ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL OF SCIENCE ENGINEERING AND TECHNOLOGY

DIRAC SYSTEMS IN TERMS OF THE BERRY GAUGE FIELDS AND EFFECTIVE FIELD THEORY OF A TOPOLOGICAL INSULATOR

Ph.D. THESIS

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Department of Physics Engineering

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ABBREVIATIONS

TRI	**:** Time Reversal Invariant
SO	**:** Spin-Orbit
SOI	**:** Spin-Orbit Interaction
TRB	**:** Time Reversal Breaking
QHE	**:** Quantum Hall Effect
SQHE	**:** Spin Quantum Hall Effect

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DIRAC SYSTEMS IN TERMS OF THE BERRY GAUGE FIELDS AND EFFECTIVE FIELD THEORY OF A TOPOLOGICAL INSULATOR

SUMMARY

Dirac systems in terms the of Berry gauge fields and the effective field theory of a time-reversal invariant topological insulator are investigated. Dirac systems or Dirac-like systems are non-relativistic systems, e.g. condensed matter systems, where the description of the physical system is given by either the massive or massless Dirac Hamiltonian. The Dirac systems investigated in this thesis are the time-reversal invariant topological insulators. A topological insulator is a bulk insulator with conducting edge states characterized by a topological number. The first theoretical model of the time-reversal invariant topological insulators is the Kane-Mele model of graphene where the intrinsic spin-orbit interaction and time-reversal symmetry is predicted to cause a quantized spin Hall current at the edges , leading to a quantized spin Hall conductivity given by the the topological Chern number.
As the theoretical background, the explicit derivation of $2+1$ dimensional massless Dirac Hamiltonian on graphene is given. The Berry gauge field and the corresponding Berry curvature are defined for massive free Dirac Hamiltonian in arbitrary dimensions employing the Foldy-Wouthuysen transformation of the Dirac Hamiltonian. The definitions of the first and second Chern numbers in terms of Berry curvature are given.
In the first part of the thesis, a semiclassical formulation of the quantum spin Hall effect for physical systems satisfying Dirac-like equation is introduced. Quantum spin Hall effect is essentially a phenomenon in two space dimensions. In the semiclassical formulation adopted in the thesis, the position and momenta are classical phase space variables, and spin is not considered as a dynamical degree of freedom. The derivation of the matrix-valued one-form lying at the heart of the semiclassical formulation adopted is made explictly using a wave-packet constructed from the positive energy eigenstates of free Dirac equation. Defining the symplectic two-form and employing Liouville equation, the semiclassical matrix-valued equations of motion are obtained. The phase space measure, $\tilde{w}_{1/2}$, and time evolutions of phase space variables, $\dot{\tilde{x}}_i\tilde{w}_{1/2}$ and $\dot{\tilde{p}}_i\tilde{w}_{1/2}$, are obtained in terms of the phase space variables. As an introductory example, the formalism is displayed through the anamolous Hall effect. The anamolous Hall conductivity is established from the term linear in the electric field and the Berry curvature in $\dot{\tilde{x}}_i\tilde{w}_{1/2}$. The semiclassical formulation adopted is then illustrated within the Kane-Mele model of graphene in the absence and in the presence of the Rashba spin-orbit coupling term. The spin Hall current is defined with the aid of the equations for the time evolutions of phase space variables in terms of phase space variables. The spin Hall conductivity is established from the term linear in the elctric field and the Berry curvature in $\dot{\tilde{x}}_i\tilde{w}_{1/2}$. It is shown that if one adopts the correct definition of the spin current in two space dimensions, the essential part of the spin Hall conductivity is always given by the spin Chern number whether the spin is conserved or not at the quantum level. In the absence of Rashba spin-orbit coupling, the third component of spin is conserved, and the definition of the spin Hall

current is straightforward. In the presence of Rashba spin-orbit coupling, the third component of spin is not conserved so that a suitable base of spin eigenstates need to be employed to define spin Hall current. The anomalous velocity term survives in any $d+1$ spacetime dimension, since independent of the spacetime dimension and the origin of the Berry curvature in the time evolution of the coordinates there is always a term which is linear in both electric field and the Berry field strength. In the basis where a certain component of spin is diagonal this term will be diagonal.
In the second part of the thesis, a field theoretic investigation of topological insulators in $2+1$ and $4+1$ dimensions is presented using Chern-Simons theory and a method of dimensional reduction. Chern-Simons actions emerge as the effective field theories from the actions describing Dirac fermions in the presence of external gauge fields. A time-reversal invariant topological insulator model in $2+1$ dimensions is discussed and by means of a dimensional reduction the $1+1$ dimensional descendant is presented. The field strength of the Berry gauge field corresponding to the $4+1$ dimensional Dirac theory is explicitly derived through the Foldy-Wouthuysen transformation. Acquainted with it, the second Chern number is calculated for specific choices of the integration domain. The Foldy-Wouthuysen transformation which diagonalizes the Dirac Hamiltonian is proven to be a powerful tool to perform calculations in the effective field theory of the $4+1$ dimensional time-reversal invariant topological insulator. A method is proposed to obtain $3+1$ and $2+1$ dimensional descendants of the effective field theory of the $4+1$ dimensional time reversal invariant topological insulator. Inspired by the spin Hall effect in graphene, a hypothetical model of the time reversal invariant spin Hall insulator leading to a dissipationless spin current in $3+1$ dimensions is proposed. In terms of the explicit constructions presented in this thesis, one can discuss $\mathbb{Z}_2$ topological classification of TRI insulators in a tractable fashion. In principle, the approach presented can be generalized to interacting Dirac particles where the related Foldy-Wouthuysen transformation at least perturbatively exists.

BERRY AYAR ALANLARI CİNSİNDEN DİRAC SİSTEMLERİ VE BİR TOPOLOJİK YALITKANIN ETKİN ALAN KURAMI

ÖZET

Berry ayar alanları cinsinden Dirac sistemleri ve zaman tersinmesi altında değişmez bir topolojik yalıtkanın etkin alan kuramı incelenmiştir. Dirac sistemleri ya da diğer bir ismi ile Dirac-benzeri sistemler, kütleli ve ya kütlesiz Dirac Hamilton fonksiyonu ile betimlenen yoğun madde sistemleridir. Tezde incelenen Dirac sistemleri zaman tersinmesi altında değişmez kalan topolojik yalıtkanlardır. Topolojik yalıtkanlar, iç kısımlarında yalıtkan olmalarına rağmen iletken kenar durumlarına sahip olan ve topolojik değişmezler ile karakterize edilen sistemlerdir.

Maddenin simetri kırılması ile sınıflandırılması bilinmektedir. Katı-sıvı- gaz sistemleri öteleme simetrisinin kırılması ile, manyetik malzemeler, dönme simetrisinin kırılması ile ve süperiletkenlik ayar simetrisinin kırılması ile betimlenmektedir. Topolojik yalıtkanın betimlemesi simetri kırılması ile verilememektir ve böylece topolojik yalıtkan, topolojik olarak betimlenen maddenin yeni bir fazı olarak ortaya çıkmıştır. Sıradan yalıtkan topolojik olarak bakıldığında trivial bir yapıda olmasına rağmen topolojik yalıtkan trivial olmayan bir yapıdadır. Topolojik yalıtkan kavramının ortaya çıkması esas olarak kuantum Hall olayının topolojik bir faz olduğunun anlaşılması ile başlamıştır.

Klasik Hall olayında dış bir manyetik alan içerisinde ilerleyen yüklü parçacıklar, manyetik alana ve ilerleme yönüne dik bir elektrik alan ve yük akımı oluştururlar. Oluşan yük akımı ile dik elektrik alanın oranı Hall iletkenliği ile verilir. Hall iletkenliği, dış manyetik alan ile sürekli ve doğru orantılı olarak artar. İki boyutlu etkileşmeyen elektron sisteminde düşük sıcaklık ve yüksek manyetik alan altında meydana gelen kuantum Hall olayında ise kuantum Hall iletkenliği $\frac{e^2}{h}$ $'$ nin tamsayı katları olacak şekilde kuantize değerler almaktadır. Enine iletkenlikteki bu kuantizasyon 10^9 mertebesinde hassastır. Safsızlıklardan etkilenmemektedir. Kuantum Hall sisteminin oluşumu herhangi bir simetri kırılması ilkesi ile verilememiştir. Kuantum Hall iletkenliğini betimleyen kuantize tamsayının topolojik bir değişmez olduğunun gösterilmesi ile beraber kuantum Hall sistemi topolojik fazların ilk örneği olarak ortaya çıkmıştır. Topolojik değişmezler, ilgili topolojik uzaya ait olan ve sürekli deformasyonlar altında değişmez kalan sayılardır. Kuantum Hall olayının, topolojik fazların ilk örneği olarak ortaya çıkması ile yoğun madde sistemlerinin incelenmesinde geometri ve topoloji önem kazanmaya başlamıştır. İki boyutlu bir sistem olan grafen yapraklarında yük taşıyıcıların etkin olarak kütlesiz Dirac denklemini sağladığının gösterilmesi de bu gelişmede önemli bir aşama olmuştur. Zira, Dirac Hamilton fonksiyonunun topolojik özellikleri, yankı uyandıran bu gelişmeler olduğunda halihazırda önemli bir araştırma konusuydu. Berry ayar alanları, Dirac Hamilton fonksiyonu ile betimlenen yoğun madde sistemlerinin topolojik yapısını incelemek için kullanılmıştır. Berry ayar alanından elde edilen Berry eğriliği topolojik bir değişmez olan Chern sayısının hesaplanmasını sağlar. Zaman tersinmesine sahip

bir topolojik yalıtkanın Chern sayısı sıfırdan farklı çıkmaktadır.
Teorik altyapıyı oluşturmak icin öncelikle graphene üzerindeki kütlesiz $2+1$ boyutlu Dirac Hamilton fonksiyonunun çıkarımı verilmiştir. En yakın komşu etkileşmesi içeren sıkı bağlanma Hamilton yoğunluğundan başlayarak, Dirac noktaları etrafında ve sürekli limitte kütlesiz $2+1$ boyutlu Dirac Hamilton fonksiyonu elde edilir. Grafen, karbon atomlarından oluşan iki boyutlu altıgen bir örgü yapısına sahiptir. Altıgen Brillouin bölgesinin kenar noktaları Dirac noktaları olarak adlandırılır. Grafenin kuramsal açıdan önemi, enerji dağınım bağıntısının Dirac noktaları civarında lineer olması ve bu noktalar civarında yapılan yaklaşıklık ile elektronların grafen üzerinde etkin olarak $2+1$ boyutlu kütlesiz Dirac denklemini sağlamasıdır. Foldy-Wouthuysen dönüşümü, Dirac Hamilton fonksiyonunu köşegenleştirmeye yarayan bir dönüşümdür. Foldy-Wouthuysen dönüşümü kullanılarak bir ayar alanı tanımlanabilir. Bu saf bir ayar alanıdır ve ilgili eğrilik özdeş olarak sıfırdır. Foldy- Wouthuysen dönüşümü ile edilen ayar alanının pozitif enerji özdurumları üzerine izdüşümü alınırak Berry ayar alanı ve Berry ayar alanı kullanılarak ilgili Berry eğriliği tanımlanır. Bu şekilde Berry ayar alanı ve Berry eğriliği herhangi bir boyutta tanımlanabilir. $2+1$ boyutta Berry eğriliğinin entegrali birinci Chern sayısını verir. $4+1$ boyutta Berry eğriliği uygun bir şekilde entegre edilerek ikinci Chern sayısı elde edilir.
Dirac-benzeri denklem sağlayan fiziksel sistemler için kuantum spin Hall etkisinin incelemesi yarı klasik bir formulasyon ile yapılmıştır. Bu incelemede diferansiyel formlar kullanılmıştır. Kullanılan yarı klasik formulasyonda, klasik faz uzayı değişkenleri olan konum ve momentum dinamik serbestlik değişkenleri iken spin dinamik bir serbestlik derecesi olarak alınmamıştır. Spin, kullanılan yarı klasik formulasyonun matris değerli büyüklükler içermesinde kendini göstermektedir. Herhangi bir boyutta Dirac denkleminin pozitif enerji çözümleri kullanılarak kurulan dalga paketi yoluyla dalga paketinin dinamiğini betimleyen 1-form elde edilmiştir. Bu 1-form kullanılarak herhangi bir boyuttaki simplektik 2-form elde edilmiştir. $2+1$ boyutlu simplektik 2-form ve Liouville denklemi kullanılarak, yarı klasik hareket denklemleri elde edilmiştir. Bu hareket denklemlerinin yardımıyla, faz uzayı ölçüsü, konum ve momentumun zaman evrimleri için klasik faz uzayı değişkenleri konum ve momentum cinsinden yarı klasik denklemler elde edilmiştir. Spin Hall akımı faz uzayı ölçüsü ve konumun zaman evrimi ile tanımlanmıştır. Formulasyon, anomal kuantum Hall etkisi, Rashba spin yörünge etkileşmesi içeren ve içermeyen Kane-Mele modeli üzerinden örneklenmiştir. Rashba spin yörünge etkileşmesi içeren ve içermeyen Kane-Mele modeli örneklerinde kuantum seviyesinde spinin korunup korunmadığından bağımsız olarak spin Hall iletkenliğine gelen temel katkının spin Chern sayısı ile verildiği gösterilmiştir. Spin Chern sayısı, yukarı spin taşıyıcıları ile ilgili Chern sayısı ile aşağı spin taşıyıcıları ile ilgili Chern sayısının farkının yarısı olark tanımlanır.
Kane-Mele modeli, zaman tersinmesi simetrisine sahip $2+1$ boyutlu içsel spin yörünge etkileşmesi içeren grafen modelidir. Bu teorik model, grafende spin yörünge etkileşmesi sayesinde spin Hall olayının gerçekleşebileceğini öngörmektedir. Kane-Mele modeli, zaman tersinmesi simetrisine sahip topolojik yalıtkanların ilk örneğidir. Matematiksel olarak, spin yörünge etkileşmesi Dirac Hamilton yoğunluğunda kütle benzeri bir terim olarak ortaya çıkmıştır. Bu kütle benzeri terim Dirac noktaları için ters işaretli olarak gelmektedir. Ayrıca her Dirac noktasında, yukarı spin taşıyıcıları ve aşağı spin taşıyıcıları için iki ayrı Hamilton fonksiyonu mevcuttur. Spin yörünge teriminin yol açtığı enerji aralığını geçen kenar durumları kuantum spin Hall olayının oluşmasını sağlar. Kuantum spin

Hall iletkenliği, topolojik olarak korunan kenar durumları vasıtasıyla taşınan ters spin akımlarının zıt yönlü ilerlemesi ile gerçekleşmektedir ve sistemin Hamilton yoğunluğunun zaman tersinmesi simetrisine sahip olmasını gerektirmektedir. Bu model, grafendeki içsel spin yörünge etkileşmesinin çok küçük olmasından dolayı fiziksel olarak gerçeklenebilir olmamasına rağmen, zaman tersinmesi altında değişmez kalan topolojik yalıtkanların teorisinin oluşmasını sağlamıştır. Kane-Mele modeli için Foldy-Wouthuysen dönüşümleri kullanılarak Berry ayar alanı ve ilgili Berry eğriliği hesabı yapılmıştır. Ayrıca Rashba spin yörünge etkileşmesi içeren Kane-Mele modeli incelenmiştir. Rashba spin yörünge etkileşmesi ilgilenilen spin yönündeki korunumunu bozar. Sadece içsel spin yörünge etkileşmeli Kane-Mele modelinden en büyük farkı budur. Rashba spin yörünge etkileşmesi içeren Kane-Mele modeli için hem enerji özdurumları bazında hem de ilgilenilen spin bileşeninin özdurumları bazında Berry ayar alanı hesabı ve ilgili Berry eğriliği hesabı yapılmıştır. Bu model için, ilgilenilen spin bileşeninin köşegen olduğu bazda Berry eğriliği de köşegendir. Dolayısıyla spin Hall iletkenliği hesaplanabilmiştir. Kullanılan yarı klasik formulasyon ile, $2+1$ boyutta spin Hall iletkenliği hem elektrik alanda hem Berry eğriliğinde lineer olan konumun zaman evriminden elde edilmiştir. Bu anomal hız terimi herhangi bir $d+1$ boyutta mevcuttur.

