\hbar} \int_0^t dt' E_n(\mathbf{R}(t')) \right] |n(\mathbf{R}(t))\rangle \quad (1.6)$$

In above equation, the 2nd exponential is the usual dynamical phase factor that is present for the time evolution of an eigenstate. After substituting this time-dependent

eigenstate into Eq. (1.5) and multiplying with $\langle n(\mathbf{R}(t)) |$ we can write phase γ_n as,

$$\gamma_n = \int_{\mathcal{C}} d\mathbf{R} \cdot \mathcal{A}_n(\mathbf{R}) \quad (1.7)$$

where

$$\mathcal{A}_n(\mathbf{R}) = i \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} | n(\mathbf{R}) \rangle \quad (1.8)$$

is known as Berry vector potential. $\mathcal{A}_n(\mathbf{R})$ is gauge dependent and if we perform a gauge transformation such that it transforms eigenstates to,

$$|n(\mathbf{R})\rangle \rightarrow e^{i\eta(\mathbf{R})} |n(\mathbf{R})\rangle \quad (1.9)$$

and $\mathcal{A}_n(\mathbf{R})$ to,

$$\mathcal{A}_n(\mathbf{R}) \rightarrow \mathcal{A}_n(\mathbf{R}) - \nabla_{\mathbf{R}} \eta(\mathbf{R}), \quad (1.10)$$

then after transformation, the phase γ_n in Eq. (1.7) changes by $\eta(\mathbf{R}(0)) - \eta(\mathbf{R}(T))$, where $\mathbf{R}(0)$ and $\mathbf{R}(T)$ being the initial and final points of the path $\mathcal{C}$. All this has been known earlier and people have ignored this phase γ_n because there is always a gauge transformation possible for $|n(\mathbf{R})\rangle$ such that after performing this transformation the phase γ_n is canceled out along the path $\mathcal{C}$.

But Berry in 1984 revisited this problem and considered the cyclic evolution over the closed path $\mathcal{C}$ such that $\mathbf{R}(T) = \mathbf{R}(0)$. Now gauge transformation we performed earlier requires $e^{i\eta(\mathbf{R})}$ to be single valued which means that $\eta(\mathbf{R}(0)) - \eta(\mathbf{R}(T)) = 2\pi \times n$, where n is an integer. For a closed path, we can not ignore this phase because under

a gauge transformation γ_n changes as an integer multiple of 2π . This phase is now known as Berry or geometrical phase and for a closed path, it is gauge-invariant.

$$\gamma_n = \oint_{\mathcal{C}} d\mathbf{R} \cdot \mathcal{A}_n(\mathbf{R}) \quad (1.11)$$

We can use Gauss's theorem to write above equation as a surface integral of a curl,

$$\begin{aligned} \gamma_n &= \int_S d\mathbf{S} \cdot \nabla \times \mathcal{A}_n(\mathbf{R}) \\ &= \int_S d\mathbf{S} \cdot \mathbf{B}_n(\mathbf{R}) \end{aligned} \quad (1.12)$$

where $\mathbf{B}_n(\mathbf{R})$ is the Berry curvature.

$$\begin{aligned} \mathbf{B}_n(\mathbf{R}) &\equiv \nabla \times \mathcal{A}_n(\mathbf{R}) \\ &= i \langle \nabla n(\mathbf{R}) | \times | \nabla n(\mathbf{R}) \rangle \\ &= i \sum_{m \neq n} \langle \nabla n(\mathbf{R}) | m(\mathbf{R}) \rangle \times \langle m(\mathbf{R}) | \nabla n(\mathbf{R}) \rangle. \end{aligned} \quad (1.13)$$

We can use the following relation,

$$\langle m | \nabla n \rangle = \frac{\langle m | \nabla H | n \rangle}{E_n - E_m} \quad (1.14)$$

to write Berry curvature as,

$$\mathbf{B}_n(\mathbf{R}) = i \sum_{m \neq n} \frac{\langle n(\mathbf{R}) | \nabla H(\mathbf{R}) | m(\mathbf{R}) \rangle \times \langle m(\mathbf{R}) | \nabla H(\mathbf{R}) | n(\mathbf{R}) \rangle}{(E_m(\mathbf{R}) - E_n(\mathbf{R}))^2}. \quad (1.15)$$

The Berry curvature gives the Hall response of each electron state and to calculate the Hall conductivity for the whole system we need to do the sum of Berry curvature over all occupied states,

$$\sigma_{xy} = \frac{e^2}{\hbar} \frac{1}{V} \sum_{n, \mathbf{R}} \mathbf{B}_n(\mathbf{R}). \quad (1.16)$$

Recently it is observed that *non-coplanar* spin configurations in *frustrated* systems also drive AHE. When an electron moves over a path where there is a spatially varying strong magnetization then its spin will adiabatically follow the direction of magnetization. The electron will feel a fictitious magnetic field and will gain an extra Berry phase. This phase which will be equal to the solid angle subtended by this magnetization when electron follows its path then contributes to the AHE. As it depends on the topology of the magnetization pattern and not on the spin-orbit coupling hence the name Topological Hall effect (THE) has been given. In case of strong coupling between localized moments and conduction electrons, the spin of the itinerant electrons becomes enslaved to the local moment spin and effective hopping amplitude acquires a quantum mechanical phase. This phase is the vector potential generated by the local moments and corresponds to the Berry phase felt by the hopping electrons. It is also analogous to Peierls phase or Aharonov–Bohm phase induced by an external magnetic field and hence induces the Hall effect in the presence of certain spin textures. As mentioned before itinerant electron spin will follow the direction of spin of the localized moment on each site. So in the case of *non-coplanar* spin textures, the electron in its rest frame will feel a time-dependent magnetic field. This phenomenon appears in DEM – the minimal Hamiltonian that describes this model can be written as,

$$\hat{\mathcal{H}} = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c) - J_K \sum_i \mathbf{S}_i \cdot \mathbf{s}_i^c \quad (1.17)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) represents creation (annihilation) operators for an itinerant electron at the site i with spin σ and t is hopping integral. J_K is strength of Kondo-like coupling between itinerant electron spin $\mathbf{s}_i^c$ and localized spin $\mathbf{S}_i$. For strong J_K limit, the spin

of the itinerant electron is aligned parallel to the spin of localized moment at each site. In this case, the spin wavefunction of electron becomes,

$$|\chi_i\rangle = t \left[e^{ib_i} \cos \frac{\theta_i}{2}, e^{i(b_i+\phi_i)} \sin \frac{\theta_i}{2} \right], \quad (1.18)$$

where b_i is an overall phase that corresponds to gauge degrees of freedom and does not appear in the physical observables. The localized spins are considered as classical vectors and x, y, z components of these spins can be described with polar coordinates $\mathbf{S}_i = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i)$. When an electron hops from site i to site j then effective hopping matrix for this process can be written as,

$$t_{ij}^{eff} = t \langle \chi_i | \chi_j \rangle = t e^{ia_{ij}} \cos \frac{\theta_{ij}}{2} \quad (1.19)$$

In above equation, $a_{ij} = b_j - b_i$ is phase factor and θ_{ij} is the angle difference between two localized spins $\mathbf{S}_i$ and $\mathbf{S}_j$. Next, the flux that appears when an electron moves in a loop over a *non-coplanar* arrangement of spins $\mathbf{S}_i$, $\mathbf{S}_j$ and $\mathbf{S}_k$ can be calculated as,

$$\langle \mathbf{n}_i | \mathbf{n}_k \rangle \langle \mathbf{n}_k | \mathbf{n}_j \rangle \langle \mathbf{n}_j | \mathbf{n}_i \rangle = (1 + \mathbf{n}_i \cdot \mathbf{n}_j + \mathbf{n}_j \cdot \mathbf{n}_k + \mathbf{n}_k \cdot \mathbf{n}_i) \propto e^{i\Omega/2} \quad (1.20)$$

where $e^{i\Omega} = e^{2i(a_{ij}+a_{jk}+a_{ki})}$ is Berry phase gained by electron wavefunction and $\mathbf{n}_i$ is the spinor wavefunction of the spin aligned in the direction $\hat{\mathbf{n}}_i = \mathbf{S}_i / |\mathbf{S}_i|$. The imaginary part of the product of hopping integrals in Eq. (1.20) is proportional to $\mathbf{S}_i \cdot \mathbf{S}_j \times \mathbf{S}_k$ which is scalar spin chirality χ and is equal to solid angle Ω subtended by three spins. The pictorial description of this process is shown in Fig. 1.6. That means when an itinerant electron hops in a loop on a triangle where there is a *non-coplanar* arrangement of localized spins then the wavefunction of the electron gains an extra Berry phase which

is equal to the solid angle subtended by the three spins at the center of the triangle.

Figure 1.6: The figure to illustrate the extra phase $\phi = \Omega/2$ gained by an itinerant electron while traversing the closed path with a finite chirality ' χ ', figure reproduced from reference [3].

The spin chirality is a very important concept that explains THE in *frustrated* spin systems. The Berry phase will be zero for coplanar configurations as in that case chirality is zero. The *non-coplanar* arrangement generates fictitious magnetic field and affects the movement of the electrons the same way as does real magnetic field [70, 66]. The *non-coplanar* spin textures are observed in most of the *frustrated* spin systems such as triangular, kagome and pyrochlore. To observe THE at low temperatures the topological and geometrical properties of the system play an important role. Recent studies observed THE in *frustrated* double-exchange systems where this effect is related to a topologically *non-trivial* spin structure. In *frustrated* spin systems, the *chiral spin* structure is responsible for breaking the time-reversal (**T**) symmetry as well as parity (**P**) symmetry which in turn bring about THE even in the absence of magnetic field.

Figure 1.7: Energy spectrum plotted as a function of momentum along symmetric points in the 1st Brillouin Zone (BZ) including Kondo-like interaction term with triple- q order stabilized at $\mathbf{q} = (\pi, 0)$, $(0, \pi)$ and $(0, 0)$. (a) when $t = t' = 1.0$ and $J_K = 3.0$ (b) when $t = 1.0$, $t' = 0.25$ and $J_K = 8.0$.

1.5 Filling Factor for Itinerant Electrons

We plan to explore the topological phases in SS-KLM both at *insulating* and *metallic* limits. Fig. 1.7a shows the energy spectrum calculations for Eq. (1.17) at $t = t' = 1.0$ and $J_K = 3.0$. The energy spectrum is gapped at half-filling indicating the *insulating* state. Without Dzyaloshinskii-Moriya interaction (DMI), we found that at half-filling the parent ground state is AFM. Using MC calculations in Chapter 5, we discussed the role of DMI how it induces the *chiral phases*. So it was very natural to start the discussion at half filling where we have *insulating* phase and parent ground state is coplanar. In Chapter 6, we choose $n_e = 1/4$ and $3/4$, where $n_e = \frac{1}{2N} \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma}$ is the

number density of itinerant electrons and N is the total number of sites. For these filling factors the spectrum is gapless as can be seen in Fig. 1.7b where we have plotted energy spectrum at $t = 1.0$, $t' = 0.25$ and $J_K = 8.0$. The one-quarter filling is chosen to study the *metallic* behavior at relatively low commensurate filling while $n_e = 3/4$ explores the *metallic* behavior at relatively high commensurate filling away from *insulating* phase at $n_e = 1/2$. For these commensurate fillings, we found out that unlike *insulating* phase here we do not need DMI to stabilize the *non-coplanar* orderings.

1.6 Purpose and Organization of this Thesis

Our aim is to study extensively the exotic and novel phases which emerge due to the interaction between localized spins and itinerant electron spins on geometrically *frustrated* SSL. The particular focus and objective is to find the parametric regimes where *chiral* spin textures are stabilized. We will try to understand the mechanism behind the emergence of these topologically *non-trivial* phases and to control their occurrence by external parameters such as magnetic field, frustration and thermal fluctuations.

The organization of this thesis is as follows. The model that will be used in most parts of this thesis is SS-KLM that we will introduce in Chapter 2. In order to study the magnetic and electronic properties of SS-KLM, we will use an unbiased classical Monte Carlo (MC) method alongside some approximate methods such as truncated polynomial expansion method (TPEM) and traveling cluster approximation (TCA) to reach to larger lattice sizes. All these methods and variational calculations method (VCM) that we have used to study the phase diagram of the above-mentioned model will be discussed in detail in Chapter 2.

Next moving on to Chapter 3 we will present the results for integer quantum Hall effect (IQHE) on SSL. The role of different parameters such as frustration, disorder and temperature on Hall and longitudinal conductivity will be discussed thoroughly. In Chapter 4 we will use VCM to study the phase diagram of SS-KLM. The stabilization of different *non-coplanar* configurations such as a peculiar *canted-Flux* state will be discussed. Chapter 5 is dedicated to the study of the robustness of this *canted-Flux* state as a function of temperature and magnetic field at half filling of itinerant electrons. The results for topological phase transition and ground states with different *non-coplanar* characters while varying magnetic field will be presented in detail.

Chapter 6 is devoted to the study of the emergence of *chiral* phases at one-quarter and three-quarter filling of itinerant electrons. The mechanism of these phases and the role of thermal fluctuation, frustration and magnetic field leading to different topological phase transitions will be presented in this Chapter. The last Chapter is dedicated to discussion, summary and future work.

Model and Numerical Methods

2.1 Introduction

The electronic systems where a different degree of freedom (DOF) are coupled *strongly* has become exciting field of research both from the theoretical and experimental point of view [71, 72, 73]. An example for such systems is Ferromagnetic Kondo Lattice or double exchange systems where there exists a *strong* on-site interaction between localized moments and itinerant electrons in addition to a tight binding term for itinerant electrons [74, 75, 76]. To study these systems theoretically is a challenging task since multiple DOF are involved in these systems such as charge, spin and orbital and treating them equally is very difficult. Therefore, different approximations have been used to study these systems. One of the approximations that have been used quite extensively is to separate between the *fast* and *slow* dynamics of DOF [77, 78]. In these systems, the dynamics of the large localized moments is *slow* as compared to the itinerant electrons dynamics and can be treated as classical adiabatical fields on each site.

This separation between *slow* and *fast* dynamics allows studying the ground state of these systems with the help of mean-field theory as classical fields are frozen and *irrelevant*. But at finite temperature the fluctuations of these fields become relevant and itinerant electrons respond to these fluctuations in a precise manner so mean-field approximations become invalid at finite temperature. Different numerical methods are used to study the thermodynamics properties of these systems. In this Chapter, we present the detailed introduction of one of such method, classical Monte Carlo (MC) method. The method can be used to study finite size lattices of these systems where the trace over the classical fields is replaced by a stochastic sampling [79, 20]. The computational complexity for this method scales as $\mathcal{O}(N^4)$, where N is the size of the lattice. So we are restricted to only small lattice sizes and suffer from finite-size effects. In order to study large lattice sizes, we have used sophisticated methods such as truncated polynomial expansion method (TPEM) and travelling cluster approximation (TCA). For both of these methods the computational complexity scales *linearly* $\mathcal{O}(N)$ with the system size. We have discussed in detail the theoretical basis for these methods in the upcoming sections.