Ayrıca, $2+1$ ve $4+1$ boyutta Chern-Simons kuramı ve bir boyut indirgeme yöntemi ile topolojik yalıtkanların alan kuramsal bir incelemesi sunulmuştur. Chern-Simons eylemleri, dış ayar alanları içeren Dirac eylemlerinin etkin alan kuramları olarak ortaya çıkar. Etkin alan kuramı, ilgili yol entegralinde fermiyon serbestlik dereceleri entegre edilerek elde edilir. Öncellikle, $2+1$ boyutta zaman tersinme simetrisi içermeyen kuantum Hall olayının topolojik alan kuramı incelenmiştir. $2+1$ boyutlu zaman tersinmesi simetrisine sahip bir topolojik yalıtkanın etkin alan kuramı $2+1$ boyutlu Chern-Simons kuramı ile verilmiştir. $2+1$ boyutlu Chern-Simons kuramı birinci Chern sayısı ile orantılıdır ve $2+1$ boyutlu Chern-Simons eyleminden elde edilen akım ifadesinde birinci Chern sayısı yer alır. Boyutsal indirgeme yöntemi kullanılarak ve yük kutuplanması açıkca elde edilerek $2+1$ boyutlu Chern-Simons kuramından elde edilen $1+1$ boyutlu bir kuram sunulmuştur. Daha sonra temel topolojik yalıtkanı betimlediği gösterilen $4+1$ boyutlu Chern-Simons kuramı incelenmiştir. $4+1$ boyutlu kütle benzeri terim içeren Dirac kuramının Foldy-Wouthuysen dönüşümü kullanılarak elde edilen Berry ayar alanı ve ilgili Berry eğriliğinin hesabı ayrıntılı olarak sunulmuştur. Bu Berry ayar alanı Abelyen olmayan bir ayar alanıdır. İlgili Berry eğriliği kullanılarak ikinci Chern sayısı hesaplanmıştır. $4+1$ boyutlu zaman tersinmesi simetrisine sahip bir topolojik yalıtkanın etkin alan kuramı $4+1$ boyutlu Chern-Simons kuramı ile verilmiştir. $4+1$ boyutlu Chern-Simons kuramının katsayısı ikinci Chern sayısı ile orantılıdır ve $4+1$ boyutlu Chern-Simons eyleminden elde edilen akım ifadesinde ikinci Chern sayısı yer alır. Bu etkin alan kuramından boyut indirgeme yöntemi kullanılarak $3+1$ ve $2+1$ boyutlu kuramlar elde edilmiştir. Grafendeki kuantum spin Hall olayından esinlenerek, $3+1$ boyutta yitimsiz spin Hall akımına yol açan, zaman tersinme simetrisine sahip kuramsal bir topolojik yalıtkan modeli öne sürülmüştür. $2+1$ boyutlu indirgenmiş eylemde yer alan ayar alanlarının açık formu elde edilmiştir. Modelin zaman tersinme simetrisi açıkca gösterilmiştir. Sunulan ayrıntılı çıkarımlar topolojik yalıtkanların $\mathbb{Z}_2$ sınıflandırılmasını takip edilebilir bir şekilde tartışılmasını sağlamaktadır. Bu bölümde sunulan yaklaşımın Foldy-Wouthuysen dönüşümünün pertürbatif olarak geçerli olduğu etkileşim içeren Dirac sistemlerine de genelleştirilmesi prensipte mümkündür.

1. INTRODUCTION

Dirac-like systems in terms of Berry gauge fields and the effective field theory of a time-reversal invariant topological insulator is investigated in this thesis. Dirac-like systems (Dirac systems) arise in non-relativistic condensed matter systems, where charge carriers effectively obey either the massless or the massive Dirac-like equation. Polyacetylene is one of the first examples of such systems [1–3], where Dirac Hamiltonian in $1+1$ dimensions arises. Graphene, with its honeycomb structure of carbon atoms, is an example of Dirac systems in $2+1$ spacetime dimensions [4]. The Dirac Hamiltonian in two space dimensions was derived starting from the tight-binding model with on-site and nearest neighbor interactions for electrons in a planar honeycomb lattice in [5]. The on-site interaction was chosen such that it led to masses with opposite signs for the two sublattices of the hexagonal lattice. Inspecting the energy band structure, one finds that there are two inequivalent degeneracy points in the Brilliuon zone where the conduction and valance bands meet. These points are named Dirac points because by an expansion around these points and dealing with the the low-energy or the continuum limit, the massive Dirac Hamiltonian is obtained. However, considering only the nearest neighbor interaction, massless Dirac Hamiltonian is obtained, yielding a linear energy dispersion. The Dirac equation was shown to emerge for the electrons on planar graphene also in [6]. In section 2 of the thesis, derivation of Dirac Hamiltonian on graphene for three different choices of lattice vectors are given based on [4, 5, 7].

The Kane-Mele model of graphene [8] is a quantum mechanical model of the electrons on graphene which comprises of all the contributions coming from the sublattices, the Dirac points and the spin degrees of freedom by introducing an intrinsic spin-orbit interaction which acts as a mass term in the Dirac-like Hamiltonian. The time-reversal invariant intrinsic spin orbit interaction introduced by Kane-Mele induces masses with opposite signs on the two Dirac points. The model predicts the formation of dissipationless quantized spin current perpendicular to an external in-plane electric field, namely the quantum spin Hall effect. The model also predicts that the

quantum spin Hall insulator state, characterized by the quantum spin Hall current, is topologically distinct from a band insulator state. Quantum spin Hall effect, introduced by Kane-Mele is based on Haldane's model of quantum Hall effect without Landau levels [9], where a periodic magnetic field with zero net flux through the unit cell of the honeycomb lattice was introduced. Thus, this spinless model of Haldane necessarily breaks time reversal symmetry. Haldane's model takes into consideration on-site interaction, nearest neighbor and the next nearest neighbor interactions on the honeycomb lattice, the last of which violates particle-hole symmetry.

The topological nature of the quantum Hall effect was first pointed out by Thouless et al in [10] using linear response theory where it was shown that the quantum Hall conductivity, calculated by the Kubo formula, is characterized by an integer. Then, in [11] the connection between the Berry phase and the quantized integer of the quantum Hall conductivity was discovered. In [12], it was explictly demonstrated that this integer is the first Chern number within differential geometry employing fiber bundle theory. Since the wavefunctions in the magnetic Brillouin zone (reciprocal crystal momentum space) have non-trival topological character, the associated gauge field induces a non-zero topological number.

Topological nature of the Hall effect is well exhibited in terms of the Berry phases. In [13], Berry describes how a quantum mechanical system which has a parameter evolving adiabatically around a cyclic path acquires a geometrical phase besides the dynamical phase. The concept of geometrical phase was already discussed in the context of classical mechanics using parallel transport and holonomy. Some of the prominent examples from classical mechanics are Hannay's angle and Foucault's pendulum and Pancharatnam's angle in optics. A brief review of geometrical phases in physics can be found in [14]. In section 2 of the thesis, the Berry gauge fields and field strengths obtained through the Foldy-Wouthuysen transformation of the Dirac Hamiltonian are introduced.

The semiclassical equations of motion are altered drastically in the presence of the Berry gauge fields. For a formulation, see [15] and the references therein. For electrons, the semiclassical equations yield an anomalous velocity term which leads to the anomalous Hall conductivity. In fact, ignoring the spin of electrons the Hall conductivity can be written in terms of the Berry curvature on the Fermi surface as described in [16, 17]. A complete list of references for the Berry phase effects

in this context can be found in the review [18]. Considering the electrons with spin, a generalization to the spin Hall effect was discussed in [19]. The spin Chern number was introduced in [20]. In [21, 22], the Berry gauge field was derived using a wavepacket constructed from Bloch wavefunctions.

In Section 3, a semiclassical formulation of the quantum spin Hall effect for physical systems satisfying a Dirac-like equation is presented [23]. The semiclassical formulation is carried out using differential forms. Quantum spin Hall effect is essentially a phenomena in two space dimensions. In the semiclassical formulation adopted, the position and momenta are classical phase space variables. Spin is not considered as a dynamical degree of freedom, however it shows up in the matrix-valuedness of the equations of motion. The derivation of the matrix-valued one-form lying at the heart of our semiclassical formulation is established by a wave-packet constructed from the positive energy eigenstates of free Dirac equation. Then, we define the symplectic two-form and employ the Liouville equation to derive the semiclassical matrix-valued equations of motions in arbitrary dimensions. The investigation of chiral kinetic theory within this semiclassical approximation was given in [24]. We define the spin current with the aid of these equations and obtain the spin Hall conductivity. It is demonstrated that the main contribution to the spin Hall conductivity is given by the spin Chern number whether the related spin component is conserved or not at the quantum level. The formulation is illustrated within the Kane-Mele model of graphene in the absence and presence of the Rashba spin-orbit coupling term. The presence of the Rashba spin-orbit coupling term depicts itself in the non-conservation of the third component of spin which is conserved in its absence. The Kane-Mele model of spin Hall effect in $2+1$ dimensions is the first theoretical model of time-reversal invariant topological insulators. A time-reversal invariant topological insulator is a bulk insulator with conducting edge states characterized by topological numbers [25–27]. In the Kane-Mele model of graphene, a quantized spin Hall current at the edges is predicted due to the intrinsic spin-orbit coupling and the time-reversal symmetry. It furnishes a quantized spin Hall conductivity given by the topological Chern number. The Kane-Mele model paved the way to the theoretical prediction of the topological insulator phase in 3d materials [28] which was observed for the first time in [29]. They can be classified by a new topological invariant called $\mathbb{Z}_2$ [30]. As discussed, the role of topological invariants were already investigated

in the context of quantum Hall effect. Moreover, in $2+1$ dimensions a topological gauge theory is generated by integrating out the massive Dirac fermion fields coupled to Abelian gauge fields in the related path integral [31–33]. It is described by the $2+1$ dimensional Chern-Simons action whose coefficient is the winding number of the noninteracting massive fermion propagator which is equal to the first Chern number resulting from the Berry gauge field [13, 18] of the quantum Hall states. One can also derive the time reversal invariant spin Hall current of the Kane-Mele model by calculating the related first Chern numbers [34]. Therefore, the Hall current can be acquired from a topological field theory which manifestly violates time reversal symmetry [35, 36].

In $4+1$ dimensions, Chern-Simons action generated by the massive fermions coupled to Abelian gauge fields, is manifestly time-reversal invariant. Qi-Hughes-Zhang [37] designated it as the effective topological field theory of the fundamental time-reversal invariant topological insulator in $4+1$ dimensions. They demonstrated that for the band insulators which can be deformed adiabatically to a flat band model, the coefficient of the effective action is equal to the second Chern number given by the related non-Abelian Berry vector fields. The equivalence of the coefficients of the induced Chern-Simons actions with the Chern numbers is presented in [38] in a straightforward manner by employing the Foldy-Wouthuysen transformation. The $3+1$ and $2+1$ dimensional descendant theories are generated by dimensional reduction from the $4+1$ dimensional action of the massive Dirac fields coupled to external gauge fields.

In Section 4, a field theoretic investigation of topological insulators in $2+1$ and $4+1$ dimensions is provided by employing Chern-Simons theory. It is based on the approach of [37] but applied to the continuous Dirac theory and also a slightly modified method is proposed to introduce the descendant theories which permits us to derive explicitly the related physical objects like polarizations. Moreover, a hypothetical model of time-reversal invariant spin Hall effect in $3+1$ dimensions is positted which may be useful to understand some aspects of physically realizable three dimensional topological insulators described in [39–41]. We introduce the Berry gauge fields corresponding to Dirac fermions through the Foldy-Wouthuysen transformation. The $2+1$ dimensional topological field theory of the integer quantum Hall effect is recalled. It guides us to construct the time-reversal invariant spin quantum Hall effect

in graphene which is a model of $2+1$ dimensional topological insulator. Then, the dimensional reduction to $1+1$ dimensions by obtaining the one dimensional charge polarization is presented explicitly. The $4+1$ dimensional Chern-Simons field theory which was shown to describe the fundamental topological insulator is introduced. The field strengths of the related Berry gauge fields needed to provide the second Chern number are derived and dimensional reduction to $3+1$ dimensions is discussed. By imitating the approach of [8], a hypothetical model in $4+1$ dimensions is theorized which yields a time reversal invariant spin Hall current in $3+1$ dimensions by means of the dimensional reduction. A dimensional reduction procedure to $2+1$ dimensions which provides explicit forms of the gauge field components which take part in the descendant action is presented. In the last section, the results which we obtained are discussed.

2. DIRAC HAMILTONIAN, FOLDY-WOUTHUYSEN TRANSFORMATION, AND THE BERRY GAUGE FIELDS IN D-DIMENSIONS

Graphene is a single layer of graphite. Its structure consists of hexagons arranged as a honeycomb with carbon atoms sitting at every corner of the hexagonal structure. The honeycomb lattice is a superposition of two triangular sublattices . The carbon atoms in the first sublattice are named type A atoms and the carbon atoms in the second sublattice are named type B atoms. In the following discussion, the sublattices will be briefly refered to as sublattice A and sublattice B. The derivation of the Dirac Hamiltonian will be presented for three different choices of the unit cell basis vectors. Starting from the tight-binding Hamiltonian which has only the nearest-neighbor hopping term, the massless Dirac-like Hamiltonian will be derived. The bonds formed by $2p_z$ orbital electrons are called π bonds. They occur perpendicular to the two-dimensional graphene plane. The hopping in the tight-binding Hamiltonian results from the overlap of $2p_z$ orbital wavefunctions of spinless electrons in the hexagonal lattice. The nearest-hopping term refers to hopping between nearest atoms in the hexagonal lattice, therefore it actually relates the two sublattices of the graphene sheet. Passing to the reciprocal momentum space (k-space), the energy dispersion is obtained. The roots of the energy dispersion relation are where the conduction and valence bands meet. These points in k-space are called degenarcy points. They occur at the corners of the hexagonal Brillouin zone. Two of these points are inequivalent and their choice depends on the choice of unit cell basis vectors. In the continuum limit, only states around the degenarcy points contribute to the dynamics and an expansion around these points yields the Dirac-like Hamiltonians. Therefore, these degenarcy points are also refered to as Dirac points. The energy dispersion is linear around the Dirac points and is usually referred to as the Dirac cone. As will be apparent in the derivation, the Dirac-like Hamiltonians do not actually incorporate spin like the relativistic Dirac Hamiltonian. It incorporates sublattice degrees of freedom in the context of graphene. The sublattice degrees of freedom are therefore refered to as pseudo-spin.

2.1 Derivation of Dirac Hamiltonian on graphene à la Semenoff

The basis vectors for A lattice are chosen as

$$\boldsymbol{a}_1 = \frac{a}{2}\left(\sqrt{3}, -1\right),\ \boldsymbol{a}_2 = a\,(0,1)\,.$$

Here a is distance between two atoms in the same lattice as shown in Figure 2.1.

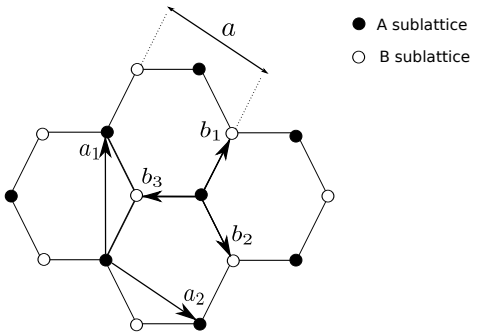

Figure 2.1: Honeycomb lattice 1.

Type A sites are generated by linear combinations of $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$. The position of the three nearest neighbors of A, i.e. the type B atoms, are

$$\boldsymbol{b}_1 = \frac{a}{2}\left(\frac{1}{\sqrt{3}}, 1\right),\ \boldsymbol{b}_2 = \frac{a}{2}\left(\frac{1}{\sqrt{3}}, -1\right),\ \boldsymbol{b}_3 = \frac{a}{\sqrt{3}}\,(-1,0)\,. \tag{2.1}$$

Type B sites are genarated by linear combinations of $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{b}_i$ with i=1, 2, 3.

The Brillouin zone is defined through the reciprocal lattice vectors, which are related to the basis vectors via the relation $\boldsymbol{a}_i \cdot \boldsymbol{R}_j = 2\pi\delta_{ij}$. The reciprocal lattice vectors are

$$\boldsymbol{R}_1 = \frac{4\pi}{\sqrt{3}a}\,(1,0)\,,\ \boldsymbol{R}_2 = \frac{2\pi}{\sqrt{3}a}\left(1, \sqrt{3}\right). \tag{2.2}$$

The Brillouin zone is a hexagon in the reciprocal space as depicted in the Figure 2.2.

The tight-binding Hamiltonian with only the nearest-neighbor hopping term is

$$H_{TB} = \alpha \sum_{\boldsymbol{A},j} (a^{\dagger}_{\boldsymbol{A}}\ b_{\boldsymbol{A}+\boldsymbol{b}_j} + b^{\dagger}_{\boldsymbol{A}+\boldsymbol{b}_j}\ a_{\boldsymbol{A}}). \tag{2.3}$$

α is the nearest-neighbor hopping energy, which is given by overlap integrals of π orbital electron wavefunctions. $a^{\dagger}_{\boldsymbol{A}}$ and $a_{\boldsymbol{A}}$ are creation and annihilation operators for electrons at site A. $b^{\dagger}_{\boldsymbol{A}+\boldsymbol{b}_j}$ and $b_{\boldsymbol{A}+\boldsymbol{b}_j}$ are creation and annihilation operators for electrons at site B. $\boldsymbol{A}$ designates the position of electrons in the A lattice, and the

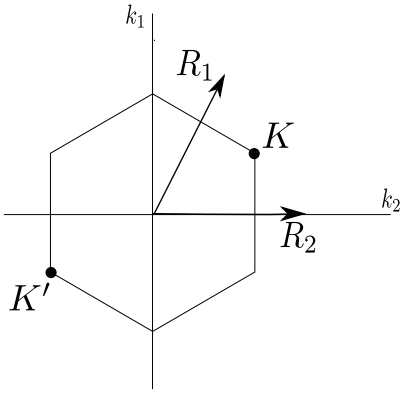

Figure 2.2: Brillouin zone 1 and degeneracy points.

position of electrons in the B lattice are given by $\boldsymbol{A}+\boldsymbol{b}_j$. The Fourier transformations of these operators are

$$a^\dagger_{\boldsymbol{A}} = \int_{BZ} \frac{d^2k}{(2\pi)^2} e^{-i\boldsymbol{k}\cdot\boldsymbol{A}} a^\dagger_{\boldsymbol{k}}, \quad b^\dagger_{\boldsymbol{A}+\boldsymbol{b}_j} = \int_{BZ} \frac{d^2k}{(2\pi)^2} e^{-i\boldsymbol{k}\cdot(\boldsymbol{A}+\boldsymbol{b}_j)} b^\dagger_{\boldsymbol{k}}. \tag{2.4}$$

Using these Fourier transformations, the tight-binding Hamiltonian in k-space becomes

$$\mathscr{H}_{TB} = \alpha \int_{BZ} \frac{d^2k}{(2\pi)^2} \begin{pmatrix} a^\dagger_{\boldsymbol{k}} & b^\dagger_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} 0 & \alpha\sum_j e^{i\boldsymbol{k}\cdot\boldsymbol{b}_j} \\ \alpha\sum_j e^{-i\boldsymbol{k}\cdot\boldsymbol{b}_j} & 0 \end{pmatrix} \begin{pmatrix} a_{\boldsymbol{k}} \\ b_{\boldsymbol{k}} \end{pmatrix}. \tag{2.5}$$

The energy eigenvalues are obtained as

$$E(k) = \pm\alpha^2 \left| e^{i\vec{k}\cdot\vec{b}_1} + e^{i\vec{k}\cdot\vec{b}_2} + e^{i\vec{k}\cdot\vec{b}_3} \right|. \tag{2.6}$$

The negative energy states corresponds to states in the valence band and the positive energy states correspond to states in the conduction band. Degenarcy points correspond to the roots of (2.6) where the conduction and valence bands meet. There are two inequivalent degenarcy points, named most commonly as K and K' points. The degenarcy points of graphene occur at corners of the Brillouin zone. These two inequivalent points can be chosen following [5] as

$$\boldsymbol{K} = \frac{2\pi}{\sqrt{3}a}\left(1, \frac{1}{\sqrt{3}}\right), \ \boldsymbol{K}' = -\boldsymbol{K}. \tag{2.7}$$

In Figure 2.2, the Brillouin zone and the degeneracy points are shown.

The continuum limit is where a, the distance between two atoms in the same lattice, goes to zero. In this limit, only states around the degeneracy points contribute to the dynamics. Hence, in the continuum limit, one is interested in the off-diagonal

componens of the Hamiltonian density for the K and K' valleys:

$$\begin{aligned}
\lim_{a\to 0} e^{i(\boldsymbol{k}+\boldsymbol{K})\cdot\boldsymbol{b}_j} &= \frac{\sqrt{3}a}{2}(ik_1-k_2)e^{i\frac{\pi}{3}},\ \lim_{a\to 0} e^{-i(\boldsymbol{k}+\boldsymbol{K})\cdot\boldsymbol{b}_j} = \frac{\sqrt{3}a}{2}(-ik_1-k_2)e^{-i\frac{\pi}{3}},\\
\lim_{a\to 0} e^{i(\boldsymbol{k}-\boldsymbol{K})\cdot\boldsymbol{b}_j} &= \frac{\sqrt{3}a}{2}(ik_1+k_2)e^{-i\frac{\pi}{3}},\ \lim_{a\to 0} e^{-i(\boldsymbol{k}-\boldsymbol{K})\cdot\boldsymbol{b}_j} = \frac{\sqrt{3}a}{2}(-ik_1+k_2)e^{i\frac{\pi}{3}}.
\end{aligned}$$

For the K valley, (2.5) becomes

$$\begin{aligned}
H_1^K &= \alpha\frac{\sqrt{3}a}{2}\int\frac{d^2k}{(2\pi)^2}\begin{pmatrix}a^\dagger_{\boldsymbol{k}-\boldsymbol{K}} & b^\dagger_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix}\begin{pmatrix}0 & (-ik_1-k_2)e^{i\frac{2\pi}{3}}\\ (ik_1-k_2)e^{-i\frac{2\pi}{3}} & 0\end{pmatrix}\begin{pmatrix}a_{\boldsymbol{k}-\boldsymbol{K}}\\ b_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix}\\
&= \alpha\frac{\sqrt{3}a}{2}\int\frac{d^2k}{(2\pi)^2}\begin{pmatrix}a^\dagger_{\boldsymbol{k}-\boldsymbol{K}} & b^\dagger_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix}e^{i\frac{\pi}{3}\sigma_3}\begin{pmatrix}0 & -ik_1-k_2\\ ik_1-k_2 & 0\end{pmatrix}e^{-i\frac{\pi}{3}\sigma_3}\begin{pmatrix}a_{\boldsymbol{k}-\boldsymbol{K}}\\ b_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix}\\
&\equiv \alpha\frac{\sqrt{3}a}{2}\frac{d^2k}{(2\pi)^2}\bar{\Psi}_1(-i\sigma_1k_1-i\sigma_2k_2)\Psi_1. \qquad \textbf{(2.8)}
\end{aligned}$$

Thus, the Dirac Hamiltonian density for the K valley is

$$H^K = v_F\gamma^\mu k_\mu, \qquad \textbf{(2.9)}$$

with the following definition of the spinor and its Dirac conjugate:

$$\Psi_1 = \sqrt{\frac{\sqrt{3}a\alpha}{2}}e^{-i\frac{\sigma_3\pi}{3}}\begin{pmatrix}a_{\boldsymbol{k}-\boldsymbol{K}}\\ b_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix},\ \bar{\Psi}_1 = \sqrt{\frac{\sqrt{3}a\alpha}{2}}\begin{pmatrix}a^\dagger_{\boldsymbol{k}-\boldsymbol{K}} & b^\dagger_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix}e^{i\frac{\sigma_3\pi}{3}}\gamma_0. \qquad \textbf{(2.10)}$$

The gamma matrices are chosen as $\gamma^\mu = (\sigma_3, i\sigma_1, i\sigma_2)$, with $\mu = 0,1,2$. They satisfy the Clifford algebra with the anti-commutation relation $\{\gamma^\mu,\gamma^\nu\} = 2g^{\mu\nu}$. The metric is Minkowski with signature $(+,-,-)$. Here $k_\mu = (0,-\boldsymbol{k})$, since in this derivation on-site interaction which would give rise to a mass is not included in the initial tight-binding Hamiltonian. v_F is the effective velocity with which electrons on graphene travel and is given in terms of α and a as $v_F = \alpha\frac{\sqrt{3}a}{2}$. For the K' valley, (2.5) becomes

$$\begin{aligned}
H_2^{K'} &= \alpha\frac{\sqrt{3}a}{2}\int\frac{d^2k}{(2\pi)^2}\begin{pmatrix}a^\dagger_{\boldsymbol{k}+\boldsymbol{K}} & b^\dagger_{\boldsymbol{k}+\boldsymbol{K}}\end{pmatrix}\begin{pmatrix}0 & (-ik_1+k_2)e^{-i\frac{2\pi}{3}}\\ (ik_1+k_2)e^{i\frac{2\pi}{3}} & 0\end{pmatrix}\begin{pmatrix}a_{\boldsymbol{k}+\boldsymbol{K}}\\ b_{\boldsymbol{k}+\boldsymbol{K}}\end{pmatrix}\\
&= \alpha\frac{\sqrt{3}a}{2}\int\frac{d^2k}{(2\pi)^2}\begin{pmatrix}a^\dagger_{\boldsymbol{k}-\boldsymbol{K}} & b^\dagger_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix}e^{-i\frac{\pi}{3}\sigma_3}\begin{pmatrix}0 & -ik_1-k_2\\ ik_1-k_2 & 0\end{pmatrix}e^{i\frac{\pi}{3}\sigma_3}\begin{pmatrix}a_{\boldsymbol{k}-\boldsymbol{K}}\\ b_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix}
\end{aligned}$$

It is observed that $\sigma_1e^{-i\frac{\pi}{3}\sigma_3}\sigma_1 = e^{i\frac{\pi}{3}\sigma_3}$.

$$\begin{aligned}
H_2^{K'} &= \alpha\frac{\sqrt{3}a}{2}\int\frac{d^2k}{(2\pi)^2}\begin{pmatrix}a^\dagger_{\boldsymbol{k}-\boldsymbol{K}} & b^\dagger_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix}\sigma_1e^{i\frac{\pi}{3}\sigma_3}\begin{pmatrix}0 & ik_1+k_2\\ -ik_1+k_2 & 0\end{pmatrix}e^{-i\frac{\pi}{3}\sigma_3}\sigma_1\begin{pmatrix}a_{\boldsymbol{k}-\boldsymbol{K}}\\ b_{\boldsymbol{k}-\boldsymbol{K}}\end{pmatrix}\\
&\equiv \alpha\frac{\sqrt{3}a}{2}\int\frac{d^2k}{(2\pi)^2}\bar{\Psi}_2(i\sigma_1k_1+i\sigma_2k_2)\Psi_2
\end{aligned}$$

Thus, the Dirac Hamiltonian density for the K' valley is

$$H^{K'} = -v_F\gamma^\mu k_\mu, \qquad \textbf{(2.11)}$$

with the following definition of the spinor and its Dirac conjugate:

$$\Psi_2 = \sqrt{\frac{\sqrt{3}a\alpha}{2}} e^{-i\frac{\sigma_3\pi}{3}} \sigma_1 \begin{pmatrix} a_{\boldsymbol{k}-\boldsymbol{K}'} \\ b_{\boldsymbol{k}-\boldsymbol{K}'} \end{pmatrix}, \; \bar{\Psi}_2 = \sqrt{\frac{\sqrt{3}a\alpha}{2}} \begin{pmatrix} a^\dagger_{\boldsymbol{k}-\boldsymbol{K}'} & b^\dagger_{\boldsymbol{k}-\boldsymbol{K}'} \end{pmatrix} \sigma_1 e^{i\frac{\sigma_3\pi}{3}} \gamma_0.$$

Hence, the Dirac-like Hamiltonian on graphene in the continuum limit takes the form

$$H = \int \frac{d^2k}{(2\pi)^2} [\bar{\Psi}_1 H^K \Psi_1 + \bar{\Psi}_2 H^{K'} \Psi_2]. \tag{2.12}$$

2.2 Derivation of Dirac Hamiltonian on graphene à la Novoselov et al

The basis vectors for A lattice are

$$\boldsymbol{a}_1 = \frac{a_l}{2}\left(3, \sqrt{3}\right), \;\; \boldsymbol{a}_2 = \frac{a_l}{2}\left(3, -\sqrt{3}\right)$$

Here a_l is distance between two carbon atoms in the hexagonal lattice, e.g. lattice spacing. For graphene, this lattice spacing is approximately 1.42 Å in literature. Type A sites are generated by linear combinations of $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$. The position of the three nearest neighbors of A, i.e. the type B atoms, are

$$\boldsymbol{b}_1 = \frac{a_l}{2}\left(1, \frac{1}{\sqrt{3}}\right), \; \boldsymbol{b}_2 = \frac{a_l}{2}\left(1, -\frac{1}{\sqrt{3}}\right), \; \boldsymbol{b}_3 = a_l(-1, 0). \tag{2.13}$$

The basis vectors are depicted in Figure 2.3. Type A sites are generated by linear

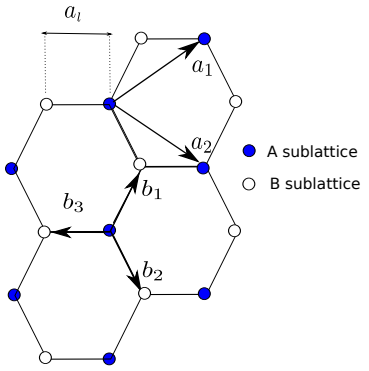

Figure 2.3: Honeycomb lattice 2.

combinations of the basis vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$. Type B sites are genarated by linear combinations of $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{b}_i$ with i=1,2,3. The extended Brillouin zone defined via the reciprocal lattice vectors

$$\boldsymbol{R}_1 = \frac{2\pi}{3a_l}\left(1, \sqrt{3}\right), \; \boldsymbol{R}_2 = \frac{2\pi}{3a_l}\left(1, -\sqrt{3}\right) \tag{2.14}$$

is a hexagon. The extended Brillouin zone is a rhombus. The degeneracy points reside at the corners of the hexagonal Brillouin zone, and can be chosen following [4] as

$$\boldsymbol{K} = \frac{2\pi}{\sqrt{3}a_l}\left(1, \frac{1}{\sqrt{3}}\right), \; \boldsymbol{K'} = \frac{2\pi}{\sqrt{3}a_l}\left(1, -\frac{1}{\sqrt{3}}\right). \tag{2.15}$$

The Brillouin zone and the degeneracy points are depicted in Figure 2.4.

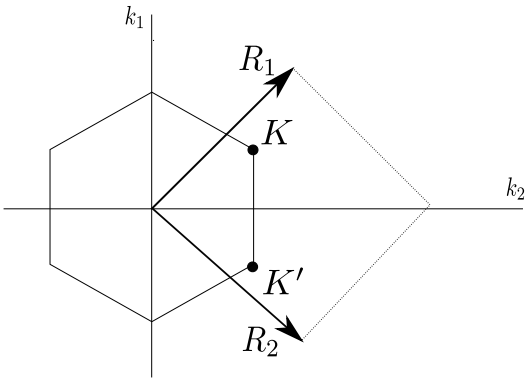

Figure 2.4: Brillouin zone 2 and degeneracy points.