2.2 Model Hamiltonian

In order to study the novel magnetic and transport properties that arise due to the interaction between spin and charge degrees of freedom on geometrically frustrated SSL, we consider here Kondo Lattice Model (KLM) or also known as DEM with classical localized spins. The Hamiltonian describing the SS-KLM with additional terms – DMI and an external magnetic field can be written as,

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_e + \underbrace{\hat{\mathcal{H}}_{ex} + \hat{\mathcal{H}}_{DM} + \hat{\mathcal{H}}_h}_{\hat{\mathcal{H}}_c} \quad (2.1)$$

where,

$$\hat{\mathcal{H}}_e = - \sum_{\langle ij \rangle, \alpha} t_{ij} (c_{i\alpha}^\dagger c_{j\alpha} + h.c.) - J_K \sum_i \mathbf{S}_i \cdot \mathbf{s}_i^c \quad (2.2)$$

is the electronic part of the Hamiltonian that has the itinerant electron hopping term together with a second term that describes the on-site interaction between these electrons and the localized spins. In above equation, t_{ij} is the hopping integral, $\langle ij \rangle$ represents the pair of sites on the bond while J_K is the Kondo-like interaction parameter whose sign is *irrelevant* in the current study since eigenstates that correspond to different signs are related by a global gauge transformation.

The last three terms in Eq. (2.1) constitute the classical spin part $\hat{\mathcal{H}}_c$ of the total Hamiltonian. All the terms in this part are dependent only on the classical localized spins. The 1st term in $\hat{\mathcal{H}}_c$ represents the Heisenberg exchange interaction between the localized spins.

$$\hat{\mathcal{H}}_{ex} = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad (2.3)$$

where J_{ij} is the exchange constant between spins on the bond $\langle ij \rangle$. While the 2nd term is the DMI the origin of this term can be explained on the basis that the systems we focus on (rare-earth elements) have larger spin-orbit interaction and large nuclear charge. In mathematical form, we can represent DMI as,

$$\mathcal{H}_{DM} = \sum_{\langle i,j \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j). \quad (2.4)$$

where D_{ij} is the DM vector which is determined by the crystal symmetry of the lattice. The full detail about this term is explained in Chapter 4. The last term is the Zeeman energy term for the localized spins due to an external (longitudinal) magnetic field.

$$\mathcal{H}_h = -h^z \sum_i S_i^z \quad (2.5)$$

Since the localized spins carry large magnetic moments and the electronic spin states are driven solely by the local moments so we only consider the effect of external magnetic field on them and ignore the effect on the itinerant electrons.

2.3 Numerical Methods

In order to study the above Hamiltonian for magnetic and electronic properties, we make use of an unbiased MC method [9, 80, 81, 82]. In this method, we treat the localized spins as classical fields that interact with the fermions. The dynamics of the large localized moments is *slow* as compared to itinerant electrons. The localized spins are treated as classical vectors of unit length and x, y, z components of the localized spin are $\mathbf{S}_i = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i)$. Replacing the itinerant electron spin $\mathbf{s}_i^c = c_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{i,\beta}$, the electronic part of the Hamiltonian becomes bilinear in fermionic operators where $\boldsymbol{\sigma}_{\alpha\beta}$ are the vector elements of usual Pauli matrices. The basis used are the one-electron basis, in that case, $\hat{\mathcal{H}}^e$ can be represented as $2N \times 2N$ matrix for a fixed configuration of classical localized spins, where N is the total number of sites.

In order to investigate the thermodynamic properties we write the partition function for the whole system which consists of two traces i.e.,

$$Z = \text{Tr}_c \text{Tr}_f \exp(-\beta[\hat{\mathcal{H}}_e(\phi) - \mu n_e]) \cdot \exp(-\beta[\hat{\mathcal{H}}_c(\phi)]) \quad (2.6)$$

where Tr_c and Tr_f represent the traces over the classical localized spin degrees of freedom and fermionic degrees of freedom respectively. ϕ represent the different configurations of the localized spins. Tr_f can easily be calculated by the eigenvalues of Hamiltonian $\hat{\mathcal{H}}_e$ matrix for a particular configuration of localized spins as,

$$\text{Tr}_f \exp(-\beta[\hat{\mathcal{H}}_e(\phi) - \mu \hat{n}_e]) = \prod_{\nu} (1 + \exp[-\beta(\varepsilon_{\nu} - \mu)]) \quad (2.7)$$

where μ is the chemical potential, $\beta = 1/T$ is inverse temperature and $\hat{n}_e = \frac{1}{2N} \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}$ is the number density operator for itinerant electrons. Replacing above equation in Eq. (2.6) the partition function for the whole system can be written as,

$$Z = \text{Tr}_c \exp[-S_{\text{eff}}(\phi) - \beta\{\hat{\mathcal{H}}_c(\phi)\}] \quad (2.8)$$

where

$$S_{\text{eff}}(\phi) = - \sum_{\nu} \log(1 + \exp[-\beta(\varepsilon_{\nu} - \mu)]) = \sum_{\nu} F(\varepsilon_{\nu}(\phi)) \quad (2.9)$$

is effective action and

$$F(y) = -\log[1 + e^{-\beta(y-\mu)}]. \quad (2.10)$$

The grand canonical trace over localized spin degrees of freedom can be calculated with the help of MC method and for a particular configuration of localized spins the probability distribution can be written as,

$$P(\phi) \propto \exp[-S_{\text{eff}}(\phi) - \beta\{\hat{\mathcal{H}}_c(\phi)\}] \quad (2.11)$$

To calculate Boltzmann weight or action we use different methods as explained below.

2.3.1 Exact Diagonalization

The simplest way to calculate the $P(\phi)$ is the exact diagonalization-MC method (ED-MC) – where the eigenvalues ε_ν are calculated by diagonalizing the Hamiltonian matrix $\hat{\mathcal{H}}_c(\phi)$. The process flow for the ED-MC is as follows,

- (1) We start with a random configuration for the classical variables and store them in an array $S[\]$. Next, we generate the full Hamiltonian $H_{\text{full}}(S[\])$ and diagonalize it to calculate the Boltzmann weight given by Eq. (2.11).
- (2) We select a site randomly and update the classical variables on that site. We generate again the $H_{\text{full}}(S[\])$ for this update and find the Boltzmann weight.
- (3) In the last step, we accept or reject this update based on Metropolis algorithm.

The disadvantage of calculating S_{eff} with ED-MC is the higher computational complexity. The computational complexity for the diagonalization of the Hamiltonian matrix to calculate eigenvalues is $\mathcal{O}(N_{\text{dim}}^3)$, where $N_{\text{dim}} = 2N$. The MC updates are done locally and the total computational complexity for one MC step varies like $\mathcal{O}(N^4)$ as $N_{\text{dim}} \propto N$. That means the calculations with ED-MC can be done for only small lattice sizes. To go to large system sizes we used the following alternative methods.

2.3.2 Polynomial Expansion Method (PEM)

The PEM replaces the exact diagonalization for polynomial expansion. In this method, the Boltzmann weight and effective action, that are calculated very frequently in MC calculations, are expanded in terms of polynomials. The polynomial expansion method accelerates the calculation of above mentioned two quantities. As suggested by Furukawa *et al.* the function $F(y)$ in Eq. (2.10) can be expanded by a series of polynomials $T_m(y)$

$$F(y) = \sum_{m=0}^{\infty} f_m T_m(y) \quad (2.12)$$

to abridge the computational complexity [83]. The effective action $S_{\text{eff}}(\phi)$ can also be written in terms of polynomials as,

$$S_{\text{eff}}(\phi) = \sum_m f_m \mu_m \quad (2.13)$$

where,

$$\mu_m = \sum_{\nu=1}^{N_{\text{dim}}} T_m(\varepsilon_{\nu}(\phi)) = \text{Tr} T_m(\hat{\mathcal{H}}_e(\phi)) \quad (2.14)$$

are polynomial moments that are calculated by trace and simple matrix operations of $\hat{\mathcal{H}}_e(\phi)$. So expanding the effective action $S_{\text{eff}}(\phi)$ by a series of polynomials help us to get Boltzmann weights by simple matrix operations for each update of localized spins. We use Chebyshev polynomials to expand the effective action as expansion coefficient f_m decays in an exponential way for $m \gg 1$. The detail about Chebyshev polynomials is provided in appendix B. As the orthonormal condition for Chebyshev polynomials is defined within the range $-1 \leq y \leq 1$ so we have to rescale our Hamiltonian ma-

trix so that eigenvalues satisfy $-1 \leq \varepsilon_\nu(\phi) \leq 1$. Using the orthonormal condition of Chebyshev polynomials we can write Eq. (2.14) as,

$$\mu_m = \int_{-1}^1 d\varepsilon D_\phi(\varepsilon) T_m(\varepsilon) \quad (2.15)$$

where $D_\phi(\varepsilon)$ are the density of states (DOS) for eigenvalues of the Hamiltonian matrix $\hat{\mathcal{H}}_e(\phi)$, defined by the following equation,

$$D_\phi(\varepsilon) = \sum_\nu \delta(\varepsilon - \varepsilon_\nu(\phi)) \quad (2.16)$$

To implement the algorithm we use the orthonormal basis vectors $v(k, m)$ and calculate the trace in Eq. (2.14) as,

$$\mu_m = \sum_k \tilde{\mu}_m(k), \quad \tilde{\mu}_m(k) \equiv (e(k), v(k, m)) \quad (2.17)$$

here $(,)$ indicates an inner product between two basis vectors and

$$v(k, m) \equiv T_m(\mathcal{H}_e)v(k, 0) \quad (2.18)$$

In order to calculate different $v(k, m)$ we use the recursion relation for the Chebyshev polynomials and for the simplicity of calculation unit vectors are used such that

$$v_i(k, 0) = e_i(k) \equiv \delta_{ik},$$

$$v(k, 1) = \hat{\mathcal{H}}v(k, 0), \quad v_i(k, m) = 2 \sum_j \hat{\mathcal{H}}_{ij} v_j(k, m-1) - v_i(k, m-2) \quad (2.19)$$

To calculate $\tilde{\mu}_m(k)$ in Eq. (2.17) we have to perform the matrix-vector operations recursively and computational complexity for these operations scales as $\mathcal{O}(N)$ as our

Hamiltonian matrix is sparse. For the calculation of $\tilde{\mu}_m(k)$ up to $m = M$, the total computational complexity is $\mathcal{O}(MN)$. We can get μ_m after evaluating the trace operation in Eq. (2.17) which scales as $\mathcal{O}(N)$ that means the complexity to calculate the Boltzmann weight is $\mathcal{O}(MN^2)$. Then for each MC step with local updates, the total complexity with PEM is $\mathcal{O}(MN^3)$ as compared to $\mathcal{O}(N^4)$ in the case of ED-MC. For the cases where $M \ll N$ PEM is useful over ED-MC.

2.3.3 Truncated Polynomial Expansion Method (TPEM)

An additional improvement over the PEM was introduced recently on the basis of two truncations (i) of matrix-vectors products and (ii) of the trace difference in action for MC updates. After doing these truncations the resulting algorithm TPEM has a CPU time which scales *linearly* with the system size [4]. In order to explain these two truncations in detail let us take a simple model as an example which is quite similar to what we have in Eq. (1.1).

$$H_{ij}(\phi) = \begin{cases} g\phi_i & \text{for } i = j, \\ -t & \text{for } i \text{ and } j \text{ are nearest neighbors,} \\ 0 & \text{otherwise.} \end{cases} \quad (2.20)$$

where t is the hopping matrix to nearest neighbors and g is the itinerant electron coupling constant to the on-site adiabatical fields ϕ_i .

(i) Truncation of vector-matrix Products

As mentioned earlier to calculate $\tilde{\mu}_m(k)$ in Eq. (2.17) we need to find matrix-vector products that scale as $\mathcal{O}(N)$. We can perform a truncation method to reduce the complexity of these products. For the orthonormal set defined as $e_i(k) \equiv \delta_{ik}$, $v_i(k, 0)$ is non-zero only when $i = k$ but $v_i(k, 1) \neq 0$ not only for $i = k$ but also for nearest neighbors from the definition of Hamiltonian (2.20). Due to the sparse Hamiltonian matrix, we do not need to calculate all other vector elements. So computational complexity can be reduced if we just keep track of non-zero vector elements of $v_i(k, m - 1)$, that later can be used to calculate the elements of $v_i(k, m)$.

The vector-products defined in Eq. (2.17) are like diffusive propagation of a wavefunction. Initially, $v(k, 0) = e(k)$ represents an electron localized at site k and each time we operate with $\mathcal{H}$ to get $v(k, m)$ electron moves to nearest neighbor sites. So operating with the Hamiltonian spreads out the non-zero vector elements of $v_i(k, m)$ this process is illustrated in Fig. 2.1. We define the distance between k^{th} site and l^{th} site by $|l - k|$ as the minimum number of steps it will take for an electron to hop from k^{th} site to l^{th} site. In Fig. 2.1 $R_o(m)$ represents the maximum distance that an electron can hop when the initial state is operated by the Hamiltonian matrix m times. There is no contribution to the calculation of vector-matrix products from the sites outside the range of propagation $R_o(m)$. We just need to perform these calculations only to the neighbors of site k which obey the condition $|l - k| \leq R_o(m)$. This also reduces the computational complexity of calculating $\tilde{\mu}_m(k)$ from $\mathcal{O}(MN)$ to $\mathcal{O}(M^{d+1})$, d being the dimension of the lattice. Until now we have not done any approximation and the results are exact.

Figure 2.1: The snapshot that illustrate the propagation of vector-matrix product elements. The vertical axis indicates the number of multiplication steps while the circles on horizontal axis represent sites. The darkness of these circles shows the amplitude of non-zero elements of vector-matrix products on that site. The initial site is represented by index k while the hatched circle at site l indicates the position where Hamiltonian matrix element is updated. The figure is reproduced from reference [4].

In the next step, we select a threshold ϵ_{pr} where the elements of the matrix-vector product are restricted. In the Fig. 2.1 $R_\epsilon(m)$ represent the maximum range of propagation for which $v_i(k, m) \geq \epsilon_{pr}$ and if $|l - k| > R_\epsilon(m)$ we neglect the contributions of these elements towards the calculation of $\tilde{\mu}_m(k)$ and $v_i(k, m + 1)$. Generally, the diffusion length is proportional to square root of number of steps i.e., $R_\epsilon(m) \propto \sqrt{m}$. So the introduction of threshold ϵ_{pr} and range $R_\epsilon(m)$ leave the number of sites contributing to the calculation of $\tilde{\mu}_m(k)$ to scale as $\mathcal{O}(M^{d/2})$. After doing this truncation the computational complexity to calculate $\tilde{\mu}_m(k)$ scales as $\mathcal{O}(M^{d/2+1})$ as compared to $\mathcal{O}(MN)$ for PEM. We can apply this procedure to any general case where the index for fermion degree of freedom include spin, orbital and site.