The tight-binding Hamiltonian with the only the nearest-neighbor hopping term is

$$H_{TB} = -\alpha \sum_{\boldsymbol{A},j} (a^\dagger_{\boldsymbol{A}} \, b_{\boldsymbol{A}+\boldsymbol{b}_j} + b^\dagger_{\boldsymbol{A}+\boldsymbol{b}_j} \, a_{\boldsymbol{A}}). \tag{2.16}$$

α is the nearest-neighbor hopping energy. The k-space Hamiltonian is obtained through the Fourier transformations (2.4).

$$\mathscr{H}_{TB} = -\alpha \int_{BZ} \frac{d^2k}{(2\pi)^2} \begin{pmatrix} a^\dagger_{\boldsymbol{k}} & b^\dagger_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} 0 & \alpha \sum_j e^{i\boldsymbol{k}\cdot\boldsymbol{b}_j} \\ \alpha \sum_j e^{-i\boldsymbol{k}\cdot\boldsymbol{b}_j} & 0 \end{pmatrix} \begin{pmatrix} a_{\boldsymbol{k}} \\ b_{\boldsymbol{k}} \end{pmatrix}. \tag{2.17}$$

The off-diagonal componens of the Hamiltonian density for the K and K' valleys in the continuum limit yield

$$\begin{aligned} \lim_{a_l \to 0} e^{i(\boldsymbol{k}-\boldsymbol{K})\cdot\boldsymbol{b}_j} &= \frac{3a_l}{2}(k_1 - ik_2)e^{i\frac{\pi}{6}}, \; \lim_{a_l \to 0} e^{-i(\boldsymbol{k}-\boldsymbol{K})\cdot\boldsymbol{b}_j} = \frac{3a_l}{2}(k_1 + ik_2)e^{-i\frac{\pi}{6}}, \\ \lim_{a_l \to 0} e^{i(\boldsymbol{k}-\boldsymbol{K'})\cdot\boldsymbol{b}_j} &= \frac{3a_l}{2}(k_1 + ik_2)e^{i\frac{\pi}{6}}, \; \lim_{a_l \to 0} e^{-i(\boldsymbol{k}-\boldsymbol{K'})\cdot\boldsymbol{b}_j} = \frac{3a_l}{2}(k_1 - ik_2)e^{-i\frac{\pi}{6}}. \end{aligned}$$

For the K valley, (2.17) becomes

$$\begin{aligned} H_1^K &= \frac{3a_l\alpha}{2} \int \frac{d^2k}{(2\pi)^2} \begin{pmatrix} a^\dagger_{\boldsymbol{k}-\boldsymbol{K}} & b^\dagger_{\boldsymbol{k}-\boldsymbol{K}} \end{pmatrix} e^{i\frac{\pi}{12}\sigma_3} \begin{pmatrix} 0 & k_1 - ik_2 \\ k_1 + ik_2 & 0 \end{pmatrix} e^{-i\frac{\pi}{12}\sigma_3} \begin{pmatrix} a_{\boldsymbol{k}-\boldsymbol{K}} \\ b_{\boldsymbol{k}-\boldsymbol{K}} \end{pmatrix}, \\ &\equiv \frac{3a_l\alpha}{2} \int \frac{d^2k}{(2\pi)^2} \Psi^\dagger_{\boldsymbol{k}-\boldsymbol{K}} (\sigma_1 k_1 + \sigma_2 k_2) \Psi_{\boldsymbol{k}-\boldsymbol{K}}. \end{aligned}$$

Then, the Dirac-like Hamiltonian density for the K valley is

$$H_{\boldsymbol{k}-\boldsymbol{K}} = v_F(\sigma_1 k_1 + \sigma_2 k_2) \tag{2.18}$$

with $v_F = \frac{3a_l\alpha}{2}$ and the spinor

$$\Psi_{\boldsymbol{k}-\boldsymbol{K}} = e^{-i\frac{\pi}{12}\sigma_3}\begin{pmatrix} a_{\boldsymbol{k}-\boldsymbol{K}} \\ b_{\boldsymbol{k}-\boldsymbol{K}} \end{pmatrix}.$$

For the K' valley, (2.17) becomes

$$\begin{aligned} H_2^{K'} &= \frac{3a_l\alpha}{2}\int \frac{d^2k}{(2\pi)^2}\begin{pmatrix} a^\dagger_{\boldsymbol{k}-\boldsymbol{K}'} & b^\dagger_{\boldsymbol{k}-\boldsymbol{K}'} \end{pmatrix} e^{-i\frac{\pi}{12}\sigma_3}\begin{pmatrix} 0 & k_1+ik_2 \\ k_1-ik_2 & 0 \end{pmatrix} e^{i\frac{\pi}{12}\sigma_3}\begin{pmatrix} a_{\boldsymbol{k}-\boldsymbol{K}'} \\ b_{\boldsymbol{k}-\boldsymbol{K}'} \end{pmatrix}, \\ &\equiv \frac{3a_l\alpha}{2}\int \frac{d^2k}{(2\pi)^2}\Psi^\dagger_{\boldsymbol{k}-\boldsymbol{K}'}(\sigma_1k_1-\sigma_2k_2)\Psi_{\boldsymbol{k}-\boldsymbol{K}'}. \end{aligned}$$

Then, the Dirac-like Hamiltonian density for the K' valley is

$$H_{\boldsymbol{k}-\boldsymbol{K}'} = v_F(\sigma_1k_1-\sigma_2k_2) \tag{2.19}$$

with $v_F = \frac{3a_l\alpha}{2}$ and the spinor

$$\Psi_{\boldsymbol{k}-\boldsymbol{K}'} = e^{i\frac{\pi}{12}\sigma_3}\begin{pmatrix} a_{\boldsymbol{k}-\boldsymbol{K}'} \\ b_{\boldsymbol{k}-\boldsymbol{K}'} \end{pmatrix}.$$

v_F is the Fermi velocity which is estimated to be on the order $10^6 m/s$. The interesting feature about this Fermi velocity is that it is a constant like the velocity of light, it does not depend on momentum or energy. It is given in terms of the lattice spacing and the nearest-neighbor hopping parameter. As a result, the effective Hamiltonian on graphene takes the form

$$H = \int \frac{d^2k}{(2\pi)^2}[\Psi^\dagger_{\boldsymbol{k}-\boldsymbol{K}}H_{\boldsymbol{k}-\boldsymbol{K}}\Psi_{\boldsymbol{k}-\boldsymbol{K}} + \Psi^\dagger_{\boldsymbol{k}-\boldsymbol{K}'}H_{\boldsymbol{k}-\boldsymbol{K}'}\Psi_{\boldsymbol{k}-\boldsymbol{K}'}]. \tag{2.20}$$

2.3 Derivation of Dirac Hamiltonian on graphene à la Gusynin et al

The basis vectors for A lattice are chosen as [7]

$$\boldsymbol{a}_1 = \frac{a}{2}\left(1,\sqrt{3}\right),\ \boldsymbol{a}_2 = \frac{a}{2}\left(1,-\sqrt{3}\right).$$

Here a is distance between two carbon atoms in the same lattice. It is $\sqrt{3}$ times the lattice spacing, a_l. Type A sites are generated by linear combinations of $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$. The position of the three nearest neighbors of A, i.e. the type B atoms, are

$$\boldsymbol{b}_1 = a\left(0,\frac{1}{\sqrt{3}}\right),\ \boldsymbol{b}_2 = -\frac{a}{2}\left(-1,\frac{1}{\sqrt{3}}\right),\ \boldsymbol{b}_3 = -\frac{a}{2}\left(1,\frac{1}{\sqrt{3}}\right). \tag{2.21}$$

Type B sites are genarated by linear combinations of $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{b}_i$ with i=1, 2, 3. The basis vectors are depicted in the Figure 2.5.

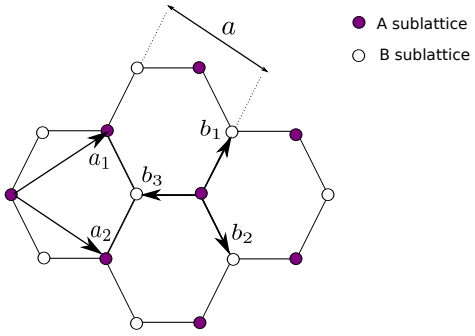

Figure 2.5: Honeycomb lattice 3.

The extended Brillouin zone defined via the reciprocal lattice vectors

$$\boldsymbol{R}_1 = \frac{2\pi}{a}\left(1, \frac{1}{\sqrt{3}}\right), \; \boldsymbol{R}_2 = \frac{2\pi}{a}\left(1, -\frac{1}{\sqrt{3}}\right) \tag{2.22}$$

is a rhombus. The Brillouin zone is a hexagon.

The degeneracy points reside at the corners of the hexagonal Brillouin zone, and can be chosen following [7] as

$$\boldsymbol{K} = \frac{4\pi}{3a}(1,0), \; \boldsymbol{K'} = -\frac{4\pi}{3a}(1,0). \tag{2.23}$$

The Brillouin zone and the choice of degeneracy points are depicted in the Figure 2.6. The tight-binding Hamiltonian in momentum space is

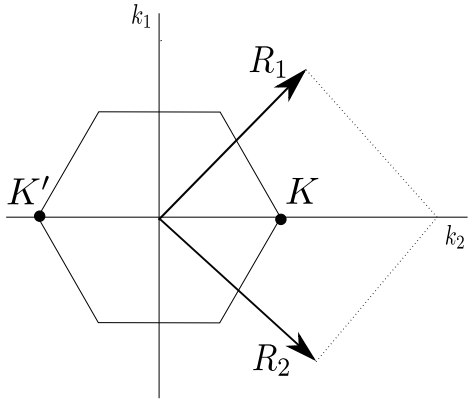

Figure 2.6: Brillouin zone 3 and degeneracy points.

$$\mathscr{H}_{TB} = -t\int_{BZ}\frac{d^2k}{(2\pi)^2}\begin{pmatrix} a_{\boldsymbol{k}}^\dagger & b_{\boldsymbol{k}}^\dagger \end{pmatrix}\begin{pmatrix} 0 & \sum_j e^{i\boldsymbol{k}\cdot\boldsymbol{b}_j} \\ \sum_j e^{-i\boldsymbol{k}\cdot\boldsymbol{b}_j} & 0 \end{pmatrix}\begin{pmatrix} a_{\boldsymbol{k}} \\ b_{\boldsymbol{k}} \end{pmatrix}. \tag{2.24}$$

where the nearest-neigbor hopping parameter t comes with a minus sign. The off-diagonal componens of the Hamiltonian density for the K and K' valleys yield

in the continuum limit

$$\begin{aligned}
\lim_{a\to 0} e^{i(\boldsymbol{k}+\boldsymbol{K})\cdot\boldsymbol{b}_j} &= \frac{a\sqrt{3}}{2}(-k_1+ik_2),\ \lim_{a\to 0} e^{-i(\boldsymbol{k}+\boldsymbol{K})\cdot\boldsymbol{b}_j} = \frac{a\sqrt{3}}{2}(-k_1-ik_2),\\
\lim_{a\to 0} e^{i(\boldsymbol{k}+\boldsymbol{K'})\cdot\boldsymbol{b}_j} &= \frac{a\sqrt{3}}{2}(k_1+ik_2),\ \lim_{a\to 0} e^{-i(\boldsymbol{k}+\boldsymbol{K'})\cdot\boldsymbol{b}_j} = \frac{a\sqrt{3}}{2}(k_1-ik_2).
\end{aligned}$$

For the K valley, (2.24) becomes

$$\begin{aligned}
H_{k+K} &= \frac{at\sqrt{3}}{2}\int \frac{d^2k}{(2\pi)^2}\begin{pmatrix} a^\dagger_{\boldsymbol{k}+\boldsymbol{K}} & b^\dagger_{\boldsymbol{k}+\boldsymbol{K}}\end{pmatrix}\begin{pmatrix} 0 & k_1-ik_2\\ k_1+ik_2 & 0\end{pmatrix}\begin{pmatrix} a_{\boldsymbol{k}+\boldsymbol{K}}\\ b_{\boldsymbol{k}+\boldsymbol{K}}\end{pmatrix},\\
&\equiv \frac{at\sqrt{3}}{2}\int \frac{d^2k}{(2\pi)^2}\Psi^\dagger_{\boldsymbol{k}+\boldsymbol{K}}(\sigma_1k_1+\sigma_2k_2)\Psi_{\boldsymbol{k}+\boldsymbol{K}}.
\end{aligned}$$

Then, the Dirac-like Hamiltonian density for the K valley is

$$H_{\boldsymbol{k}+\boldsymbol{K}} = v_F(\sigma_1k_1+\sigma_2k_2) \tag{2.25}$$

with $v_F = \frac{at\sqrt{3}}{2}$ and the spinor

$$\Psi_{\boldsymbol{k}+\boldsymbol{K}} = \begin{pmatrix} a_{\boldsymbol{k}+\boldsymbol{K}}\\ b_{\boldsymbol{k}+\boldsymbol{K}}\end{pmatrix}.$$

For the K' valley, (2.24) becomes

$$\begin{aligned}
H_{k+K'} &= \frac{at\sqrt{3}}{2}\int \frac{d^2k}{(2\pi)^2}\begin{pmatrix} a^\dagger_{\boldsymbol{k}+\boldsymbol{K'}} & b^\dagger_{\boldsymbol{k}+\boldsymbol{K'}}\end{pmatrix}\begin{pmatrix} 0 & -k_1-ik_2\\ -k_1+ik_2 & 0\end{pmatrix}\begin{pmatrix} a_{\boldsymbol{k}+\boldsymbol{K'}}\\ b_{\boldsymbol{k}-\boldsymbol{K'}}\end{pmatrix},\\
&\equiv \frac{at\sqrt{3}}{2}\int \frac{d^2k}{(2\pi)^2}\Psi^\dagger_{\boldsymbol{k}+\boldsymbol{K'}}(-\sigma_1k_1+\sigma_2k_2)\Psi_{\boldsymbol{k}+\boldsymbol{K'}}.
\end{aligned}$$

Then, the Dirac-like Hamiltonian density for the K' valley is

$$H_{\boldsymbol{k}+\boldsymbol{K'}} = v_F(-\sigma_1k_1+\sigma_2k_2), \tag{2.26}$$

with $v_F = \frac{at\sqrt{3}}{2}$ and the spinor

$$\Psi_{\boldsymbol{k}+\boldsymbol{K'}} = \begin{pmatrix} a_{\boldsymbol{k}+\boldsymbol{K'}}\\ b_{\boldsymbol{k}+\boldsymbol{K'}}\end{pmatrix}.$$

As a result, the effective Hamiltonian on graphene takes the form

$$H = \int \frac{d^2k}{(2\pi)^2}[\Psi^\dagger_{\boldsymbol{k}+\boldsymbol{K}}H_{\boldsymbol{k}+\boldsymbol{K}}\Psi_{\boldsymbol{k}+\boldsymbol{K}} + \Psi^\dagger_{\boldsymbol{k}+\boldsymbol{K'}}H_{\boldsymbol{k}+\boldsymbol{K'}}\Psi_{\boldsymbol{k}+\boldsymbol{K'}}]. \tag{2.27}$$

Investigating the Hamiltonian densities (2.25) and (2.26), one can observe that they can elegantly be treated in one Hamiltonian density in the form

$$H_G = v_F(\sigma_1\otimes\tau_3k_1+\sigma_2\otimes\mathbf{1}_\tau k_2), \tag{2.28}$$

incorporating all degrees of freedom discussed in this section. The Pauli matrices σ_i describe the two sublattices A and B and $\tau_3 = diag(1,-1)$ describes the K and K' valleys. Then, the corresponding Hamiltonian is

$$H \equiv \int \frac{d^2k}{(2\pi)^2} \Psi_G^\dagger H_G \Psi_G, \tag{2.29}$$

with four-component spinors $\Psi_G^\dagger = \left(a^\dagger_{\boldsymbol{k}+\boldsymbol{K}} \quad b^\dagger_{\boldsymbol{k}+\boldsymbol{K}} \quad a^\dagger_{\boldsymbol{k}+\boldsymbol{K}'} \quad b^\dagger_{\boldsymbol{k}+\boldsymbol{K}'}\right)$.

There are numerous articles on graphene, where the derivation of the Dirac-like Hamiltonian is presented. In this section, three of the most prominent ones were presented. The point is that the choice of unit cell basis vectors determines the position of Dirac points in the k-space and therefore affects the representation of Dirac matrices. Semenoff's derivation was originally done to comment on the parity anomaly in $2+1$ quantum field theory, therefore it is relativistic. The derivation of Novoselov et al was discussed in this section to present another perspective and because of the fact that the discussion of electronic properties of graphene usually is based on this derivation. The result of the derivation of Gusynin et al enables one to smoothly relate to Kane-Mele model on graphene, which will be broadly investigated in the rest of the thesis.

2.4 Foldy-Wouthuysen transformation and Berry gauge fields

In this section, the Foldy-Wouthuysen transformation of the Dirac Hamiltonian and Berry gauge field in terms of Foldy-Wouthuysen transformation will be presented. Relativistic electrons of charge $e > 0$ with a characteristic velocity like the velocity of light c or the effective velocity v_F as in graphene will be considered. To retain the formulation general, $\hbar = c = v_F = 1$, as well as $e = 1$. The constants will be recuperated when needed. The free, massive electrons are described by the Dirac Hamiltonian

$$H = \boldsymbol{\alpha} \cdot \boldsymbol{k} + \beta m. \tag{2.30}$$

In this section vectors are d-dimensional, like the momentum $\boldsymbol{k}$ whose components are denoted k_I; $I = 1, \cdots, d$. The Hamiltonian (2.30) can be diagonalized as

$$UHU^\dagger = E\beta, \tag{2.31}$$

where E is the total energy

$$E = \sqrt{k^2 + m^2}, \tag{2.32}$$

and U is the unitary Foldy-Wouthuysen transformation

$$U = \frac{\beta H + E}{\sqrt{2E(E+m)}}.$$

Through the transformation U a pure gauge field can be introduced as

$$\mathscr{A}^U = iU(\boldsymbol{k})\frac{\partial U^\dagger(\boldsymbol{k})}{\partial \boldsymbol{k}}. \tag{2.33}$$

Pure gauge field is a gauge field whose curvature vanishes. The Berry gauge field $\mathscr{A}$ is obtained by projecting (2.33) onto the positive energy eigenstates of the Dirac Hamiltonian (2.30). One can be convinced that eliminating the negative energy states is equivalent to the adiabatic approximation by revoking its similarity to suppression of the interband interactions in molecular problems [42]. Thus, we define the Berry gauge field as

$$\boldsymbol{A} \equiv P\mathscr{A}^U P, \tag{2.34}$$

where P is the projection operator onto the positive energy subspace. This definition of the Berry gauge field is valid irrespective of the dimensions of the Hamiltonian (2.30). In order to derive $\boldsymbol{A}$ explicitly let us adopt the following $2^N \times 2^N$; $N = [\frac{d}{2}]$, dimensional realizations of $\boldsymbol{\alpha}$ and β

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\rho} \\ \boldsymbol{\rho}^\dagger & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.35}$$

Here $\boldsymbol{\rho}$ and the unit matrix 1 are $2^{N-1} \times 2^{N-1}$ dimensional. In the representation (2.35) the gauge field (2.33) becomes

$$\mathscr{A}_I^U = \frac{i}{2E^2(E+m)}\left[E(E+m)\alpha_I\beta + \beta\boldsymbol{\alpha}\cdot\boldsymbol{k}k_I - iE\sigma_{IJ}k_J\right], \tag{2.36}$$

where $\sigma_{IJ} \equiv -\frac{i}{2}[\alpha_I, \alpha_J]$. Therefore, the Berry gauge field (2.34) results to be

$$A_I = -\frac{i}{4E(E+m)}(\rho_I\rho_J^\dagger - \rho_J\rho_I^\dagger)k_J. \tag{2.37}$$

Although the field strength of (2.36) vanishes because of being a pure gauge field, the Berry curvature

$$G_{IJ} = \frac{\partial A_J}{\partial k_I} - \frac{\partial A_I}{\partial k_J} - i[A_I, A_J], \tag{2.38}$$

is non-vanishing in general.

When in $2n+1$ dimensional space-time where $n = 1, 2\cdots$, the Berry curvature (2.38) can be employed to define the Chern number which is the integrated Chern character, as [43]

$$N_n = \frac{1}{(4\pi)^n n!}\int_{\mathscr{M}_{2n}} d^{2n}k\ \varepsilon_{I_1I_2\cdots I_{2n}}\mathrm{tr}\left\{G_{I_1I_2}\cdots G_{I_{2n-1}I_{2n}}\right\}. \tag{2.39}$$

For $2+1$ dimensional systems the Berry gauge field is Abelian, so that $G_{ab} = \partial A_b/\partial k_a - \partial A_a/\partial k_b$, where $a,b = 1,2$, and the first Chern number is

$$N_1 = \frac{1}{4\pi}\int d^2k\varepsilon_{ab}\mathrm{tr}G_{ab}. \tag{2.40}$$

In $4+1$ dimensions one introduces the second Chern number as

$$N_2 = \frac{1}{32\pi^2}\int d^4k\varepsilon_{ijkl}\mathrm{tr}\{G_{ij}G_{kl}\}, \tag{2.41}$$

where $i,j,k,l = 1,2,3,4$.

3. RELATION BETWEEN THE SPIN HALL CONDUCTIVITY AND THE SPIN CHERN NUMBER FOR DIRAC-LIKE SYSTEMS

In ferromagnets, in response to the electric field a spontaneous Hall current can be generated. A semiclassical formulation of this anomalous Hall effect was given in [16] within the Fermi liquid theory. There, the anomalous Hall conductivity was calculated considering the equations of motion in the presence of the Berry gauge fields derived from the Bloch wave function. When this system is subjected to an external magnetic field, the definition of the particle density and the electric current should be made appropriately. Nevertheless, the computed value of the anomalous Hall conductivity remains unaltered [17, 44, 45]. Hall currents without a magnetic field can be generated also in fermionic systems described by Dirac-like Hamiltonians [9]. Taking into account the spin of electrons, these systems yield Hall currents due to the spin transport which is known as the spin Hall effect [8] or Chern insulator. We would like to present a semiclassical formulation of the spin Hall conductivity using a differential form formalism for fermions which are described by Dirac-like Hamiltonians.

In semiclassical kinetic theory, the spin degrees of freedom can be considered by treating them as dynamical variables. However to calculate the spin Hall conductivities it would be more appropriate to keep the Hamiltonian and the related Berry gauge fields as matrices in “spin indices". In this respect a differential form formalism was presented in [24]. Dynamical variables in this semiclasical formalism are the usual space coordinates and momenta but the symplectic form is matrix valued. We will show that this formalism is suitable to calculate the spin Hall conductivity for Dirac-like systems. We deal with electrons, so that without loss of generality we consider the third component of spin denoted by S_z, whose explicit form depends on the details of the underlying Dirac-like Hamiltonian. When the third component of spin is conserved at the quantum level, constructing the spin current is straightforward. However, spin Hall effect can persist even if the third component of spin is not conserved. In the latter case semiclassical definition of the spin Hall conductivity is not very clear. Within the Kane-Mele model of graphene ($2+1$ dimensional topological

insulator) [8] it was argued that one cannot anymore use the Berry curvature to obtain the main contribution to the spin Hall effect when the spin nonconserving Rashba term is present [46]. We will show that even for the systems where the spin is not a good quantum number, it is always possible to establish the leading contribution to the spin Hall effect in terms of the Berry field strength derived in the appropriate basis. Moreover, we will demonstrate that it is always given in terms of the spin Chern number which is defined to be one half the difference of the Chern numbers of spin-up and spin-down sectors [20]. A similar claim was made in [47] by employing the Green function within the Kubo formalism.

The formulation will be illustrated within the Kane-Mele model of graphene: When only the intrinsic spin-orbit coupling is present, the third component of the spin is a good quantum number and the spin Hall conductivity can be acquired straightforwardly in terms of the Berry curvature [34]. When the Rashba term is switched on, the third component of spin ceases to be conserved. Nevertheless, we will show that by choosing the correct basis one can still establish the leading contribution to the spin Hall conductivity by the Berry curvature. It is given by the spin Chern number calculated in [48].

The starting point of the method is the matrix valued symplectic form [15, 24]. We will show that it can be obtained in terms of the wave packets formed by the positive energy solutions of Dirac-like equations adapting the formalism of [21, 22]. The formalism of deriving the velocities of phase space variables in terms of the phase space variables themselves will be presented in Section 3.2. It leads to the anomalous Hall effect straightforwardly as we will discuss briefly in Section 3.3. Definition of the spin current is presented in Section 3.4. It is shown that if one adopts the correct definition of the spin current in two space dimensions the essential part of the spin Hall conductivity is always given by the spin Chern number. We will illustrate the method by applying it to the Kane-Mele model first in the absence and then in the presence of Rashba coupling.

3.1 Wave-packet dynamics

Dirac equation possesses negative and positive energy solutions. Obviously one can form a wave packet by superposing only positive energy solutions. However, relativistic invariance of the Dirac theory demands to superpose both positive and negative solutions. Nevertheless by ignoring the relativistic momenta one can deal with only a wave packet composed of positive energy solutions. Indeed this is the starting point of the semiclassical approximation. We denote the spinor corresponding to a positive energy solution of Dirac equation by $u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)$, which is a function of the momentum $\boldsymbol{p}$, and the position of the wave packet center in coordinate space $\boldsymbol{x}_c$:

$$H_0(\boldsymbol{p})u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c) = E_\alpha u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c);\ E_\alpha > 0.$$

The normalization is

$$u^{\dagger(\alpha)}(\boldsymbol{p},x_c)u^{(\beta)}(\boldsymbol{p},x_c) = \delta_{\alpha\beta}. \tag{3.1}$$

Let us consider the following wave packet obtained by superposing only positive energy solutions labeled by the superscript α,

$$\Psi_{\boldsymbol{x}} \equiv \Psi_{\boldsymbol{x}}(\boldsymbol{p}_c,\boldsymbol{x}_c) = \int [dp]|a(\boldsymbol{p},t)|e^{-i\gamma(\boldsymbol{p},t)}\sum_\alpha \xi_\alpha \psi_{\boldsymbol{x}}^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c), \tag{3.2}$$

where $[dp]$ denotes the measure of the d dimensional momentum space. The distribution $|a(\boldsymbol{p},t)|e^{-i\gamma(\boldsymbol{p},t)}$ has a peak at the wave packet center $\boldsymbol{p}_c$ and satisfies $\int |a|^2[dp] = 1$. The expansion coefficients ξ_α are also normalized, $\sum_\alpha |\xi_\alpha|^2 = 1$. $\psi_{\boldsymbol{x}}^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)$ is composed of two parts

$$\psi_{\boldsymbol{x}}^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c) = u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)\phi_{\boldsymbol{x}}(\boldsymbol{p}), \tag{3.3}$$

with

$$\phi_{\boldsymbol{x}}(\boldsymbol{p}) = \frac{1}{(2\pi)^{d/2}}e^{-i\boldsymbol{p}\cdot\boldsymbol{x}}.$$

The normalization is

$$\int [dp]\phi_{\boldsymbol{x}}^\star(\boldsymbol{p})\phi_{\boldsymbol{y}}(\boldsymbol{p}) = \delta(\boldsymbol{x}-\boldsymbol{y}).$$

When the position operator, $\hat{\boldsymbol{x}}$ acts on $\phi_{\boldsymbol{x}}(\boldsymbol{p})$ we get

$$\hat{\boldsymbol{x}}\phi_{\boldsymbol{x}}(\boldsymbol{p}) = i\frac{\partial}{\partial \boldsymbol{p}}\phi_{\boldsymbol{x}}(\boldsymbol{p}) = \boldsymbol{x}\phi_{\boldsymbol{x}}(\boldsymbol{p}).$$

and the completeness relation is $\int [dx]\phi^{\star}_{\boldsymbol{x}}(\boldsymbol{p})\phi_{\boldsymbol{x}}(\boldsymbol{q}) = \delta(\boldsymbol{p}-\boldsymbol{q})$. As a result of these definitions, (3.3) has the following normalization

$$\int [dx]\psi^{\dagger(\alpha)}_{\boldsymbol{x}}(\boldsymbol{p},\boldsymbol{x}_c)\psi^{(\beta)}_{\boldsymbol{x}}(\boldsymbol{q},\boldsymbol{x}_c) = \delta_{\alpha\beta}\delta(\boldsymbol{p}-\boldsymbol{q}). \tag{3.4}$$

We would like to calculate the expectation value of the position operator over the wave packet (3.2). The calculation proceeds as follows; we first calculate $\hat{x}\Psi_{\boldsymbol{x}}$, in which we use

$$\hat{\boldsymbol{x}}\psi^{(\alpha)}_{\boldsymbol{x}} = u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)\hat{\boldsymbol{x}}\phi_{\boldsymbol{x}}(\boldsymbol{p}) = u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)\boldsymbol{x}\phi_{\boldsymbol{x}}(\boldsymbol{p}) = u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)(i\frac{\partial}{\partial \boldsymbol{p}})\phi_{\boldsymbol{x}}(\boldsymbol{p}).$$

Integrating by parts, we obtain

$$\begin{aligned}
\hat{\boldsymbol{x}}\Psi_{\boldsymbol{x}} &= -i\int [dp]\frac{\partial |a(\boldsymbol{p},t)|}{\partial \boldsymbol{p}}e^{-i\gamma(\boldsymbol{p},t)}\sum_{\alpha}\xi_{\alpha}u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)\phi_{\boldsymbol{x}}(\boldsymbol{p}) \\
&- \int [dp]|a(\boldsymbol{p},t)|\frac{\partial \gamma(\boldsymbol{p},t)}{\partial \boldsymbol{p}}e^{-i\gamma(\boldsymbol{p},t)}\sum_{\alpha}\xi_{\alpha}u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)\phi_{\boldsymbol{x}}(\boldsymbol{p}) \\
&- i\int [dp]|a(\boldsymbol{p},t)|e^{-i\gamma(\boldsymbol{p},t)}\sum_{\alpha}\xi_{\alpha}\frac{\partial u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)}{\partial \boldsymbol{p}}\phi_{\boldsymbol{x}}(\boldsymbol{p}).
\end{aligned}$$

Then we reach the following result

$$\begin{aligned}
\int [dx]\Psi^{\dagger}_{\boldsymbol{x}}\hat{x}\Psi_{\boldsymbol{x}} &= -i\int [dp]|a(\boldsymbol{p},t)|\frac{\partial |a(\boldsymbol{p},t)|}{\partial \boldsymbol{p}} \\
&- \int [dp]|a(\boldsymbol{p},t)|^2\frac{\partial \gamma(\boldsymbol{p},t)}{\partial \boldsymbol{p}} - i\int [dp]|a(\boldsymbol{p},t)|^2\sum_{\alpha,\beta}\xi^{*}_{\beta}u^{\dagger(\beta)}(\boldsymbol{p},\boldsymbol{x}_c)\frac{\partial u^{(\alpha)}(\boldsymbol{p},\boldsymbol{x}_c)}{\partial \boldsymbol{p}}\xi_{\alpha}.
\end{aligned} \tag{3.5}$$

The first term vanishes since $\int |a|^2[dp] = 1$. The second and the third terms are obtained using (3.4). The distribution has the mean momentum, $\boldsymbol{p}_c$ defined through

$$\boldsymbol{p}_c = \int [dp]\boldsymbol{p}|a(\boldsymbol{p},t)|^2.$$

Thus, for any function $f(\boldsymbol{p})$, we get

$$f(\boldsymbol{p}_c) = \int [dp]f(\boldsymbol{p})|a(\boldsymbol{p},t)|^2. \tag{3.6}$$

Using the definition (3.6) in (3.5), and observing that the expectation value of the position operator over the wave packet (3.2) is $\boldsymbol{x}_c$, which is the center of the wave packet in coordinate space, $\boldsymbol{x}_c = \int [dx]\Psi^{\dagger}_{\boldsymbol{x}}\hat{x}\Psi_{\boldsymbol{x}}$, we obtain

$$\boldsymbol{x_c} = -\frac{\partial \gamma_c}{\partial \boldsymbol{p}_c} - i\sum_{\alpha,\beta}\xi^{*}_{\beta}u^{\dagger(\beta)}(\boldsymbol{p}_c,\boldsymbol{x}_c)\frac{\partial}{\partial \boldsymbol{p}_c}u^{(\alpha)}(\boldsymbol{p}_c,\boldsymbol{x}_c)\xi_{\alpha}. \tag{3.7}$$