(ii) Truncation of Trace Operations

To calculate effective action S_{eff} from Eq. (2.13) and Eq. (2.14) we need to perform trace operations throughout the Hilbert space and it costs $\mathcal{O}(N)$ computational complexity. This complexity can be reduced by performing a truncation for the trace operations. We can write the probability for MC update where an old configuration ϕ is changed to a new configuration ϕ' as,

$$\frac{P(\phi')}{P(\phi)} = \exp(-\Delta S_{eff}) \quad (2.21)$$

where ΔS_{eff} represents the difference in effective action and in the polynomial expansion up to order M , it can be written as,

$$\Delta S_{eff} \simeq \sum_{m=0}^M f_m \sum_k^{N_{dim}} \Delta \tilde{\mu}_m(k) \quad (2.22)$$

where,

$$\Delta \tilde{\mu}_m(k) = (e(k), v'(k, 0) - (e(k), v(k, 0)) \quad (2.23)$$

We consider the Hamiltonian in Eq. (2.20) and make an update on site l by changing ϕ to ϕ' i.e., $\phi_i = \phi'_i$ if $i \neq l$. The change in the Hamiltonian matrix exists only for l, l^{th} element and it remains same for all other elements. Now we choose another site k which is far away from site l such that $|k - l| > R_o(m)$, for this case $v(k, m) = v'(k, m)$ and $\Delta \tilde{\mu}_m(k) = 0$. So in order to make $\Delta \tilde{\mu}_m(k) \neq 0$ we need to have k site in the vicinity of l so that propagation can reach to this site within M steps. That means we can restrict the summation over k in Eq. (2.22) just to the neighborhood of l that satisfies $|k - l| \leq R_o(m)$. Similarly, we can restrict the trace operations in the subspace

of $\mathcal{O}(M^d)$ so that the computational complexity to calculate these operations reduces from $\mathcal{O}(N)$ to $\mathcal{O}(M^d)$ without doing any approximation.

Next similar to what we did in the truncation of matrix-vector products we choose a threshold ϵ_{tr} for trace operations. If the site k is not in the close vicinity of the site l where update is made then the propagation of $v(k, m)$ and $v'(k, m)$ is restricted to a subspace and the change between these two elements is very small. That means $v(k, m) \simeq v'(k, m)$ within the error threshold ϵ_{tr} , and $\Delta\tilde{\mu}_m(k) = \mathcal{O}(\epsilon_{tr})$ is satisfied. We only need to consider the contribution of those sites in the neighborhood of l where propagation can reach in M steps. Due to the diffusive nature of this propagation, the sites that contribute to the calculation of $\Delta\tilde{\mu}_m(k)$ are $\mathcal{O}(M^{d/2})$. That means the computational complexity to do these trace operations is reduced from $\mathcal{O}(N)$ to $\mathcal{O}(M^{d/2})$ with an error of $\mathcal{O}(\epsilon_{tr})$. So performing both these truncations reduce the CPU time for one MC update from $\mathcal{O}(MN^2)$ to $\mathcal{O}(M^{2d+1})$.

2.3.4 Traveling Cluster Approximation (TCA)

In this method motivated by the fact that a single MC update made at site R_i does not propagate too far from the updating site we construct a cluster around the site to be updated [84, 85]. The total number of sites of this cluster is $N_c = L_c^2$ for a square lattice, where L_c is the linear dimension of the cluster. The key difference between ED-MC and TCA is that rather than diagonalizing the full Hamiltonian we only diagonalize the cluster Hamiltonian to accept or reject the update made at a particular site. As a consequence the computational complexity of diagonalizing the Hamiltonian changes from $\mathcal{O}(N^3)$ to $\mathcal{O}(N_c^3)$. The analytic reasoning behind this method comes from the

fact of *nearsightedness* of electronic matter. This method has been used to study the similar type of models [86, 87]. We move this update sequentially over the whole lattice creating cluster around the update site each time. The computational costs for calculating the effective action and MC update under the current scheme are $\mathcal{O}(N_c^3)$ and $\mathcal{O}(NN_c^3)$. Similar to what we did in ED-MC we store the random configuration for classical variables at each site in an array $S[]$ while for cluster located at site i the variables are stored in an array $C[i]$. The flowchart for TCA has the following steps,

- (1) During one MC step, we loop over all the sites sequentially in the system and for each site we build a cluster around that and generate the array $C[i]$ from $S[]$.
- (2) We calculate the Hamiltonian for this cluster $H_{clus}(C[i])$ and diagonalize it to find the Boltzmann weight.
- (3) Now we update the classical variables at the chosen site and generate again $H_{clus}(C[i])$. We re-diagonalize this Hamiltonian to find the Boltzmann weight for the update.
- (4) In order to accept or reject we use the Metropolis algorithm and if the update is accepted then we change the classical variables in array $S[]$. The whole process is repeated for all the sites in the lattice.

In this scheme, the equilibration MC updates are made at a particular temperature and the final configurations of the localized spins are used to diagonalize the full Hamiltonian and to calculate the observables quantities. The geometry of the cluster is same as that of the system and also periodic boundary conditions are used. These conditions help to recover the full energy spectrum in the limit where cluster size approaches the

actual size of the system. The computational complexity for each method is illustrated in the table 2.1.

Table 2.1: Computational complexity for each method

Algorithm	$v(k, m)$	Trace	ΔS_{eff}	Total
ED-MC	$\dots$	$\dots$	$\mathcal{O}(N^3)$	$\mathcal{O}(N^4)$
PEM	$\mathcal{O}(MN)$	$\mathcal{O}(N)$	$\mathcal{O}(MN^2)$	$\mathcal{O}(MN^3)$
TPEM	$\mathcal{O}(M^{d+1})$	$\mathcal{O}(M^d)$	$\mathcal{O}(M^{2d+1})$	$\mathcal{O}(M^{2d+1}N)$
TCA	$\dots$	$\dots$	$\mathcal{O}(N_c^3)$	$\mathcal{O}(N_c^3 N)$

2.4 Simulated Annealing Method

To do MC calculations using ED-MC, TPEM, TCA we used *simulated annealing* method. For this method, we start at a relatively high temperature $T = 0.1$ with random localized spin configuration and run the system for equilibration and then use final configuration of this temperature to do the equilibration at $T = 0.08$. We repeat this process with a step of temperature $\Delta T = 0.02$ finally calculating the thermal averages of the observables at $T = 0.02$. Measurements are done for 40,000 MC steps after 2000 – 60,000 steps for thermalization. We have divided the data into 40 different bins to calculate the average value and error from the standard deviation.

2.5 Variational Calculation Method (VCM)

To study the ground state phase diagrams of the model at $T = 0$ we used the variational calculation method [88]. In these calculations, we chose some ordered magnetic states comprising of coplanar and *non-coplanar* states and calculated the energy for all them as a function of chemical potential μ . Next, we also calculated the number density of itinerant electrons n by varying μ . The ground state is then obtained by comparing the energies of different states and then mapping this onto the phase diagram of n versus μ . The phase separation between different states is characterized by the jump of n , as the system is not stable and can not have a fixed number density in this region.

2.6 Observables

The thermodynamic quantities that depend on localized spins are calculated by the thermal averages of spin configurations while the quantities that are associated with itinerant electrons are calculated from the eigenvalues and eigenfunctions of $\hat{\mathcal{H}}_e$. The method used to calculate observables is that initially, we select a random configuration of localized spins ϕ and calculate Boltzmann action $S_{eff}(\phi)$ for this configuration. Next, we change the orientation of a localized spin by selecting it randomly and call this new configuration as ϕ' and then calculate the difference between the two actions $\Delta S_{eff} = S_{eff}(\phi') - S_{eff}(\phi)$. At the end, this new configuration is accepted or rejected based on Metropolis algorithm. This step is repeated first to equilibrate the system and after that, we start measuring the observable quantities.

In order to distinguish between different magnetic orderings we have calculated the spin structure factor for localized spins which is the Fourier transform of spin-spin correlation function,

$$S(\mathbf{q}) = \frac{1}{N} \sum_{i,j} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \exp[i\mathbf{q} \cdot \mathbf{r}_{ij}] \quad (2.24)$$

where $\mathbf{r}_{ij}$ is the position vector from i^{th} to j^{th} site and $\langle \rangle$ represent the thermal averages over the grand canonical ensemble. We have also calculated the magnetization per site,

$$m = \sqrt{\left\langle \left(\frac{\sum_i \mathbf{S}_i}{N} \right)^2 \right\rangle} \quad (2.25)$$

to describe the evolution under varying magnetic field. To elucidate the difference between topological trivial and *non-trivial* states we have calculated the local scalar chirality. On a triangle, the chirality is defined as,

$$\chi_{\triangle} = \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k) \quad (2.26)$$

This quantity is zero for collinear or coplanar magnetic states such as FM, AFM, Flux states etc and is non-zero for well known *non-coplanar* states such as all-out, 2-in 2-out and 3-in 1-out states. As an additional characterization of the spin configuration, we measure the circulation of the in-plane components around each square plaquette as,

$$f_m = \sum_{\square} \mathbf{S}_i \cdot \mathbf{r}_{ij} \quad (2.27)$$

where $\mathbf{S}_i$ is the spin at site i and $\mathbf{r}_{ij}$'s are the vectors connecting sites i and j around the square plaquette in a counter-clockwise direction. A non-zero circulation identifies a

flux configuration of the local moments.

To study the transport properties we have calculated the transverse and longitudinal conductivities using the standard Kubo formalism [89]. The derivation for transverse conductivity starting from linear response theory is presented in appendix A closely following the reference [90]. In this formalism the real-space version of both conductivities can be written as,

$$\sigma_{xy} = \frac{ie^2\hbar}{N} \sum_m \sum_{n \neq m} (f_m - f_n) \frac{\langle m | v_x | n \rangle \langle n | v_y | m \rangle}{(\mathcal{E}_m - \mathcal{E}_n)^2 + \eta^2} \quad (2.28)$$

$$\sigma_{xx} = \frac{e^2\hbar}{N} \sum_m \sum_{n \neq m} \left(\frac{f_m - f_n}{\mathcal{E}_m - \mathcal{E}_n} \right) \frac{\eta}{(\mathcal{E}_m - \mathcal{E}_n)^2 + \eta^2} \times |\langle m | v_x | n \rangle|^2 \quad (2.29)$$

Where σ_{xy} and σ_{xx} are transverse and longitudinal conductivities respectively. In above equations indices m and n represent the sum over all energy levels, N is the total number of sites, $f_m(n)$ is the Fermi distribution function for energy $\mathcal{E}_m(n)$, $|m\rangle$ and $|n\rangle$ are single-particle eigenstates corresponding to energy $\mathcal{E}_m$ and $\mathcal{E}_n$ and η is the scattering rate. v_x and v_y are velocity operators in x and y directions that can be expressed as,

$$v_x = \frac{it}{\hbar} \sum_{j,\sigma} (c_{j,\sigma}^\dagger c_{j+x,\sigma} - h.c.) \quad (2.30)$$

$$v_y = \frac{it}{\hbar} \sum_{j,\sigma} (c_{j,\sigma}^\dagger c_{j+y,\sigma} - h.c.) \quad (2.31)$$

where t is the hopping matrix along x and y directions. The more details about the parameters used in the Hamiltonian are presented in each Chapter.

Integer Quantum Hall Effect On Shastry-Sutherland Lattice

We investigate the role of external magnetic field, frustration and temperature on the transport properties of itinerant electrons. For that matter, we leave out the localized degree of freedom in the SS-KLM and just focus on itinerant electrons. The Hamiltonian then reduces to a tight binding model subject to a longitudinal magnetic field in the z -direction. In this case, the transfer matrix elements in the x -direction are real and in the y -direction, these elements are complex accompanied by Peierls phase factors. The energy spectrum splits into degenerate Landau levels depending upon the magnitude of magnetic flux. The topological properties of Landau levels are related to quantization of *transverse* conductivity – IQHE. The basic experimental feature of the IQHE is the vanishing longitudinal resistivity (dissipation-less flow) along the edges of sample and quantization of the Hall conductivity in steps of e^2/h . The most remarkable characteristic of IQHE is that quantization exists over a finite range of physical parameters such as magnetic field, temperature, strength of on-site potential and car-

rier density n_e . There is a finite probability for the states to return to a specific site in a long time limit in a *strongly* disordered system. These states are localized states and for these states, the conductivity vanishes at zero temperature. But in the case of weak disorder there are extended states that do not decay exponentially and for them, the static conductivity is non-zero at zero temperature. These extended states also play an important role in the quantization of the Hall conductivity [91]. The finite disorder potential breaks the translational invariance and helps in the quantization of Hall *plateaus* in the presence of magnetic field. Without disorder, the *plateau*-like behavior disappears and we get classical Hall effect. It is verified that with the increase of the random on-site potential the more localized states are developed and extended states become narrow in size. There is no effect on the width of the *plateaus* as there is a current compensation process. Our results indicate that the Hall conductivity shows IQHE even when we have zero disorder potential but a small degree of frustration. The *transverse* conductivity increase in multiples of e^2/h as a function of Fermi energy. The width of the Hall *plateaus* decreases when the strength of frustration parameter is increased that means there is no current compensation process involved here. Moreover, the quantization of the Hall conductivity vanishes when we have very high degree of frustration in our system. We have also obtained IQHE in the presence of non-zero on-site disorder potential. The longitudinal conductivity for a small value of disorder potential is non-zero only when Fermi energy lies in one of Landau levels. The *plateaus* in the Hall conductivity start to disappear when the temperature is increased.

3.1 Model Hamiltonian

We consider spinless tight binding model on SSL in the presence of a magnetic field B that is applied in the z -direction. The number of sites along x and y directions are L_x and L_y respectively. The Hamiltonian for such a system can be written as,

$$\hat{\mathcal{H}} = \left(t \sum_{\langle ij \rangle} c_i^\dagger c_j + t \sum_{\langle\langle ij \rangle\rangle} e^{i\theta_{ij}} c_i^\dagger c_j + t' \sum_{\langle\langle\langle ij \rangle\rangle\rangle} c_i^\dagger c_j + h.c. \right) + \sum_i w_i c_i^\dagger c_i \quad (3.1)$$

where $\langle \cdot \rangle$, $\langle\langle \cdot \rangle\rangle$ and $\langle\langle\langle \cdot \rangle\rangle\rangle$ represent the pair of sites along x , y and diagonal directions on SSL respectively. The operator $c_i^\dagger (c_i)$ annihilates (creates) an electron on site i . The hopping matrix along axial bonds is t while for SSL bonds it is t' . The last term denotes the on-site disorder potential energy and the magnitude of this energy is randomly distributed between $-W/2$ to $W/2$. We have incorporated a phase θ_{ij} in the presence of magnetic field B and for Landau gauge $A = (0, Bx)$ it will be non-zero only when an electron hops along the y -direction. In this case, the phase factor becomes $\theta_{ij} = 2\pi i\phi$, where i is the x co-ordinate of the site and ϕ is magnetic flux per plaquette.

3.2 Method

In order to study above model for the transport properties, we have calculated the longitudinal and *transverse* conductivities using Kubo formalism [89]. We have written the expressions for these conductivities in section 2.6. Recalling those expressions for this particular model we have,

$$\sigma_{xy} = \frac{ie^2\hbar}{N} \sum_m \sum_{n \neq m} (f_m - f_n) \frac{\langle m | v_x | n \rangle \langle n | v_y | m \rangle}{(\mathcal{E}_m - \mathcal{E}_n)^2 + \eta^2} \quad (3.2)$$

$$\sigma_{xx} = \frac{e^2\hbar}{N} \sum_m \sum_{n \neq m} \left(\frac{f_m - f_n}{\mathcal{E}_m - \mathcal{E}_n} \right) \frac{\eta}{(\mathcal{E}_m - \mathcal{E}_n)^2 + \eta^2} \times |\langle m | v_x | n \rangle|^2 \quad (3.3)$$

and current operators then become,

$$v_x = \frac{i}{\hbar} \left(t \sum_{a,b} c_{a,b}^\dagger c_{a+1,b} + \frac{t'}{\sqrt{2}} \sum_{a,b} c_{a,b}^\dagger c_{a+1,b+1} - \frac{t'}{\sqrt{2}} \sum_{a,b} c_{a,b}^\dagger c_{a-1,b+1} - h.c. \right) \quad (3.4)$$

$$v_y = \frac{i}{\hbar} \left(t \sum_{a,b} c_{a,b}^\dagger c_{a,b+1} e^{-i\theta_a} + \frac{t'}{\sqrt{2}} \sum_{a,b} c_{a,b}^\dagger c_{a+1,b+1} + \frac{t'}{\sqrt{2}} \sum_{a,b} c_{a,b}^\dagger c_{a-1,b+1} - h.c. \right) \quad (3.5)$$

where the terms having t' in the numerator in both expressions are due to the projections of diagonal bonds on x and y -axis. The matrix elements of v_x and v_y with respect to eigenvectors $|m\rangle$ and $|n\rangle$ then become,

$$\begin{aligned} \langle m | v_x | n \rangle &= \frac{it}{\hbar} \sum_{a,b} ((A_{a,b}^m)^* A_{a+1,b}^n - h.c.) + \\ &\quad \frac{it'}{\sqrt{2}\hbar} \sum_{a,b} ((A_{a,b}^m)^* A_{a+1,b+1}^n - (A_{a,b}^m)^* A_{a-1,b+1}^n - h.c.) \end{aligned} \quad (3.6)$$

$$\begin{aligned} \langle m | v_y | n \rangle &= \frac{it}{\hbar} \sum_{a,b} ((A_{a,b}^m)^* A_{a,b+1}^n e^{-i\theta_a} - h.c.) + \\ &\quad \frac{it'}{\sqrt{2}\hbar} \sum_{a,b} ((A_{a,b}^m)^* A_{a+1,b+1}^n + (A_{a,b}^m)^* A_{a-1,b+1}^n - h.c.) \end{aligned} \quad (3.7)$$

where we have expressed the eigenfunctions in terms of Wannier states and $A_{a,b}^m$ and $A_{a,b}^n$ correspond to the coefficients of these states. Substituting both these equations in Eq. (3.2) and Eq. (3.3) we have final expressions for *transverse* and longitudinal conductivities.

$$\begin{aligned} \sigma_{xy} = & -\frac{e^2}{h} \frac{2\pi i}{N} \sum_m \sum_{n \neq m} \frac{(f_m - f_n)}{(\mathcal{E}_m - \mathcal{E}_n)^2 + \eta^2} \times \\ & \left(t \sum_{a,b} (A_{a,b}^m)^* A_{a+1,b}^n + \frac{t'}{\sqrt{2}} \sum_{a,b} (A_{a,b}^m)^* A_{a+1,b+1}^n - \frac{t'}{\sqrt{2}} \sum_{a,b} (A_{a,b}^m)^* A_{a-1,b+1}^n - h.c. \right) \times \\ & \left(t \sum_{a,b} (A_{a,b}^n)^* A_{a,b+1}^m e^{-i\theta_a} + \frac{t'}{\sqrt{2}} \sum_{a,b} (A_{a,b}^n)^* A_{a+1,b+1}^m + \frac{t'}{\sqrt{2}} \sum_{a,b} (A_{a,b}^n)^* A_{a-1,b+1}^m - h.c. \right) \end{aligned} \quad (3.8)$$

$$\begin{aligned} \sigma_{xx} = & \frac{e^2}{h} \frac{2\pi}{N} \sum_m \sum_{n \neq m} \left(\frac{f_m - f_n}{\mathcal{E}_m - \mathcal{E}_n} \right) \frac{\eta}{(\mathcal{E}_m - \mathcal{E}_n)^2 + \eta^2} \times \\ & \left| \left(t \sum_{a,b} (A_{a,b}^m)^* A_{a+1,b}^n + \frac{t'}{\sqrt{2}} \sum_{a,b} (A_{a,b}^m)^* A_{a+1,b+1}^n - \frac{t'}{\sqrt{2}} \sum_{a,b} (A_{a,b}^m)^* A_{a-1,b+1}^n - h.c. \right) \right|^2 \end{aligned} \quad (3.9)$$

These two expressions are computationally very efficient to calculate the conductivities for larger lattice sizes. 1st we diagonalize the Hamiltonian in Eq. (3.1) to get eigenvalues and eigenfunctions and then insert them in above two equations to calculate conductivities.

3.3 Results

We have done conductivity calculations on 60×60 square lattice that corresponds to 30×30 SSL. We set $e = h = 1$ and t as the unit for energy. The values of the other parameters used in the calculations are given in each section.

3.3.1 Role of Frustration

We start with looking at the energy spectrum without any disorder on-site potential. In Fig. 3.1 we have plotted energy spectrum for different values of t' . The sharp lines show the location of energy eigenvalues. For $t' = 0$ these levels are highly degenerate. The degeneracy of these levels depends upon the value of magnetic field. These levels are similar to the Landau levels that are observed in the case of 2DEG. The only difference being the energy levels in case of continuum 2DEG are evenly spaced while for a finite SSL the energy spacing is non-uniform. Including a non-zero t' the degeneracy of the Landau levels will be lifted. This is shown in Fig 3.1 by superimposing the new gray color lines on the black lines ($t' = 0$). The original sharp energy levels now split into sub-levels keeping the total number of levels constant. Also with the increase of t' the broadening of the levels increases and when $t' = 0.5$ these levels start overlapping with each other.

In Fig. 3.2 we have plotted *transverse* conductivity as a function of Fermi energy ϵ_f . There is a quantum phase transition from an insulating phase where conductivity is zero to a conducting phase where conductivity is 1 when we change the Fermi energy. We can also observe the quantization of the conductivity. The value of the *transverse* conductivity at *plateaus* is ne^2/h , where n is the number of occupied Landau levels. The number of Hall *plateaus* depend upon the magnetic field as ϕ fixes the total number of Landau levels. Whenever Fermi energy passes through a Landau level then the increase in *transverse* conductivity is e^2/h . The width of Hall *plateaus* is not robust against the frustration parameter which in this case is ratio t'/t – it decreases with the increase of t'/t . The current compensation process discussed in continuum limit for

Figure 3.1: Energy spectrum for 20×20 SSL when $t = 1.0$ and $\phi = 0.1$ (a) for $t' = 0.0$ (b) for $t' = 0.1$ (c) for $t' = 0.25$ and (d) for $t' = 0.5$.

the case of non-zero random potential is not present here. As mentioned in previous paragraph when we increase the value of t'/t the Landau levels starts to broaden and eventually overlap. In case of small degree of frustration t'/t the electrons do not have enough energy to move to a higher energy band as the gap between Landau levels is very large. But at high value of t'/t , the bands start overlapping making it possible for electrons to hop between different energy levels which result in the decrease in width of the *plateaus* and finally at very high value these *plateaus* disappear.

Figure 3.2: Transverse conductivity as a function of Fermi energy for different values of t' at $T = 0.01$ and $w = 0$. The calculations are done on 30×30 SSL when $t = 1.0$ and $\phi = 0.1$.

3.3.2 Role of Disorder

We have also explored the role of disorder on the energy spectrum of our model in Fig. 3.3 where we have plotted energy levels for three different values of the strength of disorder. This disorder could be due to impurities or due to the interaction of the system with a potential. We have modeled this type of disorder by including a random on-site potential. In the presence of disorder potential, the degeneracy of the Landau levels will be lifted. This comes from quantum perturbation theory, any perturbation that does not preserve any symmetry will break the degeneracies. The second effect of disorder in the current model is that it splits the energy levels into localized states and extended states. The states at the far edge of the band are localized states while the states close to the center of the band are extended states.

The distinction between localized and extended states is very important for un-

Figure 3.3: The plots illustrating the energy spectrum for 20×20 SSL when $t = 1.0$, $\phi = 0.1$, $t' = 0$ and (a) $w = 0$ (b) $w = 1.0$ (c) $w = 2.0$. It is clear from the diagrams that with the increase of disorder strength the broadening of energy levels increases.

derstanding the behavior of conductivity. Only the extended states contribute to the conductivity as these states transport charge from one side of the system to another. To investigate the behavior of conductivities we have plotted Hall and longitudinal conductivities in Fig. 3.4a and Fig. 3.4b respectively for different values of the strength of disorder. The Hall conductivity shows *plateaus* behavior as a function of Fermi energy, these *plateaus* correspond to the quantization of the Hall conductivity. The conductivity increases in steps of e^2/h whenever Fermi energy passes through a Landau level, which is characteristic of IQHE. The value of the conductivity at each *plateau* is ne^2/h , where n is the number of filled Landau levels.

For longitudinal conductivity to be non-zero there should be an inelastic scattering of the electrons. For scattering to happen electron should jump from an occupied state to an empty state. The electrons in filled level can not scatter to unfilled Landau levels as there is an energy gap and thermal energy of electrons is very small to cross this gap. This leads to very large scattering time. Recently it is observed that when-

Figure 3.4: The plots of (a) *transverse* conductivity (b) *longitudinal* conductivity for different values of disorder potential. The conductivities are calculated on 30×30 SSL keeping $t = 1.0$, $t' = 0.1$, $\phi = 0.1$ and $T = 0.01$.

ever Fermi level lies in *plateau* region then backscattering processes are completely suppressed as there is no overlap between current carrying states [92]. Due to this suppression of backscattering processes, the longitudinal conductivity becomes zero whenever Fermi energy lies in a *plateau* region. But when the Fermi energy lies within a Landau level then the backscattering processes are allowed and we get non-zero longitudinal conductivity this behavior is shown in Fig. 3.4b. With the increase of the disorder potential, the localized states increase in size while extended states at the center of the energy levels become narrow in size. The width of Hall *plateaus* is robust against this change as the contribution from extended states will enhance and compensate the lost due to the additional localized states. This phenomenon known as current compensation is already studied in the case of continuum model [93]. More-

over, it is observed that with the increase of strength of disorder the highest *plateaus* in the Hall conductivity start to disappear systematically. Like in our case at $W = 2$ first 3rd *plateau* vanishes and when we further increase W to 3 then 2nd *plateau* vanishes too. This process of destruction of *plateaus* with the increase of disorder can be explained on the basis of the merging of extended states. At a low value of disorder, the density of localized states peaks at the center of Landau levels and these peaks are separated by *plateaus* of localized states. When the strength of disorder is increased then the distribution of the extended states changes and the higher peaks start to merge with each other and causes the highest *plateau* to disappear [94].

3.3.3 Role of Temperature

The effect of temperature on the Hall and longitudinal conductivities are illustrated in Fig. 3.5 where we have plotted *transverse* and longitudinal conductivities while varying the Fermi energy at three different values of the T keeping $t = 1.0$, $t' = 0.1$, $\phi = 0.1$ and $w = 1.0$. With the increase of the temperature, the width of the Hall *plateaus* starts shrinking and at a sufficiently high value of T these *plateaus* disappear. This effect is due to Fermi distribution function, at $T = 0$ this has value 1 for the states below Fermi energy and 0 for the states above Fermi energy. So whenever Fermi energy passes through a Landau level there will be a sharp jump. The Fermi distribution function at finite temperatures start to smear out that is why the width of the Hall *plateaus* decreases as we increase T . The electrons get thermal energy $k_B T$ and jump to extended state region this results in gradual disappearance of Hall *plateaus*. While longitudinal conductivity caused due to the hopping of electrons in extended states becomes

non-zero throughout the range of the Fermi energy. This phenomenon where quantization of the Hall conductivity vanishes as temperature increases has been observed experimentally also [95, 96, 97, 98].

Figure 3.5: (a) Transverse conductivity (b) longitudinal conductivity as a function of Fermi energy for three different values of T keeping $t' = 0.1$ and $w = 1.0$. The calculations are done on 30×30 SSL when $t = 1.0$ and $\phi = 0.1$.

3.4 Summary

To summarize, we have studied the IQHE on SSL using a single band tight-binding model in the presence of a longitudinal magnetic field within non-interacting electron picture. We have numerically calculated the Hall and longitudinal conductivities using Kubo formalism. The effect of different parameters involved in the model Hamiltonian such as disorder, temperature and strength of frustration has been discussed in

details. The physical behavior of Hall and longitudinal conductivities in the current discrete model is quite similar to what has been observed in the continuum limit of such type of models.

Phase Diagram of Shastry-Sutherland Kondo Lattice Model: A Variational Calculation Study

Our plan in this Chapter is to identify ranges of parameters that stabilize topologically *non-trivial chiral* ground states. Owing to a large number of parameters involved, the SSL-KLM is expected to have an extremely rich phase diagram with multiple competing ground state phases stabilized in different parameter regimes. With that in mind and following previous studies on similar models [88, 23, 99], we explore the ground state phase diagram of this model with variational calculations and find out the parameters space where *chiral* spin phases are stabilized. Next step would be to find the stability of these states against thermal fluctuations which we carry out in the next two Chapters using MC simulations. We explore the SSL-KLM over a wide range of Hamiltonian parameters such as electronic filling factor, strength of the Kondo interaction between itinerant electrons and local moments, DMI as well as the ratio of the

Heisenberg interaction between the local moments. Using a variational ansatz, we compare the energies for a variety of commonly observed ground state phases and determine the state with minimum energy. While such an approach may not always yield the true ground state, it is an effective way of identifying parameter regimes with maximum susceptibility towards the desired ground states. Our results suggest that *chiral* spin arrangements are stabilized over a large range of parameters when we include the DMI. We have obtained a previously unknown *non-coplanar canted-Flux* state which is stabilized not only for *insulating* phases but also for *metallic* phases.