We define $\gamma_c \equiv \gamma(\boldsymbol{p}_c, t)$. We would like to define the one-form η through $d\mathscr{S}$,

$$d\mathscr{S} = \int [dx] \Psi^\dagger_{\boldsymbol{x}} (id - H_0 dt) \Psi_{\boldsymbol{x}} = d\gamma_c + \sum_{\alpha\beta} \xi^*_\alpha \eta^{\alpha\beta} \xi_\beta .$$

We start by computing

$$\begin{aligned} d\Psi_{\boldsymbol{x}} &= dt \frac{\partial \Psi_{\boldsymbol{x}}}{\partial t} + d\boldsymbol{x}_c \frac{\partial \Psi_{\boldsymbol{x}}}{\partial \boldsymbol{x}_c} \\ &= dt \int [dp] \frac{\partial}{\partial t} |a(\boldsymbol{p},t)| e^{-i\gamma(\boldsymbol{p},t)} \sum_\alpha \xi_\alpha u^{(\alpha)}(\boldsymbol{p}, \boldsymbol{x}_c) \phi_{\boldsymbol{x}}(\boldsymbol{p}) \\ &- idt \int [dp] |a(\boldsymbol{p},t)| \frac{\partial \gamma(\boldsymbol{p},t)}{\partial t} e^{-i\gamma(\boldsymbol{p},t)} \sum_\alpha \xi_\alpha u^{(\alpha)}(\boldsymbol{p}, \boldsymbol{x}_c) \phi_{\boldsymbol{x}}(\boldsymbol{p}) \\ &+ d\boldsymbol{x}_c \int [dp] |a(\boldsymbol{p},t)| e^{-i\gamma(\boldsymbol{p},t)} \sum_\alpha \xi_\alpha \frac{\partial}{\partial \boldsymbol{x}_c} u^{(\alpha)}(\boldsymbol{p}, \boldsymbol{x}_c) \phi_{\boldsymbol{x}}(\boldsymbol{p}). \end{aligned}$$

So that we obtain

$$\int [dx] \Psi^\dagger_{\boldsymbol{x}} i d\Psi_{\boldsymbol{x}} = dt \frac{\partial \gamma_c}{\partial t} + id\boldsymbol{x}_c \sum_{\alpha\beta} \xi^*_\beta u^{\dagger(\beta)}(\boldsymbol{p}_c, \boldsymbol{x}_c) \frac{\partial}{\partial \boldsymbol{x}_c} u^{(\alpha)}(\boldsymbol{p}_c, \boldsymbol{x}_c) \xi_\alpha .$$

To transform the first term, we use $d\gamma_c = dt \frac{\partial \gamma_c}{\partial t} + d\boldsymbol{p}_c \frac{\partial \gamma_c}{\partial \boldsymbol{p}_c}$ and (3.7). Then

$$\int [dx] \Psi^\dagger_{\boldsymbol{x}} i d\Psi_{\boldsymbol{x}} = d\gamma_c + d\boldsymbol{p}_c \cdot \boldsymbol{x}_c + id\boldsymbol{p}_c \sum_{\alpha\beta} \xi^*_\beta u^{\dagger(\beta)} \frac{\partial}{\partial \boldsymbol{p}_c} u^{(\alpha)} \xi_\alpha + id\boldsymbol{x}_c \sum_{\alpha\beta} \xi^*_\beta u^{\dagger(\beta)} \frac{\partial}{\partial \boldsymbol{x}_c} u^{(\alpha)} \xi_\alpha$$

This is a convenient point to define the following matrix valued Berry gauge fields

$$iu^{\dagger(\alpha)}(\boldsymbol{p}_c, \boldsymbol{x}_c) \frac{\partial}{\partial \boldsymbol{x}_c} u^{(\beta)}(\boldsymbol{p}_c, \boldsymbol{x}_c) = \boldsymbol{a}^{\alpha\beta}, \tag{3.8}$$

$$iu^{\dagger(\alpha)}(\boldsymbol{p}_c, \boldsymbol{x}_c) \frac{\partial}{\partial \boldsymbol{p}_c} u^{(\beta)}(\boldsymbol{p}_c, \boldsymbol{x}_c) = \boldsymbol{A}^{\alpha\beta}. \tag{3.9}$$

The Dirac-like free Hamiltonian only depends on the derivatives with respect to $\boldsymbol{x}$, so that we get

$$\int [dx] \Psi^\dagger_{\boldsymbol{x}} H_0(\frac{\partial}{\partial \boldsymbol{x}}) \Psi_{\boldsymbol{x}} = \sum_{\alpha\beta} \xi^*_\alpha E_\alpha(\boldsymbol{p}_c) \delta^{\alpha\beta} \xi_\beta .$$

Thus, by defining $H_0^{\alpha\beta} = E_\alpha \delta^{\alpha\beta}$, we obtain

$$d\mathscr{S} = \int [dx] \Psi^\dagger_{\boldsymbol{x}} (id - H_0 dt) \Psi_{\boldsymbol{x}} = d\gamma_c + \sum_{\alpha\beta} \xi^*_\alpha \Big(d\boldsymbol{p}_c \cdot \boldsymbol{x}_c \delta^{\alpha\beta} + d\boldsymbol{x}_c \boldsymbol{a}^{\alpha\beta} + d\boldsymbol{p}_c \boldsymbol{A}^{\alpha\beta} - H_0^{\alpha\beta} dt \Big) \xi_\beta .$$

Then we can define the matrix valued one-form $\eta^{\alpha\beta}$ as,

$$\eta^{\alpha\beta} = \delta^{\alpha\beta} \boldsymbol{x}_c \cdot d\boldsymbol{p}_c + \boldsymbol{a}^{\alpha\beta} \cdot d\boldsymbol{x}_c + \boldsymbol{A}^{\alpha\beta} \cdot d\boldsymbol{p}_c - H_0^{\alpha\beta} dt, \tag{3.10}$$

which governs dynamics of the wave-packet.

Before moving onto the semiclassical formalism stemming from the matrix valued

one-form, $\eta^{\alpha\beta}$. Here, an alternative derivation will be presented. The derivation starts from the following wave-packet

$$\tilde{\Psi}_{\boldsymbol{x}} \equiv \tilde{\Psi}_{\boldsymbol{x}}(\boldsymbol{p}_c, \boldsymbol{x}_c, t) = \sum_{\alpha} \xi_{\alpha}(\boldsymbol{p}_c, t) u^{(\alpha)}(\boldsymbol{p}_c, \boldsymbol{x}_c) e^{-i\boldsymbol{p}_c \cdot \boldsymbol{x}}, \tag{3.11}$$

The normalization of $u^{(\alpha)}(\boldsymbol{p}_c, \boldsymbol{x}_c)$ is given by (3.1). The one-form η is defined through $d\mathscr{S}$,

$$d\mathscr{S} = \int [dx] \delta(\boldsymbol{x} - \boldsymbol{x}_c) \tilde{\Psi}^{\dagger}_{\boldsymbol{x}} (id - H_0 dt) \tilde{\Psi}_{\boldsymbol{x}} = i \sum_{\alpha} \xi^*_{\alpha} d\xi_{\alpha} + \sum_{\alpha\beta} \xi^*_{\alpha} \eta^{\alpha\beta} \xi_{\beta}.$$

The exact derivative of (3.11) yields

$$\begin{aligned} d\tilde{\Psi}_{\boldsymbol{x}} &= dt \frac{\partial \tilde{\Psi}_{\boldsymbol{x}}}{\partial t} + d\boldsymbol{x}_c \frac{\partial \tilde{\Psi}_{\boldsymbol{x}}}{\partial \boldsymbol{x}_c} + d\boldsymbol{p}_c \frac{\partial \tilde{\Psi}_{\boldsymbol{x}}}{\partial \boldsymbol{p}_c} \\ &= dt \sum_{\alpha} \frac{\partial \xi_{\alpha}}{\partial t} u^{(\alpha)} e^{-i\boldsymbol{p}_c \cdot \boldsymbol{x}} + d\boldsymbol{x}_c \sum_{\alpha} \xi_{\alpha} \frac{\partial u^{(\alpha)}}{\partial \boldsymbol{x}_c} e^{-i\boldsymbol{p}_c \cdot \boldsymbol{x}} + d\boldsymbol{p}_c \sum_{\alpha} \frac{\partial \xi_{\alpha}}{\partial \boldsymbol{p}_c} u^{(\alpha)} e^{-i\boldsymbol{p}_c \cdot \boldsymbol{x}} \\ &+ d\boldsymbol{p}_c \sum_{\alpha} \xi_{\alpha} \frac{\partial u^{(\alpha)}}{\partial \boldsymbol{p}_c} e^{-i\boldsymbol{p}_c \cdot \boldsymbol{x}} + d\boldsymbol{p}_c \sum_{\alpha} \xi_{\alpha} u^{(\alpha)} (-i\boldsymbol{x}) e^{-i\boldsymbol{p}_c \cdot \boldsymbol{x}}. \end{aligned}$$

Thus,

$$\begin{aligned} \int [dx] \delta(\boldsymbol{x} - \boldsymbol{x}_c) \tilde{\Psi}^{\dagger}_{\boldsymbol{x}} id\tilde{\Psi}_{\boldsymbol{x}} = idt \sum_{\alpha} \xi^*_{\alpha} \frac{\partial \xi_{\alpha}}{\partial t} &+ id\boldsymbol{x}_c \sum_{\alpha\beta} \xi^*_{\alpha} u^{\dagger(\alpha)} \frac{\partial u^{(\beta)}}{\partial \boldsymbol{x}_c} \xi_{\beta} + d\boldsymbol{p}_c \boldsymbol{x}_c \\ &+ id\boldsymbol{p}_c \sum_{\alpha} \xi^*_{\alpha} \frac{\partial \xi_{\alpha}}{\partial \boldsymbol{p}_c} + id\boldsymbol{p}_c \sum_{\alpha\beta} \xi^*_{\alpha} u^{\dagger(\alpha)} \frac{\partial u^{(\beta)}}{\partial \boldsymbol{p}_c} \xi_{\beta} \end{aligned}$$

Using the definitions of Berry gauge fields given in (3.8), (3.9), and defining $H_0^{\alpha\beta} = E_{\alpha} \delta^{\alpha\beta}$, the following expression is obtained

$$d\mathscr{S} = i \sum_{\alpha} \xi^*_{\alpha} d\xi_{\alpha} + \sum_{\alpha\beta} \xi^*_{\alpha} \Big(\delta^{\alpha\beta} id + d\boldsymbol{p}_c \cdot \boldsymbol{x}_c \delta^{\alpha\beta} + d\boldsymbol{x}_c \boldsymbol{a}^{\alpha\beta} + d\boldsymbol{p}_c \boldsymbol{A}^{\alpha\beta} - H_0^{\alpha\beta} dt \Big) \xi_{\beta}.$$

Ignoring the time dependence, (3.10) is obtained straightforwardly.

3.2 Semiclassical formalism

In the previous section, the semiclassical theory established in terms of the wave packet composed of positive energy solutions is presented. It yields a semiclassical description of the system whose dynamics is governed by gauge fields which are matrices labeled by “spin indices". It is so called because the basis of the wave packets are solutions of a Dirac-like Hamiltonian. Obviously range of this index depends on the spacetime dimension as well as on the intrinsic properties of the system considered.

In d+1 dimensions, the following matrix valued one-form is dealt with,

$$\eta_H = p_a dx_a + [ea_a^{ext}(x,t) + a_a(x,p)]dx_a + A_a(x,p)dp_a - H(x,p)dt.$$

(x_a, p_a); $a = 1,2,...,d$, denote the classical phase space variables and $e > 0$, is the electron charge. $a_a(x,p,t)$ and $A_a(x,p,t)$ are the matrix-valued Berry gauge potentials. $H(x,p) = H_0(\boldsymbol{p}) - ea_0^{ext}(\boldsymbol{x})$ comprises of H_0, which is the diagonalized Dirac-like free Hamiltonian projected on positive energies, and the electromagnetic scalar field a_0^{ext}. We suppress the unit matrices. The related symplectic two-form is defined by

$$\begin{aligned} w_H &= d\eta_H - i\eta_H \wedge \eta_H \\ &= dp_a \wedge dx_a + F + G + M - \left(e\frac{\partial a_a^{ext}}{\partial t} + \frac{\partial H}{\partial x_a} - i[H, a_a] \right) dx_a \wedge dt \\ &\quad - \left(\frac{\partial H}{\partial p_a} + i[H, A_a] \right) dp_a \wedge dt. \end{aligned} \tag{3.12}$$

For $a_a = 0$, this coincides with the matrix-valued two form considered in [24]. $F = \frac{1}{2}F_{ab}dx_a \wedge dx_b$, $G = \frac{1}{2}G_{ab}dp_a \wedge dp_b$, and $M = \frac{1}{2}M_{ab}dp_a \wedge dx_b$ are the two-forms with the following components,

$$\begin{aligned} F_{ab} &= \frac{\partial a_b}{\partial x_a} - \frac{\partial a_a}{\partial x_b} - i[a_a, a_b] + e\left(\frac{\partial a_b^{ext}}{\partial x_a} - \frac{\partial a_a^{ext}}{\partial x_b} \right), \\ M_{ab} &= \frac{\partial a_b}{\partial p_a} - \frac{\partial A_a}{\partial x_b} - i[A_a, a_b], \\ G_{ab} &= \frac{\partial A_b}{\partial p_a} - \frac{\partial A_a}{\partial p_b} - i[A_a, A_b]. \end{aligned}$$

In order to obtain the equations of motion, we introduce the matrix valued vector field

$$\tilde{v} = \frac{\partial}{\partial t} + \dot{\tilde{x}}_a \frac{\partial}{\partial x_a} + \dot{\tilde{p}}_a \frac{\partial}{\partial p_a}. \tag{3.13}$$

Here, $(\dot{\tilde{x}}_a, \dot{\tilde{p}}_a)$ are the matrix-valued time evolutions of the phase space variables (x_a, p_a). This is analogous to the situation in the canonical formulation of the Dirac particle where the velocities are matrices though the phase space variables are ordinary vectors. The equations of motion are derived by demanding that the interior product of w_H, (3.12), with the matrix-valued vector field $\tilde{v}$, (3.13), vanish:

$$i_{\tilde{v}} w_H = 0.$$

The resulting equations are

$$\begin{aligned} \dot{\tilde{p}}_a &= \dot{\tilde{x}}_c F_{ac} + e_a - M_{ca}\dot{\tilde{p}}_c, \\ \dot{\tilde{x}}_a &= G_{ca}\dot{\tilde{p}}_c - f_a - \dot{\tilde{x}}_c M_{ac}, \end{aligned}$$

where we defined

$$\begin{aligned} e_a &\equiv e\mathscr{E}_a + i[H_0, a_a], \\ f_a &\equiv -\frac{\partial H_0}{\partial p_a} + i[H_0, A_a], \end{aligned}$$

in terms of the external electric field $\mathscr{E}_a = \partial a_0^{ext}/\partial x_a - \partial a_a^{ext}/\partial t$.