4.1 Model

We study SS-KLM with additional DMI – the total Hamiltonian for this model can be written as,

$$\hat{\mathcal{H}} = \underbrace{- \sum_{\langle i,j \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - J_K \sum_i \mathbf{S}_i \cdot \mathbf{s}_i^c}_{\hat{\mathcal{H}}_e} + \underbrace{\sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle i,j \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)}_{\hat{\mathcal{H}}_c} \quad (4.1)$$

The first two terms make up the electronic part of the Hamiltonian $\hat{\mathcal{H}}_e$ where we have the tight-binding term for itinerant electron and a Kondo-like interaction between these electrons and localized spins. $\langle i, j \rangle$ denotes the bonds on the SSL, where NN are axial bonds and NNN are alternate diagonal bonds and t_{ij} describes the hopping matrix of itinerant electrons on these SSL bonds. We treat the localized spins $\mathbf{S}_i$ as classical vectors of unit length. In this limit, the sign of J_K is irrelevant. The third term in Eq. (4.1) represent AFM Heisenberg interaction between the localized spins. The

last term is the DMI and more detail about this interaction on NN and NNN bonds is presented in caption of Fig. 4.1. Hereafter the primed parameters represent the interactions on diagonal bonds while the unprimed are for axial bonds. We choose $t = 1$ as the energy unit.

Figure 4.1: DMI defined on the unit cell of SSL where direction of arrow from site i to j indicates the direction of cross product $\mathbf{S}_i \times \mathbf{S}_j$. The red arrows represent the in-plane components of $\mathbf{D}$ while $\otimes$ and $\odot$ represent into and out-of-plane components of $\mathbf{D}$. Blue arrows indicate the in-plane components of $\mathbf{D}'$ on the diagonal bonds. The directions of x, y and z -axes are also mentioned.

4.2 Method

We study the phase diagram of the Hamiltonian written in Eq. (4.1) as a function of itinerant electron number density n_e and Kondo interaction J_K with the help of variational ansatz at $T = 0$. In order to do that, we estimate the total energy of the system

for different configurations of localized moments and then identify the most energetically favorable state having the minimum energy between all of them. By replacing the itinerant electron spin as $\mathbf{s}_i^c = c_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{i,\beta}$ the electronic part of the Hamiltonian in Eq. (4.1) becomes quadratic in fermionic operators, where $\boldsymbol{\sigma}_{\alpha\beta}$ are vector elements of usual Pauli matrices. This transformation also helps us to write this part as $2N \times 2N$ matrix for a particular configuration of the localized spins using single particle basis. The electronic energy for a specific ordering of localized spins can then be calculated by diagonalizing this matrix. The energy that corresponds to the localized spin part of the Hamiltonian $\hat{\mathcal{H}}_c$ is obvious to calculate once we have specified the ordering of these classical spins. The total average energy then can be written as,

$$\langle E \rangle = \sum_i f(\epsilon_i) \epsilon_i + \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle i,j \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) \quad (4.2)$$

where $f(\epsilon)$ is the Fermi distribution function and at $T = 0$ this will be non-zero only when $\epsilon \leq \epsilon_f$.

In the calculations, we considered 9 different ordered configurations of localized spins including coplanar and *non-coplanar* states. These states are shown in Fig. 4.2, where AFM, FM, Flux, stripe and 3:1 collinear are all coplanar ordered states while all-out, 2-in 2-out and 3-in 1-out are *non-coplanar* states. We have also chosen a *canted-Flux* state that may arise due to the interplay between the Heisenberg and the DMI. For the phase diagram as a function of n_e , we need to look at the relationship between n_e and chemical potential μ . Generally, the phase transition between different magnetic states is discontinuous accompanied by a jump of n_e . We have obtained the ground state by comparing energies of all these ordered states by varying μ . We have also

Figure 4.2: Different ordered configurations used in the variational calculations (a) AFM state (b) FM state (c) coplanar Flux state (d) stripe state (e) 3:1 collinear state (f) all-out state (g) 2-in 2-out (h) 3-in 1-out state (i) *canted-Flux* state (here this ground state is shown on an 8×8 lattice). From a-e are coplanar arrangements of localized spins while f-i are *non-coplanar* configurations.

calculated the electron number density n_e as a function of μ . At the end phase diagram is obtained by mapping ground state energy versus μ curve on n_e versus μ curve. The phase separation region is characterized by a jump of n_e because in this region the system is not stable and does not have a fixed number density [88, 23, 99].

4.3 Results and Discussions

We have performed the above mentioned variational calculations on finite size lattices while varying the parameters n_e , J_K , and strengths of Heisenberg exchange interaction and DM vectors. Most of the results presented were obtained for a 8×8 lattice, and they were verified on larger lattices at a few values of the parameters. Since all the states have a periodicity of at most 2 unit cells, the results from the 8×8 lattices were found to be adequate and no significant finite size effects were observed. We start our discussion with Fig. 4.3a that shows the phase diagram without DMI for $t' = 1.0$, $J = 0.1$, and $J' = 0.12$ as a function of n_e and J_K . At very small and high values of electron number density FM *metallic* ground state is stabilized and these regions become wider as J_K increases [75, 74]. These parts of the phase diagram appear as a result of double exchange mechanism. For the current value of parameters, an *insulating* AFM ground state is realized around half filling. The AFM interaction between localized spins at $n_e \simeq 1/2$ is favored as it minimizes the kinetic energy term for the itinerant electrons. The other coplanar states such as Flux, stripe and 3:1 collinear also appear in phase diagram over a quite wide range of number density and J_K . As we are interested in the phases with non-zero chirality which are absent in the Fig. 4.3a except for some small patches for all-out and *canted-Flux* states. The *canted-Flux* is a new *chiral*

phase that has not been observed earlier. At some places in the phase diagram, the ground state has a volume which is a mixture of different ordered states these regions are shown as phase separation (PS) in the figure [100, 101]. The composition of this phase separation region depends upon where it appears in the phase diagram. It is composed of the phases on both sides of the phase separation region. In the current system, these phase separations are termed as electronic phase separations because these are related to the behavior of electrons and phases in competition have different electron density. If we choose μ exactly at the phase transition point then both of the ground states will be degenerate and what we get in an MC run is a complex behavior, which can tunnel between two sectors with a different number of electrons. The number density plot versus μ shows a discontinuity at these phase separation regions.

Figure 4.3: The phase diagrams at $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$ (a) $|\mathbf{D}| = |\mathbf{D}'| = 0$ (b) $D_{\parallel} = -0.1$, $D_{\perp} = 0.1$ and $D' = -0.12$. The calculations are done on 8×8 lattice and the regions marked with a-i indicates the portions where ordered states in Fig. 4.2 are stabilized. PS describes a phase separation region.

Now we move our attention to what happens to phase diagram when we *switch on* the DMI? The results are shown in Fig. 4.3b. Clearly, DMI stabilized the states that are *non-coplanar* in nature and that is why the regions where *chiral* states are realized become wider in size. In fact what we found out is that the *canted-Flux* state is the one that now covers most part of the phase diagram. This *chiral* state that is driven by DMI replaces the AFM at $n_e = 1/2, 1/4$ and $3/4$. We focus on this state at half filling where the system is in *insulating* phase. We found out that this phase is stabilized even at finite temperature. More details will be presented in Chapter 5 where we dynamically reproduce this ground state starting from some random configurations of localized spins using MC method and will discuss its evolution as a function of magnetic field. Moreover, with the increase of the J_K interaction the portions with *canted-Flux* phase shrink and at a very high value of J_K around $n_e \simeq 1/4$ and $3/4$ what we get is a PS. FM phase appearing at small and high values of number density is robust against this DMI. Among other coplanar states that still survive in the presence of DMI are the stripe, 3:1 collinear and some portions of AFM phase.

Next, we consider the *other limit* of the Shastry-Sutherland model where the strength of the interactions on the diagonal bonds are greater than the one on the axial bonds. The interest is driven by the fact that the system is in *insulating* state at $n_e = 1/4$ and $3/4$ when *non-coplanar* order is stabilized and if Fermi level lies in one of these gaps then there is a possibility that we can realize the quantized THE. Fig. 4.4a shows the phase diagram for $t' = 2.2$, $J = 0.1$, $J' = 0.22$ and $|\mathbf{D}| = |\mathbf{D}'| = 0$. The results for FM phase are the same as observed earlier. But now at $n_e \simeq 1/2$ the ground state is not AFM but a coplanar Flux state. For this configuration, the localized spins on the SSL diagonals are anti-parallel aligned (singlet state) same like for pure SSL model

where the ground state is a direct product of singlets on these SSL diagonal bonds in *this limit*. For small values of J_K , a coplanar stripe state is observed at $n_e = 1/4$ which changes to 3:1 collinear state at high values of J_K . Similarly, at $n_e = 3/4$ the ground state is coplanar Flux state at lower J_k values and it is replaced by AFM phase when J_K increases in size. There are some regions of *non-coplanar* states such as all-out, 2-in 2-out, 3-in 1-out and *canted-Flux* in the phase diagram but not at $n_e = 1/4$ and $3/4$.

In the last part of our calculations, we *turned on* the DMI in the limit we discussed in the last paragraph to realize the *non-coplanar* ground states. The results are shown in Fig. 4.4b where phase diagram is plotted in the presence of DMI, $D_{\parallel} = -0.1$, $D_{\perp} = 0.15$ and $D' = -0.22$. Similar to what happened in the earlier case when we *switched on* the DMI here also the *canted-Flux* becomes stabilized in the wider range of electron

Figure 4.4: The Phase diagrams at $t = 1.0$, $t' = 2.2$, $J = 0.1$, $J' = 0.22$ (a) $|\mathbf{D}| = |\mathbf{D}'| = 0$ (b) $D_{\parallel} = -0.1$, $D_{\perp} = 0.15$ and $D' = -0.22$. The calculation are done on 8×8 lattice and the regions marked with a-i indicates the portions where ordered states in Fig. 4.2 are stabilized. PS describes a phase separation region.

number density. In addition to $n_e = 1/2$, this phase is stabilized at $n_e = 1/4$ and $3/4$ for small and large values of J_K . There is no significant change in the stability of other *non-coplanar* states in the presence of DMI in this case. FM phase is present at low and high values of n_e similar to what we observed earlier. The coplanar flux state is totally replaced by *canted-Flux* state. There are small patches of other coplanar states such as AFM, stripe and 3:1 collinear at some values of n_e .

4.4 Summary

We investigated the ground state phase diagram of SS-KLM with classical localized spins. This study is relevant to exploring the novel magnetic and transport properties arising from the interplay between the charge-spin coupling and geometrical frustration in rare earth tetraborides. Using variational calculations, the different *non-coplanar* arrangement of localized moments with non-zero net chirality are realized over finite ranges of interaction parameters. Electron motion through such spin textures may result in novel transport phenomena, such as THE. The inclusion of DMI further stabilizes new *canted-Flux* spin state.

Field-tuned Chiral Phase Transition in SS-KLM at half filling

In the last Chapter, we found out that topologically *non-trivial* ground state *canted-Flux* state is realized over a wide range of parametric space at $T = 0$. In this Chapter, our aim is to investigate the stability of this *chiral* state in an external magnetic field at $n_e = 1/2$ using MC method at non-zero value of temperature. Our focus is to realize topologically *non-trivial chiral* magnetic phases including *canted-Flux* state from physically relevant interactions and investigate their evolution in an external magnetic field. Does the ground state retain its *chiral* nature in the presence of a field? How does the net chirality evolve with the applied field and how is it eventually suppressed? Do the *nature* of *chiral* spin state change in the presence of an external field? These are some of the questions we address in this Chapter. Our results reveal that multiple *non-coplanar* spin arrangements including *canted-Flux* state (characterized by different values of the scalar spin chirality) with the long-range magnetic order are stabilized over an extended range of parameters. Furthermore, we are able to tune the non-

coplanarity (equivalently, the topological character) of the spin textures – changing and suppressing the net chirality – by applying an external magnetic field. This is in marked contrast to most previous studies where the *non-coplanar* textures of the local moments is imposed by extraneous factors (e.g., crystal electric field in pyrochlores) and as such, cannot be changed easily.

5.1 Model

The detail about the Hamiltonian describing the SS-KLM with additional DMI and external magnetic field is already presented in section 2.2 we write here its full form just for the sake of completeness,

$$\hat{\mathcal{H}} = - \sum_{\langle ij \rangle, \alpha} t_{ij} (c_{i\alpha}^\dagger c_{j\alpha} + h.c) - J_K \sum_i \mathbf{S}_i \cdot \mathbf{s}_i^c + \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle i,j \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) - h^z \sum_i S_i^z. \quad (5.1)$$

Throughout this chapter, the parameters with primed represent the interactions on diagonal bonds of SSL while the unprimed are for axial bonds.

5.2 Method

To investigate the above model, we used an unbiased MC method that we have introduced in Chapter 2. The results for 8×8 lattice are obtained using ED-MC (introduced in subsection 2.3.1) as it is faster for a system with less than 100 lattice sites. For larger system sizes ED-MC faces huge computational complexity issues and slows down significantly. So to investigate 12×12 lattice in this Chapter we used approximate meth-

ods like TPEM and TCA (also introduced in subsection 2.3.3 and 2.3.4 respectively) that reduce the CPU time. In case of TPEM the values of thresholds for matrix-vector product and trace used are $\epsilon_{pr} = 10^{-5}$ and $\epsilon_{tr} = 10^{-3}$ while $M = 30$ is used as a cutoff value for polynomial expansion. We made a comparison between the results obtained using these two methods to show the consistency and accuracy. We also made use of the *simulated annealing* method that is introduced in section 2.4.

5.3 Physical Observables

In order to identify different magnetic orderings, we calculate the spin structure factor as well as magnetization per unit site which are defined in Eq. (2.24) and Eq. (2.25) respectively. To elucidate the difference between topological trivial and *non-trivial* states we evaluate the local scalar chirality per unit cell defined in Eq. (2.26). Finally, as an additional characterization of the spin configuration, we measure the circulation of the in-plane components around each square plaquette defined by Eq. (2.27).

5.4 Results and Discussions

The Hamiltonian (5.1) has a large number of parameters and consequently, supports a rich array of ground state phases over different ranges of the Hamiltonian parameters. In the present Chapter, we focus our attention on the magnetic behavior at an electronic filling factor $n_e = 1/2$, for which the system is in an insulating state. The choice for the rest of the Hamiltonian parameters is motivated by experimental observation in similar systems. The electronic hopping matrix elements along the axial and

Figure 5.1: Plots of (a) static spin structure along q_x and q_y indicating the peaks appearing at $\mathbf{q} = (0, 0)$, $(0, \pi)$ and $(\pi, 0)$ for 12×12 lattice (b) The magnitudes of peaks at $\mathbf{q} = (0, 0)$, and $(\pi, 0)$ for 8×8 and 12×12 lattices at $h^z = 0$. The other interaction parameters used in calculations are $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$, $J_K = 3.0$, $D_{\parallel} = -0.1$, $D_{\perp} = 0.1$ and $D' = -0.12$.

diagonal bonds are chosen to be equal and the energy scale is fixed by setting them to unity ($t = t' = 1$). The rest of the parameters are expressed in units of t . We choose the strengths of the Heisenberg interactions between the local moments to be approximately equal along the axial and diagonal bonds as well. This choice of identical strengths of both the hopping and magnetic exchange along all the dominant bonds in the SSL is motivated by the experimental observation of approximately equal bond lengths in the rare earth tetraboride family of compounds. The value of the exchange interactions are set at $J = 0.1$ and $J' = 0.12$, to reflect the predominantly electronic character of these quantum magnets. The DMI is assumed to be largely in the plane

and perpendicular to the diagonal bonds as shown in Fig. 4.1, and the magnitude of the DM vectors (strength of DM interaction) is set at $|\mathbf{D}| = 0.17$ and $|\mathbf{D}'| = 0.12$. Finally following the experimental observation in other frustrated magnets such as the pyrochlores, the strength of the Kondo coupling is chosen to be the strongest energy scale in the problem, $J_K = 3.0$.

Figure 5.2: (a) Magnetization per unit site as a function of magnetic field for 12×12 at three different values of $D_{\parallel}$ while keeping $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$, $J_K = 3.0$, $D_{\perp} = 0.1$ and $D' = -0.12$. (b) The total chirality as a function of longitudinal magnetic field. The different interaction parameters used are $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$, $J_K = 3.0$, $D_{\parallel} = -0.1$, $D_{\perp} = 0.1$ and $D' = -0.12$.

We start our discussion by analyzing the nature of the magnetic ground state at zero field. The momentum dependence of the static spin structure factor is illustrated in Fig. 5.1a. It exhibits sharp peaks at $(\pi, 0)$ and $(0, \pi)$. There is an additional, subdominant peak at $(0, 0)$ indicating a net magnetic moment even at zero external field

[see Fig. 5.2a], despite the AFM nature of the Heisenberg interaction between the localized moments. This is due to the (relatively strong) DMI which favors an out-of-plane orientation of the spins, as well as the Kondo-like interaction between the local moments and the spin of the itinerant electrons. Nominally such features in the structure factor point towards a canted AFM state. However, the strong Kondo-like interaction precludes pure AFM ordering and hence we need to explore alternate possibilities [19]. To identify the true nature of the magnetic ground state we probe the chirality as defined in Eq. (2.26). The scalar spin chirality is non-zero for this state, indicating a *non-coplanar* component to the spin configuration [see Fig. 5.2b]. This confirms the absence of pure AFM ordering as well as establishes topologically *non-trivial chiral* nature of the spin configuration. Further insight into the character of the spin texture is obtained from the local circulation on individual plaquettes [see Fig. 5.4(a)]. The circulation is equal in magnitude and opposite in sign for the plaquettes with diagonal bonds whereas it is vanishingly small in the other plaquettes. In other words, the in-plane components of the local moments are arranged in a flux pattern on alternating plaquettes. Finally, the complete nature of the magnetic ground state is illustrated by a snapshot of the real space (periodic) equilibrium spin configuration obtained from the simulations and shown schematically in Fig. 5.3(a). The in-plane components of the local moments are arranged in a near-ideal flux pattern along with a finite out-of-plane component – that is, the magnetic ground state is in a *canted-Flux* state. Such complex spin textures are essential ingredients for the observation of THE, *chiral* spin liquid and other topologically interesting phases. In contrast to most previous studies, the *non-coplanar* spin arrangements in our study arise dynamically from the interplay between competing Heisenberg, DM and Kondo-like interactions in the presence of

geometric frustration. This enables us to control these complex magnetic orderings via an external magnetic field.

Figure 5.3: The real space configurations of local spins for 8×8 lattice shown at different values of magnetic field (a) $h^z = 0.0$ (b) $h^z = 0.8$, just prior to a phase transition (c) $h^z = 1.2$, after the phase transition point and (d) $h^z = 1.6$, when local spins are almost becoming polarized with magnetic field. The color bar besides each plot indicates the out-of-plane component of the spin vector. The different interaction parameters used are $t = t' = 1.0$, $J = 0.1$, $J' = 0.12$, $J_K = 3.0$, $D_{\parallel} = -0.1$, $D_{\perp} = 0.1$ and $D' = -0.12$.

One of the most intriguing features of the canonical (purely magnetic) Shastry-Sutherland model is the appearance of magnetization *plateaus* in an applied magnetic field. It is expected that DMI strongly modify the *plateau* structure. Our results show that the appearance and nature of the *plateaus* in the presence of simultaneous DM and

Kondo-like interactions depend on the magnitude of $D_{\perp}$ and $D_{\parallel}$. For $D_{\perp} > 0.1$ necessary to stabilize *non-coplanar* spin textures that we are interested in, the *plateaus* are completely suppressed in the absence of $D_{\parallel}$. For small values ($|D_{\parallel}| \lesssim 0.1$), there are no signatures of any *plateau*-like features in the field dependence of the uniform magnetization – m/m_s increases monotonically with increasing field strength and reaches saturation around $h_z \sim 1.7$. For $D_{\parallel} = -0.10$ signs of non-monotonicity begins to appear at $m/m_s = 0.5$ and 0.75 . Further increasing the $D_{\parallel}$ component of DMI two magnetization *plateaus* are observed at $m/m_s = 0.5$ and ~ 0.75 . The evolution of the uniform magnetization in a longitudinal magnetic field is shown in Fig. 5.2a(a) for 3 different values of $D_{\parallel}$. The strongest *plateau* appears at $m/m_s \sim 0.75$, in contrast to all other reported magnetization *plateaus* (theoretical or experimental) in the spin-only Shastry-Sutherland model and associated quantum magnets. The large value of magnetization *plateau* is a consequence of the additional canting out of the plane driven by the coupling of the local moments with the itinerant electrons as well as the strong DMI.

What is the topological character of the magnetic ground state as it is tuned by the external field? Fig. 5.2b shows the evolution of the net static spin chirality with increasing magnetic field. The ground state spin texture remains *non-coplanar* in nature over a large range of fields. The chirality increases monotonically up to a critical field of $h_{c1} \approx 1.0$, above which there is a discontinuous transition to a different *chiral* spin state with small (but still non-zero) chirality. Eventually, when the field strength is increased beyond a second critical field $h_{c2} \approx 1.5$, the ground state loses its non-coplanarity and the chirality is completely suppressed. Once again, snapshots of local spin configurations and circulation elucidate the true nature of the magnetic ground

Figure 5.4: Snapshot depicting the circulation of flux, clockwise or anticlockwise, on each plaquette of 8×8 lattice for different values of magnetic field (a) $h^z = 0.0$, (b) $h^z = 0.8$, just before the phase transition (c) $h^z = 1.2$, just after phase transition (d) $h^z = 1.6$, when almost all spins become parallel with h -field. The other interaction parameters used are the same as for Fig. 5.3.

state. Snapshots at $h = 0.8 (< h_{c1})$ reveal that the ground state remains a *canted-Flux* state for $h \leq h_{c1}$. The discontinuous transition at h_{c1} is driven by the partial breaking of the flux configuration of the in-plane components – in other words, the transition is topological in character. The moments connected by the diagonal bonds inside the plaquettes with a positive circulation still retain a large in-plane component and $(\pi, 0)$ ordering, whereas the other spins are largely polarized. The partial breaking of the flux pattern causes a drop in the circulation across the transition [see Fig. 5.4], whereas

the polarization of half the spins results in a drop in the staggered magnetization. The transition at h_{c2} is marked by the complete breaking of the flux pattern and polarization of the remaining spins. It is also observed that the results obtained with ED-MC for 8×8 lattice and with TPEM and TCA for 12×12 lattice are quite consistent that establishes the accuracy and precision of the approximate methods that we used.

5.5 Summary

To summarize, we have studied the KLM with additional DMI on the Shastry-Sutherland lattice. Our results show that complex, *non-coplanar* spin configurations can be generated dynamically from purely short range interactions and coupling to itinerant electrons. Furthermore, such *non-coplanar* structures can be tuned continually by applying an external magnetic field. These results provide an insight into the origin and nature of topologically *non-trivial* magnetic phases in *frustrated* magnets. They will also be crucial in understanding the magnetic and electronic properties of the rare earth tetraboride family of frustrated magnets.

Chiral Phase Transitions driven by Temperature, Geometrical Frustration and Magnetic Field in SS-KLM at $n_e = 1/4$ and $n_e = 3/4$

In this Chapter, we explore the SS-KLM for the stabilization of topologically *non-trivial* ground states at one-quarter and three-quarter filling of itinerant electrons. Our results reveal that *non-coplanar* ground states are realized for a wide range of parameters involved in the Hamiltonian. We discuss in detail the nature of topological phase transition as a function of thermal fluctuations, frustration and external magnetic field for both number densities of electrons.

6.1 Model

We consider the SS-KLM in the presence of a longitudinal magnetic field. The geometry of SSL has already been introduced earlier – for convenience it is depicted in Fig. 6.1. The Hamiltonian describing the system under investigation is,

$$\hat{\mathcal{H}} = - \sum_{\langle i,j \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - J_K \sum_i \mathbf{S}_i \cdot \mathbf{s}_i^c + \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - h^z \sum_i S_i^z \quad (6.1)$$

The detail about each term present in above Hamiltonian is discussed in section 2.2. From here onwards primed parameters represent interactions on diagonal bonds while unprimed are for axial bonds and we set $t = 1$ as the unit of energy.

Figure 6.1: (a) Geometry of SSL, where there are diagonal bonds on alternate plaquette in addition to axial bonds along x and y -axes. (b) 1st BZ of SSL lattice with high symmetric points mentioned.

6.2 Methods

In order to study the thermodynamic properties of the model represented by Eq. (6.1) we used the unbiased MC method that we have introduced in Chapter 2. To obtain the results for 8×8 lattice size we used ED-MC method to calculate the effective action for each MC step as it is faster for a system size comprising of 100 or less than 100 lattice sites. But for 12×12 and 16×16 lattice sizes we used TCA method, 6×6 cluster of SSL is used to calculate the effective action for one MC sweep and once the system is equilibrated then we calculated the thermal averages by diagonalizing the full Hamiltonian matrix. Moreover, we used *simulated annealing* method in our calculations which is mentioned in section 2.4.

6.3 Physical Observables

To study magnetic properties and identify different magnetic ordered states we have calculated the spin structure factor and magnetization per unit site defined in Eq. (2.24) and Eq. (2.25) respectively. To differentiate between coplanar and *non-coplanar* magnetic states we have calculated the local scalar spin chirality per unit cell defined in Eq. (2.26).

6.4 Results and Discussions

In this Chapter, we focus on studying the magnetic properties at itinerant electron densities $n_e = 1/4$ and $3/4$ for which the electronic spectrum is gapless, i.e., the ground state is metallic. Throughout this Chapter, we choose the limit of strong Kondo cou-

Figure 6.2: Plots of (a) magnetization per unit site and (b) chirality as a function of temperature T at $n_e \simeq 1/4$. The calculations are done on $L = 8 - 16$ lattice sizes keeping $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$.

pling between itinerant electrons and localized spins $J_K = 8.0$ following the lead of studies already done in this limit on other lattice structures. We start our discussion by considering the temperature dependence of magnetization per site and scalar spin chirality. Fig. 6.2a shows the results of MC calculations for magnetization per site as a function of temperature at $n_e \simeq 1/4$ (here we have introduced $\simeq$ sign because we are working in grand canonical ensemble and electron densities are controlled by the values of μ that gives number densities fluctuating within the error bars close to the required one). Initially, the magnetization decreases very slowly with decreasing temperature but around $T \simeq 0.05$ there is a significant drop in magnetization indicating a phase transition. The nature of this transition becomes much clearer if we look at Fig. 6.2b where we have shown the behavior of chirality while varying T for $n_e \simeq 1/4$.

The value of chirality is very small and it remains almost flat at higher values of temperature indicating an absence of *non-coplanar* ordering. The small values of chirality can be attributed to thermal fluctuations which are dominant at higher temperatures. But as we approach $T \simeq 0.05$ an appreciable change in chirality is indicated by a discontinuous increase in its value as seen in Fig. 6.2b. At lower temperatures, χ approaches a large value – specifying a *non-coplanar* or *chiral* phase. These results clearly demonstrate the *chiral* symmetry breaking character of the transition. Quenching the thermal fluctuations drives the system from a topologically trivial paramagnet to a topologically *non-trivial* state marked by finite chirality at low temperature.

Figure 6.3: Real space configurations of localized spins obtained from MC calculations on 8×8 lattice (a) when $T = 0.03$, after the phase transition and (b) when $T = 0.06$, prior to phase transition. The data is obtained for $n_e \simeq 1/4$ case when $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$.

We can get a better insight of this transition by closely analyzing Fig. 6.3 where we have plotted the snapshots of real space configurations of the spins obtained from MC results at two different values of T , before and after the phase transition for 8×8 lattice. It can be seen that the arrangement of the spins at $T = 0.06$ [see Fig. 6.3(b)] is random

and there is no clear pattern or order to it – a paramagnetic (PM) state. The ground state at $T = 0.03$ is an ordered one where order starts to manifest itself by aligning the spins in a flux pattern. For this flux state, the in-plane components of spins on axial bonds are orthogonal to each other while the spins on diagonal bonds are aligned anti-parallel. In contrast to earlier studies the flux state in the current model is not coplanar but the spins are tilted slightly producing an out-of-plane component also. This canting of flux state is also illustrated in Fig. 6.4 where the static spin structure is plotted as a function of momentum at $T = 0.02$ and $T = 0.06$. The spin structure factor for $T = 0.06$ has a peak of very small magnitude at $\mathbf{q} = (0, 0)$ and vanishingly small peaks at $\mathbf{q} = (0, \pi)$ and $(\pi, 0)$. But for $T = 0.02$ it exhibits a sub-dominant peak

Figure 6.4: The momentum dependence of spin structure factor for (a) $T = 0.02$, where the sharp peaks appears at $\mathbf{q} = (0, \pi)$, $(\pi, 0)$ and a small peak at $(0, 0)$ (b) $T = 0.06$, where there is just one peak at $\mathbf{q} = (0, 0)$. The results are obtained using parameters $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$ for 12×12 lattice at $n_e \simeq 1/4$.

Figure 6.5: The MC results for (a) magnetization per site (b) chirality as a function of T for $n_e \simeq 3/4$. The data is obtained while keeping $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$.

at $\mathbf{q} = (0, 0)$ in addition to sharp peaks at $(0, \pi)$ and $(\pi, 0)$ (these two peaks are the signature of pure Flux state) clearly suggesting a *canted-Flux* state. The evolution of peaks at $\mathbf{q} = (0, \pi)$ and $(\pi, 0)$ clearly suggests a phase transition as a function of T . The canting of flux state is stabilized due to the competition between AFM super-exchange interaction and the double exchange interaction (that favors the FM ordering at this filling factor) in the presence of geometrical frustration.