The Lie derivative of the volume form $\Omega_{d+1} = \frac{(-1)^{[\frac{d}{2}]}}{d!} w_H^d \wedge dt$ can be used to attain the matrix-valued velocities $(\dot{\tilde{x}}_a, \dot{\tilde{p}}_a)$ in terms of the phase space variables (x_a, p_a). It will be illustrated for $d = 2$, due to the fact that basically we are interested in $2+1$ spacetime dimensional Dirac-like systems. In $2+1$ dimensions, where the extended phase space is 5 dimensional, the volume form reads

$$\Omega_{2+1} = -\frac{1}{2} w_H \wedge w_H \wedge dt. \tag{3.14}$$

We express it through the canonical volume element of the phase space dV, as

$$\Omega_{2+1} = \tilde{w}_{1/2} dV \wedge dt, \tag{3.15}$$

where $\tilde{w}_{1/2}$ is the Pfaffian of the following 4×4 matrix,

$$\begin{pmatrix} F_{ij} & -\delta_{ij} - M_{ij} \\ \delta_{ij} + M_{ij} & -G_{ij} \end{pmatrix}.$$

We do not treat the spin indices on the same footing with the phase space indices (x_i, p_i); $i = 1, 2$. Thus the Pfaffian $\tilde{w}_{1/2}$ is a matrix in spin indices. The Lie derivative associated with the vector field (3.13) of the volume form (3.15) can be expressed formally as

$$L_v \Omega_{2+1} = (i_v d + d i_v)(\tilde{w}_{1/2} dV \wedge dt) = \left(\frac{\partial}{\partial t} \tilde{w}_{1/2} + \frac{\partial}{\partial x_i} (\dot{\tilde{x}}_i \tilde{w}_{1/2}) + \frac{\partial}{\partial p_i} (\tilde{w}_{1/2} \dot{\tilde{p}}_i) \right) dV \wedge dt. \tag{3.16}$$

Actually, to obtain it explicitly one should employ the definition (3.14) yielding

$$L_v \Omega_{2+1} = -\frac{1}{2} d w_H^2.$$

Comparing the exterior derivative of

$$\begin{aligned} w_H \wedge w_H &= dp_i \wedge dx_i \wedge dp_j \wedge dx_j + 2M \wedge dp_i \wedge dx_i + 2e_i dx_i \wedge dt \wedge dp_j \wedge dx_j \\ &+ (F f_i + f_i F) \wedge dp_i \wedge dt + (M e_i + e_i M) \wedge dx_i \wedge dt \\ &+ 2 f_i dp_i \wedge dt \wedge dp_j \wedge dx_j + F \wedge G + G \wedge F + (M f_i + f_i M) \wedge dp_i \wedge dt \\ &+ (G e_i + e_i G) \wedge dx_i \wedge dt, \end{aligned}$$

with the formal expression (3.16) one obtains the solutions

$$\tilde{w}_{1/2} = 1 - M_{ii} - \frac{1}{4}(F_{ij}G_{ij} + G_{ij}F_{ij}), \quad \textbf{(3.17)}$$

$$\dot{\tilde{x}}_i \tilde{w}_{1/2} = -f_i + (M_{ij}f_j + f_j M_{ij}) - (M_{jj}f_i + f_i M_{jj}) - \frac{1}{2}(G_{ij}e_j + e_j G_{ij}), \quad \textbf{(3.18)}$$

$$\tilde{w}_{1/2}\dot{\tilde{p}}_i = e_i - (M_{ji}e_j + e_j M_{ji}) + (M_{jj}e_i + e_i M_{jj}) + \frac{1}{2}(F_{ji}f_j + f_j F_{ji}). \quad \textbf{(3.19)}$$

These solutions are useful even for Schrödinger type Hamiltonian systems where the origin of the Berry gauge fields will be different. Indeed, to illustrate the power of the differential form method in general we would like to deal briefly with the anomalous Hall effect in two dimensions.

3.3 Anomalous Hall effect

The intrinsic anomalous Hall effect in ferromagnetic materials arise from the Berry curvature in the crystal momentum space of Bloch electrons either in the absence or in the presence of an external magnetic field [16, 17, 44, 45]. In the latter case one should define the electric current by taking corrections to the path integral measure into account. The anomalous Hall conductivity can be derived within the formalism of Section 3.2. Obviously, in this case the Berry gauge fields are derived from the occupied Bloch states. Consider the electrons which are constrained to move in the xy-plane in the presence of the constant magnetic field in the z-direction $F_{xy} = B$, and the Berry curvature G_{xy}. The equations of motion (3.17)-(3.19) become

$$\sqrt{w} = 1 - BG_{xy}, \quad \textbf{(3.20)}$$

$$\sqrt{w}\dot{x}_i = \frac{\partial H}{\partial p_i} - e\varepsilon_{ij}\mathscr{E}_j G_{xy}, \quad \textbf{(3.21)}$$

$$\sqrt{w}\dot{p}_i = e\mathscr{E}_i + \varepsilon_{ij}\frac{\partial H}{\partial p_j}B.$$

(3.20) is the correction to the path integral measure. Hence, the correct definition of electric current is

$$j_i = e\int \frac{d^2p}{(2\pi\hbar)^2}\sqrt{w}\dot{x}_i f(x,p,t),$$

where $f(x,p,t)$ is the ground state distribution (occupation) function. Plugging (3.21) into this definition one obtains the total electric current as

$$j_i = e\int \frac{d^2p}{(2\pi\hbar)^2}\left(\frac{\partial H}{\partial p_i} - e\varepsilon_{ij}\mathscr{E}_j G_{xy}\right) f(x,p,t).$$

The term proportional to the electric field yields the anomalous Hall current

$$j_i^{AH} = -e^2 \varepsilon_{ij} \mathscr{E}_j \int \frac{d^2p}{(2\pi\hbar)^2} G_{xy} f(x,p,t) \equiv \sigma_{AH} \varepsilon_{ij} \mathscr{E}_j,$$

where σ_{AH} denotes the anomalous Hall conductivity. For electrons obeying Fermi-Dirac distribution at zero temperature, the ground state distribution is given by the theta-function at the Fermi energy E_F : $f = \theta(E - E_F)$. Thus, the anamolous Hall conductivity reads

$$\sigma_{AH} = -e^2 \int_{E>E_F} \frac{d^2p}{(2\pi\hbar)^2} G_{xy}.$$

On the other hand the first Chern number, which is a topological invariant, is defined by

$$N_1 = \frac{1}{2\pi\hbar} \int d^2p G_{xy}.$$

Therefore, one concludes that the anomalous Hall conductivity

$$\sigma_{AH} = -\frac{e^2}{2\pi\hbar} N_1,$$

is a topological invariant.

3.4 Spin Hall conductivity vs spin Chern number

The semiclassical currents of the electrons obeying Dirac-like equations should be defined in terms of the velocities which are weighted with the correct measure $\dot{\tilde{x}}_a \tilde{w}_{1/2}$ which are matrices in spin indices. We only deal with the spin current generated by the third component of spin S_z, though any spin component can be studied similarly. The most convenient representation is

$$S_z = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{3.22}$$

where the dimension of the unit matrix I depends on the system considered. To define the spin current one also needs to introduce the ground state distribution functions $f^{\uparrow}(x,p,t)$ and $f^{\downarrow}(x,p,t)$ for the electrons with spin-up and spin-down. In the representation (3.22) we can define the distribution matrix by

$$f = \begin{pmatrix} f^{\uparrow} & 0 \\ 0 & f^{\downarrow} \end{pmatrix},$$

where the unit matrix I is suppressed. Now, the appropriate choice for the semiclassical spin current seems to be

$$j_a^z = \frac{\hbar}{2} \int \frac{d^d p}{(2\pi\hbar)^d} \mathrm{Tr}\left[S_z \dot{\tilde{x}}_a \tilde{w}_{1/2} f \right]. \tag{3.23}$$

Basis of the matrix representation are the positive energy solutions of the underlying Dirac-like equation (see Appendix A). If they are not eigenfunctions of the spin matrix S_z, simultaneously definition (3.23) does not make sense. Hence, to adopt (3.23) as the definition of the spin current we should choose the basis functions with a definite spin. Once this is done we can set the ground state distribution functions to unity by restricting our integrals to energies higher than the ground state energy. However, this is already the case because we deal with the wave packet composed of the positive energy solutions. Now, in $d = 2$, let us consider the spin Hall current which results from the last term in (3.18):

$$j_i^{SH} = -e\mathscr{E}_j \frac{\hbar}{2} \int \frac{d^2p}{(2\pi\hbar)^2} \mathrm{Tr}\left[S_z G_{ij} f\right] \equiv \sigma_{SH} \varepsilon_{ij} \mathscr{E}_j.$$

We are obliged to choose the basis which are spin eigenvalues so that spin Hall conductivity can be expressed as

$$\sigma_{SH} = -\frac{e}{2\pi} C_s, \tag{3.24}$$

where the spin Chern number

$$C_s = \frac{1}{2}(N^{\uparrow} - N^{\downarrow}),$$

is one half of the difference of the spin-up and spin-down first Chern numbers defined by

$$N^{\uparrow,\downarrow} = \frac{1}{2\pi\hbar} \int d^2p \ \mathrm{Tr} G_{xy}^{\uparrow,\downarrow}.$$

We demonstrated that the spin Hall conductivity is given by the spin Chern number (3.24), which is a topological invariant characterizing the spin Hall effect. Hence, it will be the main contribution to the spin Hall conductivity if the spin Hall phase exists. This is the main conclusion of this work. In the following section we will illustrate this formalism by applying it to the Kane-Mele model of graphene which is also known as Chern insulator in $2+1$ dimensions.

3.5 Kane-Mele Model

Time reversal invariant $2+1$ dimensional topological insulator can be formulated as the spin Hall effect in graphene within the Kane-Mele model described by the Hamiltonian

$$H = v_F \sigma_x \tau_z p_x + v_F \sigma_y p_y + \Delta_{SO} \sigma_z \tau_z s_z + \lambda_R (\sigma_x \tau_z s_y - \sigma_y s_x). \tag{3.25}$$

It is the effective theory of electrons on graphene with the Fermi velocity v_F. The intrinsic and Rashba spin-orbit coupling constants are denoted by Δ_{SO} and λ_R, respectively. $\sigma_{x,y,z}$ are the Pauli matrices in the representation $\sigma_z = \mathrm{diag}(1,-1)$, which act on the states of sublattices. $\tau_z = \mathrm{diag}(1,-1)$, labels the states at the Dirac points (valleys) K and K', and the Pauli matrices, $s_{x,y,z}$ act on the real spin space in the representation where the third component is diagonal $s_z = \mathrm{diag}(1,-1)$.

The main difference between the Kane-Mele model with and without the Rashba spin-orbit coupling term lies in whether the third component of spin is a good quantum number or not. In the former case s_z is conserved and application of the semiclassical approach is straightforward. However, also in the latter case the spin Hall conductivity is non-vanishing with the condition $\Delta_{SO} > \lambda_R$. We will illustrate how the semiclassical formulation can be applied in both cases and demonstrate that main contribution to the spin Hall conductivity is always given by the spin Chern number defined in [20].

3.6 Kane-Mele model without the Rashba spin-orbit interaction term

In this case the Hamiltonian is

$$H^{SO} = v_F \sigma_x \tau_z p_x + v_F \sigma_y p_y + \Delta_{SO} \sigma_z \tau_z s_z. \tag{3.26}$$

In fact, there are four different two dimensional Hamiltonians stemming from (3.26):

$$H^{SO} = \begin{pmatrix} H^{\uparrow +} & 0 & 0 & 0 \\ 0 & H^{\uparrow -} & 0 & 0 \\ 0 & 0 & H^{\downarrow +} & 0 \\ 0 & 0 & 0 & H^{\downarrow -} \end{pmatrix}.$$

These two dimensional Hamiltonians corresponding to the $\uparrow$, $\downarrow$ spin and the K, K' valley are

$$H^{\uparrow +} = v_F(\sigma_x p_x + \sigma_y p_y) + \Delta_{SO}\sigma_z, \qquad H^{\uparrow -} = v_F(-\sigma_x p_x + \sigma_y p_y) - \Delta_{SO}\sigma_z, \tag{3.27}$$

$$H^{\downarrow +} = v_F(\sigma_x p_x + \sigma_y p_y) - \Delta_{SO}\sigma_z, \qquad H^{\downarrow -} = v_F(-\sigma_x p_x + \sigma_y p_y) + \Delta_{SO}\sigma_z. \tag{3.28}$$

The effect of the spin-orbit term is to create a gap in the energy band structure of the Hamiltonians. In terms of the eigenvalues of the momenta $\hbar\boldsymbol{k}$, (3.27) and (3.28) yield the same energy distribution

$$E = \pm\sqrt{v_F^2 \hbar^2 k^2 + \Delta_{SO}^2}, \tag{3.29}$$

corresponding to particle and antiparticle (hole) states.

Note that in this section $\boldsymbol{p}$ is not a quantum operator but denotes the classical phase space variable.

We deal with four different two dimensional Dirac-like theories (3.27), (3.28), thus we should take into account the contributions arising from each of them separately. We adopt the formulation of [42] to derive the Berry gauge fields arising from each one of the two dimensional Hamiltonians (3.27), (3.28). Therefore, we should start with giving the unitary Foldy-Wouthuysen transformations $(U^{\uparrow+},U^{\uparrow-},U^{\downarrow+},U^{\downarrow-})$ corresponding to the Dirac-like Hamiltonians $(H^{\uparrow+},H^{\uparrow-},H^{\downarrow+},H^{\downarrow-})$. We would like to present them in the unified notation:

$$U \equiv \mathrm{diag}(U^{\uparrow+},U^{\uparrow-},U^{\downarrow+},U^{\downarrow-}).$$

The unitary Foldy-Wouthuysen transformation U can be engaged to define the gauge field [42, 50]

$$\mathscr{A} \equiv \mathrm{diag}(\mathscr{A}^{\uparrow+},\mathscr{A}^{\uparrow-},\mathscr{A}^{\downarrow+},\mathscr{A}^{\downarrow-}) = i\hbar U(\boldsymbol{p})\frac{\partial U^{\dagger}(\boldsymbol{p})}{\partial \boldsymbol{p}}.$$

Exploring the Dirac-like Hamiltonians (3.27), (3.28), we introduce the following Foldy-Wouthuysen transformation

$$U = \frac{1}{\sqrt{2E(E+\Delta_{so})}}\begin{pmatrix} \sigma_z H^{\uparrow+}+E & 0 & 0 & 0 \\ 0 & -\sigma_z H^{\uparrow-}+E & 0 & 0 \\ 0 & 0 & -\sigma_z H^{\downarrow+}+E & 0 \\ 0 & 0 & 0 & \sigma_z H^{\downarrow-}+E \end{pmatrix}, \tag{3.30}$$

where E is the positive energy depending on $\boldsymbol{p}$ as $E=\sqrt{v_F^2\boldsymbol{p}^2+\Delta_{so}^2}$. Observe that (3.30) is defined to satisfy

$$H^{so} = UHU^{\dagger} = E\sigma_z\tau_z s_z. \tag{3.31}$$

One can study each entry of (3.30) as in [42] and show that they lead to the gauge potential

$$\mathscr{A}^U = \frac{i\hbar}{2E^2(E+\Delta_{so})}\left[v_F E(E+\Delta_{so})\boldsymbol{\alpha}\sigma_z\tau_z s_z + v_F^3\sigma_z\tau_z s_z(\boldsymbol{\alpha}\cdot\boldsymbol{p})\boldsymbol{p} + v_F^2 E(\boldsymbol{\alpha}\cdot\boldsymbol{p})\boldsymbol{\alpha} - v_F^2\boldsymbol{p}E\right].$$

Its components can be written explicitly as [34]

$$\mathscr{A}_x^U = \frac{\hbar(v_F E(E+\Delta_{so})\sigma_y s_z - v_F^3(\sigma_y p_x - \sigma_x\tau_z p_y)s_z p_x + v_F^2 E\sigma_z\tau_z p_y)}{2E^2(E+\Delta_{so})}, \tag{3.32}$$

$$\mathscr{A}_y^U = \frac{\hbar(-v_F E(E+\Delta_{so})\sigma_x\tau_z s_z - v_F^3(\sigma_y p_x - \sigma_x\tau_z p_y)s_z p_y - v_F^2 E\sigma_z\tau_z p_x)}{2E^2(E+\Delta_{so})}. \tag{3.33}$$

Because of being a pure gauge potential the field strength of $\mathscr{A}^U$ vanishes. However, one can consider the adiabatic approximation by projecting on the positive energy states:

$$\boldsymbol{A} \equiv P\mathscr{A}^U P. \tag{3.34}$$

By inspecting the positive eigenvalues of the (3.31) one can deduce that the projection operator P is

$$P \equiv \mathrm{diag}(P_+^{\uparrow}, P_-^{\uparrow}, P_+^{\downarrow}, P_-^{\downarrow}) = \mathrm{diag}(1,0,0,1,0,1,1,0).$$

It should be noted that when projected on positive energy states only the last terms in (3.32) and (3.33) make nonvanishing contributions, so that the Abelian Berry gauge field is

$$A_i = \frac{\hbar v_F^2}{2E(E+\Delta_{SO})}\varepsilon_{ij}p_j \mathbf{1}_\tau s_z, \tag{3.35}$$

where the unit matrix $\mathbf{1}_\tau$ in the τ_z space is exhibited explicitly. It is worth emphasizing that in $\mathscr{A}$ negative energy states are present, thus it possesses twice the matrix elements of $\mathscr{A}^{\mathrm{B}}$. The nonvanishing component of the Berry curvature is given as

$$G = \hbar\left(\frac{\partial A_y}{\partial p_x} - \frac{\partial A_x}{\partial p_y}\right) \equiv \mathrm{diag}(G_+^{\uparrow}, G_-^{\uparrow}, G_+^{\downarrow}, G_-^{\downarrow}) = -\frac{\hbar^2 v_F^2 \Delta_{SO}}{2E^3}\mathbf{1}_\tau s_z. \tag{3.36}$$

The spin Hall effect in graphene can be given as [19] as

$$\sigma_{SH} = -\frac{e}{2}\int^{E_F^{(2)}} \frac{d^2p}{(2\pi\hbar)^2}\left[(G_+^{\uparrow} + G_-^{\uparrow}) - (G_+^{\downarrow} + G_-^{\downarrow})\right]. \tag{3.37}$$

$E_F^{(2)}$ denotes the highest energy level occupied in the two dimensional system. Thus, inserting (3.36) into the definition (3.37) leads to

$$\begin{aligned}\sigma_{SH} &= -\frac{e}{2}\int_{-\infty}^{E_F^{(2)}} \frac{d^2p}{(2\pi\hbar)^2}\left(-\frac{2\hbar^2 v_F^2 \Delta_{SO}}{E^3}\right) \\ &= -\frac{e}{2\pi}\frac{\Delta_{SO}}{E_F^{(2)}}.\end{aligned} \tag{3.38}$$

This in accord with the calculation of the spin Hall conductivity obtained by employing the Kubo formula which is presented in Appendix B.