Next, we move to $n_e \simeq 3/4$, we have illustrated the results obtained from MC calculations for magnetization per site and chirality while varying T in Fig. 6.5a and Fig. 6.5b respectively. A *chiral* phase transition similar to the case for $n_e \simeq 1/4$ is also observed here. However, finite size effects are much more pronounced for $n_e \simeq 3/4$ as seen in Fig. 6.5a and 6.5b. The approach to thermodynamic limit occurs much more slowly with system size. The ground state at a lower temperature is a *canted-Flux* state

Figure 6.6: Energy bands plotted along symmetric points in the 1st BZ with triple- Q order stabilized at $\mathbf{q} = (\pi, 0)$, $(0, \pi)$ and $(0, 0)$. The values of interaction parameters used are $t = 1.0$, $t' = 0.25$ and $J_K = 8.0$.

similar to the previous case. This similarity between the results for both cases can be ascribed to the symmetry of band structure at one-quarter and three-quarter filling of itinerant electrons. In Fig. 6.6 the dependence of energy spectrum along symmetric points in 1st BZ is shown when triple- Q order is stabilized. The three values of $\mathbf{q}$ used are that of *canted-Flux* state – $(0, \pi)$, $(\pi, 0)$ and $(0, 0)$. It is clear that the bands are symmetric for one-quarter and three-quarter filling of electron density.

Now we explore the role of frustration on the magnetic properties of the current model. Since t' and J' are determined by the overlap of different orbitals across the diagonal bonds, their ratio can, in principle, be different for different materials. In this study, we choose to vary t' , keeping J' constant. Both t' and J' induce frustration – the former in electron hopping and the latter in exchange interactions between local

Figure 6.7: The diagrams illustrating the frustration dependence of (a) magnetization per site and (b) chirality at $n_e \simeq 1/4$. The calculations are done keeping the values of parameters $t = 1.0$, $J = 0.1$, $J' = 0.025$, $h^z = 0$, $J_K = 8.0$ and $T = 0.02$.

moments. With varying t' , the nature of electron hopping changes from being unfrustrated at $t' = 0$ to highly frustrated at $t' \gtrsim t$, whereas the degree of frustration in the direct exchange between the local moments remain unaltered. We start with $n_e \simeq 1/4$ – Fig. 6.7a and 6.7b show the results of MC calculations for magnetization and chirality while varying the hopping integral on the diagonal bonds t' . At $t'/t = 0.0$ the ground state has a non-zero magnetization and finite chirality. The static spin structure factor for this state exhibits a small peak at $\mathbf{q} = (0, 0)$ in addition to two sharp and equal in magnitude peaks at $(0, \pi)$ and $(\pi, 0)$. Actually this is the same *canted-Flux* state that we encountered earlier. The in-plane components of the local moments are arranged in a pattern similar to a coplanar Flux state. Furthermore, the moments are tilted slightly out-of-plane due to geometrical frustration (in Heisenberg interac-

tion) and competition between FM double exchange interaction and AF Heisenberg interaction. The flux pattern consists of columnar AFM arrangements of the in-plane components with simultaneous $(\pi, 0)$ and $(0, \pi)$ ordering. With increasing t'/t , the magnetization remains constant at a value consistent with a *canted-Flux* state up to $t'/t \approx 0.75$, where there is a discontinuous transition to a state with partial polarization of the spins. m/m_s jumps to ≈ 0.4 and remains constant for $0.75 \lesssim t'/t \lesssim 1.0$. In

Figure 6.8: The snapshots of real space configurations of localized spins obtained from MC calculations on 12×12 lattice (a) when $t'/t = 0.2$, before 1st phase transition and (b) when $t'/t = 0.8$, just after the 1st phase transition (c) when $t'/t = 1.0$, just before the 2nd phase transition and (d) when $t'/t = 1.3$, just after the 2nd phase transition. The data is obtained for $n_e \simeq 1/4$ case when $J = 0.1$, $J' = 0.025$, $h^z = 0$ and $J_K = 8.0$ at $T = 0.02$.

this intermediate range of t'/t , the flux ordering is broken and the transverse components of the local moments are fully disordered. The strength of the static structure factor $S(\mathbf{q})$ is vanishingly small for the AFM ordering wave vectors $(\pi, 0)$, $(0, \pi)$ and (π, π) indicating the complete suppression of AFM ordering. This breaking of in-plane flux ordering results in an increase in the partial ordering of the longitudinal component, reflected in the increased magnetization. The chirality drops discontinuously to a very small value as a result of the breaking of the flux pattern. Upon further increasing t'/t there is a second discontinuous spin-flop transition to a canted AFM state with small magnetization. The in-plane components of the local moments are arranged in a staggered (π, π) order with a small out-of-plane component resulting from the strong double-exchange interaction. The chirality is suppressed completely indicating a pure AFM character of the ground state spin configuration. The nature of the magnetic ground states in the different regimes is, once again, confirmed by the snapshots of instantaneous spin configurations shown in Fig. 6.8. The in-plane components are seen to evolve from a flux pattern at small t'/t to completely disordered in the intermediate regime to staggered AFM order at large values of t'/t . This behavior is depicted in Fig. 6.9 where the magnitude of peaks in spin structure factor at $\mathbf{q} = (\pi, 0)$ and (π, π) are plotted while varying the frustration parameter. After the transition, the magnitude of the peak at (π, π) increases monotonically establishing the fact that with the increase of frustration the system moves towards the fully polarized AFM state.

For $n_e \simeq 3/4$ case MC results for magnetization and chirality are illustrated in Fig. 6.10a and 6.10b respectively. At $t'/t = 0$ the ground state is *canted-Flux* state similar to $n_e \simeq 1/4$ case with sharp peaks in spin structure factor at $\mathbf{q} = (0, \pi)$, $(\pi, 0)$ and

Figure 6.9: The plots for $n_e \simeq 1/4$ case of magnitude of peaks appearing in spin structure factor at $\mathbf{q} = (\pi, 0)$, $(0, 0)$ and (π, π) as a function of frustration. The MC results are obtained when $J = 0.1$, $J' = 0.025$, $h^z = 0$, $J_K = 8.0$ and $T = 0.02$.

a small sub-dominant one at $\mathbf{q} = (0, 0)$. This state is a topologically *non-trivial* state with a finite chirality as discussed earlier. Initially, increase in the magnetization is very small but around $t'/t = 0.5$ it increases appreciably indicating a phase transition. The true nature of this phase transition can be once again found when we look at the chirality plot – at the start, the change in χ is not very significant when frustration is increased. Around $t'/t = 0.5$ the chirality drops to a very low value close to zero indicating that the phase transition is of *chiral* nature. There is no peak in the structure factor at $(\pi, 0)$ or (π, π) for the intermediate state ruling out any conventional AFM order. To gain better insight into the nature of this elusive state we decided to carefully look at snapshots of real space configurations – two such configurations at two different values of t'/t are shown in Fig. 6.11(b) and (c). No clear signs of any commonly observed states are visible. With increasing t'/t , there is a moderate rise in the uniform

Figure 6.10: (a) Magnetization per site (b) chirality for $n_e \simeq 3/4$ case while varying the degree of frustration. The MC results are obtained when $J = 0.1$, $J' = 0.025$, $h^z = 0$, $J_K = 8.0$ and $T = 0.02$.

magnetization followed by another transition, to a state with very small uniform magnetization. The range of the intermediate state is much larger for this filling factor. To get further insight into this second transition we closely analyze the other plots such as of chirality, real space configurations [shown in Fig. 6.11] and magnitude of peaks in static spin structure factor [shown in Fig. 6.12]. From the chirality plot, it is obvious that the magnetically ordered state at larger t'/t is also topologically trivial as χ approaches to zero beyond the critical point. Next looking at the snapshots of real space configurations obtained from MC results we found out that the magnetic ground state is AFM because most of the localized spins present on axial bonds are aligned anti-parallel. Lastly from Fig. 6.12 it is concluded that the spin texture is clearly AFM as at critical point, there is a crossover between the magnitude of peaks in spins structure factor at $\mathbf{q} = (\pi, \pi)$ and $(0, 0)$. More and more spins on the axial bonds start to

be anti-aligned which increases the magnitude of the peak at (π, π) when we increase frustration beyond the 2nd critical point.

Finally, we investigate the role of external magnetic field in the current model both at one-quarter and three-quarter fillings of electrons. For $n_e \simeq 1/4$ the magnetic field dependence of magnetization and chirality is shown in Fig. 6.13a and 6.13b respectively. At $h^z = 0.0$ the magnetic ground state is *canted-Flux* state which we have al-

Figure 6.11: The equilibrium real space spin configurations obtained from MC calculations on 8×8 lattice (a) when $t'/t = 0.2$, before 1st phase transition and (b) when $t'/t = 0.8$, after 1st phase transition (c) when $t'/t = 1.0$, just before 2nd phase transition and (d) when $t'/t = 2.2$, after the 2nd phase transition. The data is obtained for $n_e \simeq 3/4$ case when $J = 0.1$, $J' = 0.025$, $h^z = 0.0$ and $J_K = 8.0$ at $T = 0.02$. See text for more details about these two phase transitions.

Figure 6.12: The plots for $n_e \simeq 3/4$ case of magnitude of peaks appearing in spin structure factor at $\mathbf{q} = (\pi, 0)$, $(0, 0)$ and (π, π) as a function of frustration. The MC results are obtained when $J = 0.1$, $J' = 0.025$, $h^z = 0$, $J_K = 8.0$ and $T = 0.02$.

Figure 6.13: The magnetic field dependence of (a) magnetization per site (b) chirality for $n_e \simeq 1/4$ case. The calculations are done at $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $J_K = 8.0$ and $T = 0.02$.

Figure 6.14: The magnitude of peaks in spin structure factor at $\mathbf{q} = (\pi, 0)$ and $(0, 0)$ while changing magnetic field for $n_e \simeq 1/4$ case. The MC results are obtained when $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $J_K = 8.0$ and $T = 0.02$.

ready discussed in full detail. Looking at the m/m_s plot the change in magnetization is continuous as a function of field until around $h^z = 0.2$ where it increases abruptly indicating a 1st order phase transition. Further insight into this transition can be obtained from chirality plot [Fig. 6.13b] initially the change in χ is also monotonous like magnetization when field is increased until reaching a maximum value for $h^z = 0.2$. Beyond this point, the chirality drops discontinuously to a small value (still non-zero) indicating a different *chiral* state. This establishes the topological nature of phase transition taking place between two different topological phases. Finally around $h^z = 0.3$ the chirality is completely suppressed signaling a coplanar ground state. To dig deep into the nature of this coplanar magnetic ground state we analyzed the static spin structure. Fig. 6.14 depicts the magnitude of peaks appearing in spin structure factor at $\mathbf{q} = (\pi, 0)$ and $(0, 0)$. There is an obvious crossover happening between the magni-

tude of these two peaks around critical point $h_c = 0.2$. That means the *chiral* state after phase transitions has most spins polarized ferro-magnetically. Around $h^z = 0.3$, the magnetization saturates around ~ 1.0 in other words all the spins are fully polarized in the direction of external field (fully polarized FM phase).

Next, for $n_e \simeq 3/4$ case there is a topological transition similar to $n_e \simeq 1/4$ case only difference being that the critical field shifts to $h_c \sim 0.16$ [see Fig. 6.15a and 6.15b]. The magnetic ground states are similar in nature what we obtained in the one-quarter filling case over the whole range of magnetic field. The plot of magnitudes of sharp peaks appearing in static spin structure factor [see Fig. 6.16] also confirms the order of the magnetic ground states which starting from zero field is *canted-Flux* state and beyond the critical point $h_c \sim 0.16$ it is FM state with few spins still not aligned in the

Figure 6.15: The plots depicting the behavior of (a) magnetization per site (b) chirality as a function of external magnetic field for $n_e \simeq 3/4$ case. The calculations are done at $t = 1.0$, $t' = 0.25$, $J = 0.1$, $J' = 0.025$, $J_K = 8.0$ and $T = 0.02$.

Figure 6.16: The magnetic field dependence of magnitude of peaks appearing in spin structure factor at $\mathbf{q} = (\pi, 0)$ and $(0, 0)$ for $n_e \simeq 3/4$ case. The MC results are obtained keeping parameters values at $t = 1.0$, $J = 0.1$, $J' = 0.025$, $J_K = 8.0$ and $T = 0.02$.

direction of field. But around $h^z = 0.24$ the peak at $\mathbf{q} = (0, 0)$ saturates close to ~ 1 indicating that ground state is fully polarized FM now.

6.5 Summary

To summarize we have studied in detail the SS-KLM with the help of an unbiased MC method for magnetic properties at $1/4$ and $3/4$ filling of itinerant electrons. For both the cases as a function of temperature we observed a phase transition taking place between a ground state with small chirality to *canted-Flux* state. For $n_e = 1/4$ while varying frustration parameter t'/t the *non-coplanar* states are stabilized over a wide range before a topological transition changes the *canted-Flux* state to a ground state with small *non-coplanar* character – a paramagnetic state. Further increasing the

frustration parameter the ground state changes to staggered AFM with zero chirality. Similar to $n_e = 1/4$, for $n_e = 3/4$ we observed two phase transitions when frustration parameter is increased 1st from a *canted-Flux* state (*chiral*) to a paramagnetic state with very small *non-coplanar* character and further increase in t'/t induced a 2nd phase transition from this state to a staggered AFM state. Finally when localized moments are subjected to an external magnetic field we showed that there is a topological transition for both $n_e = 1/4$ and $3/4$ cases from a *chiral* phase to a ground state with very small chirality (staggered FM state) and further increase in magnetic field results in a fully polarized FM state.

Conclusions and Outlook

Frustrated magnets have long served as a fertile ground for realizing novel magnetic phases that are not observed in their non-frustrated counterparts. In the presence of additional itinerant electrons that interact with localized moments, the system exhibits an even richer array of magnetic and electronic phases. The KLM provides the minimal model for describing such systems. The spin-charge coupling in these systems induces novel and exotic phases and unconventional phase transitions. The itinerant electrons in these systems act as mediators to establish the effective correlation between localized spins giving rise to magnetic behavior. On the other hand, the scattering of these electrons from localized moments may affect the electronic and transport properties of these systems. Additionally, geometric frustration, by its very definition, results in multiple ground state phases with nearly equal energy. Significantly, a small variation in applied magnetic field, pressure, chemical composition or other tunable parameters can alter the quantum mechanical ground state dramatically. Understanding, and, even more importantly, controlling the emergent complexity in these systems is a major challenge confronting the community of Condensed Matter Physicists. We

are still at a nascent stage in harnessing the potential of novel phases and functionalities in strongly correlated electronic systems with geometric frustration for practical applications, largely due to our incomplete knowledge of such phases and phenomena. In this thesis, we particularly discussed how the interaction between itinerant electrons and localized spins in a frustrated quantum magnet leads to stabilization of different topologically *non-trivial* ground states (*non-coplanar* configuration of localized spins).

7.1 Conclusions

In Chapter 3, we discussed the transport properties of itinerant electrons on SSL in the presence of a longitudinal magnetic field. The results suggested that for small frustration t'/t the transverse conductivity exhibits Hall *plateaus* as a function of Fermi energy. The Hall conductivity increases in multiples of e^2/h whenever Fermi energy passes through a Landau level. The width of the Hall *plateaus* decreases when frustration is increased and the *plateaus* behavior is completely suppressed once we reach the limit where the ratio $t'/t \rightarrow 1.0$. The Landau levels get broadened with the increase of frustration and eventually start to overlap which results in suppression of Hall *plateaus*. In the case of small disorder, the transverse conductivity increases in steps of ne^2/h , where n is the number of filled Landau levels – similar to the case of small frustration. Unlike frustration, the width of Hall *plateaus* is robust against the increase of disorder potential. This has to do with the current compensation process – where the enhanced effect from extended states compensates the loss due to the increase of localized states. However, the increase in disorder potential causes the destruction of

higher *plateaus* – the extended states start overlapping when the strength of disorder is increased. We also discussed the effect of temperature on Hall and longitudinal conductivity. For transverse conductivity, the *plateaus* behavior is suppressed as a function of temperature. The increase in thermal energy helps electrons to overcome the energy gap between Landau levels.

In Chapter 4, we studied the phase diagram of SS-KLM with the help of VCM. We choose different favorable spin configurations and compared their energy to find ground state. The results demonstrated that *non-coplanar* spin configurations of localized are stabilized over a wide range of parametric space. From the variational calculations, we found out that a peculiar *chiral* ground state – *canted-Flux* state can be stabilized over an extended range of the phase diagram by turning on DMI. For this spin state, the in-plane components are arranged in a flux pattern where the localized spins on the axial bonds are perpendicular to each other while the spins on the diagonal bonds are anti-parallel to each other. This state also has an out-of-plane component that emerges due to different competing interaction on geometrically frustrated lattice – these interactions include AFM Heisenberg and DM interactions between localized spins and Kondo-like interaction between localized moments and itinerant electrons.

In Chapter 5, we investigated the stability of above-mentioned *canted-Flux* state against the thermal fluctuations using an unbiased MC method at $n_e = 1/2$. The results suggested that this ground state emerges dynamically starting from random spin configurations. The static spin structure factor for localized spins exhibits a small peak at $\mathbf{q} = (0, 0)$ in addition to two sharp peaks at $\mathbf{q} = (0, \pi)$ and $(\pi, 0)$. The nature of this state was found to be topologically *non-trivial* with a finite non-zero chirality. We also showed that the ground states with non-zero chirality are stabilized over a wide range

of magnetic fields. By applying a longitudinal magnetic field we obtained a topological phase transition – the drop in chirality was discontinuous with the increase in magnetic field. Further increase in the field induced a 2nd phase transition where we got a fully polarized FM with zero chirality. We have also obtained magnetization plateaus appearing at $m/m_s \approx 0.5$ and ≈ 0.75 as a function of $D_{\parallel}$ component of DM vector. Moreover, we showed the consistency in results obtained with approximate method TPBM and TCA for 12×12 lattice sizes.

In Chapter 6, we investigated the SS-KLM for magnetic properties at $n_e \simeq 1/4$ and $n_e \simeq 3/4$ in strong J_K coupling limit. The role of thermal fluctuations, frustration and external magnetic field in stabilizing different *chiral* and non-chiral ground states was discussed. Our results suggested that at $n_e \simeq 1/4$ and $3/4$ decrease in temperature drives a phase transition to a *non-coplanar* ground state – *canted-Flux* state that we obtained in Chapter 5. The similarity between the results obtained at one-quarter and three-quarter filling of itinerant electrons can be attributed to the symmetry of bands at these fillings. The results for both the cases showed that while increasing frustration ratio t'/t we can induce a phase transition from *canted-Flux* to a paramagnetic state with small chirality. This state has no long range order except localized spins on some bonds are arranged anti-parallel to each other. Further increase in frustration results in chirality becoming exactly zero indicating a state having coplanar nature. Our results indicated that this state is staggered AFM with vanishing magnetization. Frustration can be used to change the topological character of the ground state by changing the chirality. Finally, we discussed our results obtained when an external magnetic field is applied in the z -direction for both $n_e \simeq 1/4$ and $3/4$. The results showed that there exist a phase transition taking place between *canted-Flux* and a state with small but

non-zero scalar chirality. This partially polarized FM ground state evolves as a function of magnetic field with the partial breaking of flux pattern. Further increase in magnetic field results in complete breaking of flux pattern and chirality becomes zero indicating a coplanar ground state. This ground state is fully polarized FM state where all localized spins are aligned in the direction of magnetic field.

In conclusion, we investigated the SS-KLM for magnetic properties at different number densities of itinerant electrons. To calculate thermodynamic properties throughout the thesis we used MC method along with two other approximate methods to go to larger lattice sizes. Our results indicate that topologically *non-trivial* states such as *canted-Flux* emerge as a ground state due to spin-charge coupling and geometrical frustration. The ground states with different topological character can be tuned with the help of thermal fluctuation, frustration and magnetic field at different filling of itinerant electrons.

7.2 Future Work

Currently, we are investigating the novel magnetic and electronic phases at commensurate electronic fillings in more detail; in particular, the intermediate state that appeared in our results as a function of frustrations for $n_e \simeq 1/4$ and $3/4$. In the near future, we plan to explore the emergent magnetic phases away from commensurate fillings. We have already started to study the transport properties – both longitudinal and transverse – in this model. For future work, we are interested in identifying parameter ranges for the stabilization of topologically *non-trivial* ground states at a small value of J_K . In Chapter 4 from phase diagram, we found out that *non-coplanar*

configurations are stable at this limit of J_K . Next step would be to find the stability of these ground states at finite non-zero temperature using MC methods. To summarize, we plan to explore the novel magnetic and transport properties of the SS-KLM extensively for the near future.

Appendix A

Kubo Formalism for Transverse Conductivity

Appendix A

Kubo Formalism for Transverse Conductivity

We consider the Hamiltonian that consists of an unperturbed part $\mathcal{H}_o$ and perturbed part $\mathcal{H}'(t)$,

$$\mathcal{H} = \mathcal{H}_o + \mathcal{H}'(t), \quad (\text{A.1})$$

and similarly density matrix can be split accordingly,

$$\rho = \rho_o + \rho(t). \quad (\text{A.2})$$

The density matrix for the Hamiltonian without perturbation in grand canonical ensemble can be written as,

$$\rho_o = \frac{1}{Z} \exp(-\beta[\mathcal{H}_o - \mu N]) \quad (\text{A.3})$$

where Z is grand canonical partition function, $\beta = \frac{1}{k_B T}$ is inverse temperature, μ is chemical potential and N is number operator for particles. The equation of motion for density matrix is,

$$i\hbar \frac{d\rho}{dt} = [\mathcal{H}, \rho], \quad (\text{A.4})$$

and using interaction picture we can write ρ as,

$$\rho_I(t) = \exp\left(\frac{i}{\hbar}\mathcal{H}_o\right) \rho \exp\left(-\frac{i}{\hbar}\mathcal{H}_o\right). \quad (\text{A.5})$$

Inserting above equation in Eq. (A.4) and keeping the terms linear in $\mathcal{H}'(t)$ we get the expression,

$$i\hbar \frac{d\rho_I(t)}{dt} = [\mathcal{H}'_I(t), \rho], \quad (\text{A.6})$$

Making the assumption that perturbation was turned off adiabatically at $t \rightarrow -\infty$ that is,

$$\lim_{t \rightarrow -\infty} \rho_I(t) = 0. \quad (\text{A.7})$$

we can integrate Eq. (A.6) to get the expression,

$$i\hbar \rho_I(t) = \int_{-\infty}^t dt' [\mathcal{H}'_I(t'), \rho_o], \quad (\text{A.8})$$

The expectation value of any observable O in interaction picture can be represented as,

$$\langle O(t) \rangle = \text{Tr}\{O_I(t) \rho_I(t)\} \quad (\text{A.9})$$

now assuming that in unperturbed case expectation value of an observable is zero then we can write above equation,

$$\begin{aligned} \langle O(t) \rangle &= \text{Tr}\{O_I(t) \rho_I(t)\} \\ &= -\frac{i}{\hbar} \int_{-\infty}^t dt' \text{Tr}\{[\mathcal{H}'_I(t'), \rho_o] O_I(t)\} \\ &= -\frac{i}{\hbar} \int_{-\infty}^t dt' \text{Tr}\{\rho_o [\mathcal{H}'_I(t'), O_I(t)]\} \end{aligned} \quad (\text{A.10})$$

We represent the $\mathcal{H}'(t)$ in terms of its Fourier components and make use of linearity of Eq. (A.10) to treat one component at a time. We take one component as $A \exp(-i[\omega +$

$i\eta]t)$, where η (convergence factor) is introduced to insure the boundary conditions.

Using this specific component of Fourier transform we can write Eq. (A.10) as,

$$\langle O(t) \rangle = \frac{i}{\hbar} \int_{-\infty}^t dt' \text{Tr} \{ \rho_o [A, O_I(t-t')] \} \exp(-i[\omega + i\eta]t') \quad (\text{A.11})$$

The linear response function can be defined as,

$$\langle O(t) \rangle = \int_{-\infty}^{+\infty} dt' \chi_{OA} \exp(-i[\omega + i\eta]t'). \quad (\text{A.12})$$

So we can write χ_{OA} from Eq. (A.11),

$$\chi_{OA}(t) = \frac{i}{\hbar} \text{Tr} \{ [A, \rho_o] O_I(t) \} \theta(t), \quad (\text{A.13})$$

in above equation $\theta(t)$ is Heaviside step function. Replacing the observable O with μ^{th} component of current density operator J – which can be represented as,

$$-eJ_\mu(r) = -\frac{e}{2} \sum_{i=1}^n \{ v_{i\mu} \delta(\mathbf{r} - \mathbf{r}_i) + \delta(\mathbf{r} - \mathbf{r}_i) v_{i\mu} \}, \quad (\text{A.14})$$

where v_i are velocity operators for particle i . From linear response theory the perturbed part of Hamiltonian is,

$$\mathcal{H}'(t) = e \sum_{\nu} X_{\nu} E_{\nu}(t), \quad (\text{A.15})$$

where $X_y = \sum_{i=1}^n r_{iy}$. Replacing $A = eX_y$ in Eq. (A.13) we can write conductivity σ_{xy} ,

$$\sigma_{xy}(\mathbf{r}, t) = -\frac{ie^2}{\hbar} \theta(t) \text{Tr} \{ \rho_o [X_y, J_x(\mathbf{r}, t)] \} \quad (\text{A.16})$$

To calculate trace we use the eigenstates $|n\rangle$ of $\mathcal{H}_o$, where this Hamiltonian matrix is diagonal since for these eigenstates ρ_o is also diagonal. The Schrödinger equation for this unperturbed Hamiltonian can be written as,

$$\mathcal{H}_o |n\rangle = E_n |n\rangle; n = 0, 1, 2, 3, \dots \quad (\text{A.17})$$

where E_0 is ground state and at lower temperatures the term $\langle 0|\rho_o|0\rangle$ contributes to trace in Eq. (A.16). The ground state does not contribute to current density $\langle 0|J_\mu(\mathbf{r})|0\rangle = 0$. Using interaction picture representation for $J_\mu(\mathbf{r}, t)$ Eq. (A.16) becomes,

$$\begin{aligned} \sigma_{xy}(\mathbf{r}, t) = & -\frac{ie^2}{\hbar}\theta(t) \sum_{n>0} \{ \langle 0|X_y|n\rangle \langle n|J_x(\mathbf{r})|0\rangle \exp(\frac{i}{\hbar}[E_n - E_0]t) \\ & - \langle n|X_y(\mathbf{r})|0\rangle \langle 0|J_x|n\rangle \exp(-\frac{i}{\hbar}[E_n - E_0]t) \}. \end{aligned} \quad (\text{A.18})$$

To get static conductivity $\sigma_{xy}(\mathbf{r})$ we integrate over t ,

$$\sigma_{xy}(\mathbf{r}) = \lim_{\eta \rightarrow 0+} \int_{-\infty}^{+\infty} dt e^{-\eta t} \sigma_{xy}(\mathbf{r}, t), \quad (\text{A.19})$$

where $e^{-\eta t}$ is convergence factor with $\eta > 0$. The average conductivity then can be obtained as,

$$\sigma_{xy} = \frac{1}{A} \int d\mathbf{r} \sigma_{xy}(\mathbf{r}), \quad (\text{A.20})$$

where A is the area of the system. Similarly, the total current or velocity operator can also be written as,

$$J_x = v_x = \int d\mathbf{r} J_x(\mathbf{r}). \quad (\text{A.21})$$

Making all these substitutions in Eq. (A.18) we have transverse conductivity as,

$$\sigma_{xy} = e^2 \sum_{n>0} \frac{\langle 0|X_y|n\rangle \langle n|v_x|0\rangle + \langle n|X_y|0\rangle \langle 0|v_x|n\rangle}{E_n - E_0} \quad (\text{A.22})$$

and also noting that $\dot{X}_y = v_y$ from equation of motion,

$$i\hbar v_y = i\hbar \frac{d}{dt} X_y = [X_y, \mathcal{H}_o]. \quad (\text{A.23})$$

Inserting above equation in Eq. (A.22) we are left with final expression for transverse conductivity,

$$\sigma_{xy} = \frac{ie^2\hbar}{A} \sum_{n>0} \frac{\langle 0|v_y|n\rangle \langle n|v_x|0\rangle + \langle n|v_y|0\rangle \langle 0|v_x|n\rangle}{(E_n - E_0)^2}. \quad (\text{A.24})$$

Appendix **B**

Chebyshev Polynomials

Appendix B

Chebyshev Polynomials

The recursion formula for Chebyshev polynomials is given by,

$$T_0(x) = 1, \quad T_1(x) = x,$$

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

for $-1 \leq x \leq 1$. These polynomials are even (odd)-functions for even (odd) value of n . The orthonormality condition for Chebyshev polynomials has a form,

$$\int_{-1}^1 \frac{dx}{\pi \sqrt{1-x^2}} T_n(x) T_m(x) = \begin{cases} 0, & m \neq n \\ 1, & m = n = 0 \\ 1/2, & m = n \neq 0 \end{cases}$$

The trigonometric or alternative definition of these polynomials is,

$$T_n(\cos \theta) = \cos n\theta$$

within the range $\theta = [0, \pi]$.

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