We let the Fermi energy level of graphene lie in the gap, so that in (3.38) we set $E_F^{(2)} = \Delta_{SO}$ and obtain the spin Hall conductivity as

$$\sigma_{SH} = -\frac{e}{2\pi}.$$

This is the value established in [8]. Based on the above derivation of spin Hall conductivity, in the rest of the section the semiclassical treatment presented before will be employed. U can be employed to acquire the eigenfunctions of (3.26) as

$$u^{(\alpha)}(p) = U^{\dagger} v^{(\alpha)},$$

where $v^{(1)} = (1,0\cdots,0)^T, \cdots, v^{(8)} = (0,0\cdots,1)^T$. The Hamiltonian projected on positive energy eigenstates in the presence of the external electric field $\mathscr{E}$ is

$$H_0^{SO} = (E + e\mathscr{E}\cdot\boldsymbol{x})\mathbf{1}_\tau \mathbf{1}_s.$$

In the rest of this section we will keep the unit matrices explicit. The Berry gauge field is given by (3.35). Hence, the corresponding Berry curvature is given by (3.36). In the absence of a magnetic field the phase space measure (3.17) is trivial: $\tilde{w}_{1/2} = 1$. Thus, the equations of motion (3.18)-(3.19) yield

$$\begin{aligned} \dot{\tilde{x}}_i &= -\frac{v_F^2 p_i}{E}\tau_z s_z - e\varepsilon_{ij}\mathscr{E}_j G_{xy}, \\ \dot{\tilde{p}}_i &= e\mathscr{E}_i \mathbf{1}_\tau \mathbf{1}_s. \end{aligned}$$

In the representation which we adopted the third component of spin becomes

$$S_z = \mathbf{1}_\tau s_z. \tag{3.39}$$

Note that $u^{(\alpha)}$ are also the eigenstates of the spin matrix (3.39). Therefore, the distribution matrix $f = \mathbf{1}_\tau \mathrm{diag}(f^{\uparrow}, f^{\downarrow})$ is adequate to define the spin current by

$$j_i^z = \frac{\hbar}{2}\int \frac{d^2p}{(2\pi\hbar)^2}\mathrm{Tr}\left[S_z\sqrt{w}\dot{\tilde{x}}_i f\right].$$

It yields the spin Hall current $j_i^{SH} = \sigma_{SH}\varepsilon_{ij}\mathscr{E}_j$, where the spin Hall conductivity is given by

$$\sigma_{SH} = -\frac{e\hbar}{2}\int \frac{d^2p}{(2\pi\hbar)^2}\mathrm{Tr}\left[S_z G_{xy}\right]. \tag{3.40}$$

Let us decompose (3.40) such that the contributions arising from spin subspace and K, K' valleys become apparent. One can easily observe that

$$\begin{aligned} \sigma_{SH} &= -\frac{e\hbar}{2}\int \frac{d^2p}{(2\pi\hbar)^2}(G_{xy}^{\uparrow K} - G_{xy}^{\downarrow K} + G_{xy}^{\uparrow K'} - G_{xy}^{\downarrow K'}) \\ &= -\frac{e}{4\pi}(N_1^{\uparrow K} - N_1^{\downarrow K} + N_1^{\uparrow K'} - N_1^{\downarrow K'}). \end{aligned}$$

Each contribution is associated with the first Chern number of the related subspace. This has been observed in [34] where the related Chern numbers were calculated. We

conclude that the spin Hall conductivity is proportional to the sum of the spin Chern number of the K valley, C_s^K and the spin Chern number of the K' valley, $C_s^{K'}$:

$$\sigma_{SH} = -\frac{e}{2\pi}(C_s^K + C_s^{K'}) = -\frac{e}{2\pi}C_s = -\frac{e}{2\pi}.$$

In the absence of Rashba term we defined the spin current straightforwardly since the Hamiltonian (3.26) commutes with s_z.

3.7 Kane-Mele model with Rashba spin-orbit interaction term

Although, in the presence of the Rashba term s_z does not commute with the Hamiltonian (3.25), the spin Hall effect still exists for $\Delta_{SO} > \lambda_R$ [8, 49, 51]. However, the semiclassical calculation is not clear as we discussed in Section 3.4. There we also discussed the correct definition of spin current. Nevertheless, before proceeding as indicated in Section 3.4 let us carry on with the computation of the Berry gauge field naively using the positive energy eigenfunctions of (3.25).

The K and K' subspaces corresponding to $\tau_z = \pm 1$ yield the same energy eigenvalues and eigenstates which are presented in Appendix B. Thus, it is sufficient to consider only the 4×4 Hamiltonian in K subspace denoted by H_K :

$$H_K \Phi_\alpha = E_\alpha \Phi_\alpha,$$

where $\alpha = 1, .., 4$ and the energy eigenvalues E_α are

$$\begin{aligned} E_1 &= \lambda + \sqrt{(\Delta_{SO} - \lambda)^2 + v_F^2 p^2},\ E_2 = -\lambda + \sqrt{(\Delta_{SO} + \lambda)^2 + v_F^2 p^2}, \\ E_3 &= \lambda - \sqrt{(\Delta_{SO} - \lambda)^2 + v_F^2 p^2},\ E_4 = -\lambda - \sqrt{(\Delta_{SO} + \lambda)^2 + v_F^2 p^2}. \end{aligned} \quad \textbf{(3.41)}$$

We deal with the coupling constants satisfing $\Delta_{SO} > 2\lambda_R$, so that E_1, E_2 and E_3, E_4 are positive and negative, respectively.

The diagonalized Hamiltonian is $\mathscr{H}_K^\Phi = \mathrm{diag}(E_1, E_2, E_3, E_4)$. When we project on the positive energy eigenstates and take both of the contributions coming from the K and K' subspaces, the Hamiltonian becomes

$$H_0^\Phi = \mathbf{1}_\tau \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + e\mathscr{E} \cdot \boldsymbol{x} \mathbf{1}_\tau \mathbf{1}_s.$$

The Berry gauge field turns out to be Abelian:

$$A_i^\Phi = \hbar \varepsilon_{ij} \frac{p_j}{p^2} \mathbf{1}_\tau \begin{pmatrix} -1 & 2N_1N_2 \\ 2N_1N_2 & -1 \end{pmatrix}.$$

The corresponding Berry curvature $G^{\Phi}_{xy} = (\partial_x A^{\phi}_y - \partial_y A^{\phi}_x)$, can easily be computed as

$$G^{\Phi}_{xy} = \mathbf{1}_\tau \begin{pmatrix} 0 & -\frac{2\hbar}{p}\partial_p(N_1N_2) \\ -\frac{2\hbar}{p}\partial_p(N_1N_2) & 0 \end{pmatrix}.$$

According to (3.17)-(3.19) the equations of motion calculated in the energy eigenfunction basis are

$$\begin{aligned} \dot{\tilde{x}}_i &= -\mathbf{1}_\tau v_F^2 p_i \begin{pmatrix} \frac{1}{E_1-\lambda} & 0 \\ 0 & \frac{1}{E_2+\lambda} \end{pmatrix} + 2\frac{N_1N_2}{p^2}\varepsilon_{ij}p_j(E_1-E_2)\mathbf{1}_\tau s_y - e\varepsilon_{ij}\mathscr{E}_j\mathbf{1}_\tau G^{\Phi}_{xy}, \\ \dot{\tilde{p}}_i &= e\mathscr{E}_i\mathbf{1}_\tau\mathbf{1}_s, \end{aligned}$$

where we set $\tilde{w}_{1/2} = 1$.

The spin current cannot be defined by (3.23) with a diagonal f. Choosing it diagonal would lead to a vanishing spin Hall current due to the fact that

$$\mathrm{Tr}\left[S_z G^{\Phi}_{xy}\right] = 0.$$

The difficulty stems from the fact that energy eigenfunctions are not simultaneously eigenstates of the spin operator $S_z = \mathrm{diag}(s_z, s_z)$. In K subspace eigenstates of the spin operator S_z, constructed from the energy eigenstates Φ_α, are

$$\begin{aligned} \Psi_1 &= \frac{1}{\sqrt{2}}(\Phi_1+\Phi_2),\ \Psi_2 = \frac{1}{\sqrt{2}}(\Phi_1-\Phi_2), \\ \Psi_3 &= \frac{1}{\sqrt{2}}(\Phi_3+\Phi_4),\ \Psi_4 = \frac{1}{\sqrt{2}}(\Phi_3-\Phi_4). \end{aligned}$$

Ψ_1, Ψ_2 and Ψ_3, Ψ_4 correspond to positive and negative energy sectors, respectively. They satisfy

$$S_z\Psi_{1,3} = \Psi_{1,3},\ S_z\Psi_{2,4} = -\Psi_{2,4}.$$

The Hamiltonian in Ψ_α basis is obtained by the transformation

$$\mathscr{H}^{\Psi}_K = U_\Psi H_K U^\dagger_\Psi,$$

where $U^\dagger_\Psi = \begin{pmatrix} \Psi_1 & \Psi_2 & \Psi_3 & \Psi_4 \end{pmatrix}$. Notice that U_Ψ is related to the unitary transformation that diagonalizes H_K, denoted by U_Φ, via $U_\Psi = RU_\Phi$, where $R = \begin{pmatrix} \tilde{R} & 0 \\ 0 & \tilde{R} \end{pmatrix}$ with

$$\tilde{R} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Thus we acquired

$$\begin{aligned}\mathscr{H}^{\Psi} &= (\mathbf{1}_\tau R)\mathscr{H}^{\Phi}(R\mathbf{1}_\tau) \\ &= \frac{1}{2}\begin{pmatrix} E_1+E_2 & E_1-E_2 & 0 & 0 \\ E_1-E_2 & E_1+E_2 & 0 & 0 \\ 0 & 0 & E_3+E_4 & E_3-E_4 \\ 0 & 0 & E_3-E_4 & E_3+E_4 \end{pmatrix}\mathbf{1}_\tau.\end{aligned}$$

The Hamiltonian in Ψ_α basis projected on positive energy eigenstates in the presence of external electric field $\mathscr{E}$, is

$$H_0^{\Psi} = (E_1+E_2)\mathbf{1}_\tau\mathbf{1}_s + (E_1-E_2)\mathbf{1}_\tau s_x + e\mathscr{E}\cdot\boldsymbol{x}\mathbf{1}_\tau\mathbf{1}_s.$$

The basis transformation $\tilde{R}$ sustains the connection between $\boldsymbol{A}^{\Psi}$ and $\boldsymbol{A}^{\Phi}$ via the relation $\boldsymbol{A}^{\Psi} = (\mathbf{1}_\tau\tilde{R})\boldsymbol{A}^{\Phi}(\tilde{R}\mathbf{1}_\tau)$, so that

$$A_i^{\Psi} = \hbar\varepsilon_{ij}\frac{p_j}{p^2}\mathbf{1}_\tau\begin{pmatrix} -1+2N_1N_2 & 0 \\ 0 & -1+2N_1N_2 \end{pmatrix} \equiv \mathbf{1}_\tau\begin{pmatrix} A_i^{\uparrow} & 0 \\ 0 & A_i^{\downarrow} \end{pmatrix}.$$

The corresponding Berry curvature $G_{xy}^{\Psi} = (\mathbf{1}_\tau\tilde{R})G_{xy}^{\Phi}(\tilde{R}\mathbf{1}_\tau)$ is calculated as

$$G_{xy}^{\Psi} = -\frac{2\hbar}{p}\frac{\partial(N_1N_2)}{\partial p}\mathbf{1}_\tau s_z \equiv \mathbf{1}_\tau\begin{pmatrix} G_{xy}^{\uparrow} & 0 \\ 0 & G_{xy}^{\downarrow} \end{pmatrix}.$$

Hence, the equations of motion are

$$\begin{aligned}\dot{\tilde{x}}_i &= -\mathbf{1}_\tau v_F^2 p_i\begin{pmatrix} \frac{1}{E_1-\lambda}+\frac{1}{E_2+\lambda} & \frac{1}{E_1-\lambda}-\frac{1}{E_2+\lambda} \\ \frac{1}{E_1-\lambda}-\frac{1}{E_2+\lambda} & \frac{1}{E_1-\lambda}+\frac{1}{E_2+\lambda} \end{pmatrix} - 2\frac{N_1N_2}{p^2}\varepsilon_{ij}p_j(E_1-E_2)\mathbf{1}_\tau s_y - e\varepsilon_{ij}\mathscr{E}_j G_{xy}^{\Psi}, \\ \dot{\tilde{p}}_i &= e\mathscr{E}_i\mathbf{1}_\tau\mathbf{1}_s.\end{aligned}$$

The spin Hall current can now be written as

$$j_i^{SH} = -\frac{e\hbar}{2}\varepsilon_{ij}\mathscr{E}_j\int\frac{d^2p}{(2\pi\hbar)^2}\mathrm{Tr}\left[S_z G_{xy}^{\Psi} f\right],$$

where $f = \mathbf{1}_\tau\mathrm{diag}(f^{\uparrow}, f^{\downarrow})$. Therefore, f restricts the integral to positive energies and the spin Hall conductivity becomes

$$\sigma_{SH} = -\frac{e\hbar}{2}\int\frac{d^2p}{(2\pi\hbar)^2}\left\{(G_{xy}^{K\uparrow}-G_{xy}^{K\downarrow})+(G_{xy}^{K'\uparrow}-G_{xy}^{K'\downarrow})\right\} = -\frac{e}{2\pi}(C_s^K+C_s^{K'}) = -\frac{e}{2\pi}C_s.$$

In [48] this spin Chern number is calculated as $C_s = 1$. Therefore, we conclude that

$$\sigma_{SH} = -\frac{e}{2\pi}.$$

Indeed, in [8] it was argued that the value of the spin Hall conductivity sligtly differs from this value which is confirmed either in terms of numerical methods [49] or deriving the related effective theory [51].

4. EFFECTIVE FIELD THEORY OF TIME-REVERSAL INVARIANT TOPOLOGICAL INSULATORS

The $2+1$ dimensional topological field theory of the integer quantum Hall effect is considered in Section 4.1 in order to recall how to construct the TRI spin quantum Hall effect in graphene which is a model of $2+1$ dimensional topological insulator. Then, the dimensional reduction to $1+1$ dimensions by obtaining the one dimensional charge polarization explicitly is presented. In Section 4.2, the $4+1$ dimensional Chern-Simons field theory which was shown to describe the fundamental topological insulator is considered. The field strengths of the related Berry gauge fields are derived to obtain the second Chern number and dimensional reduction to $3+1$ dimensions is studied. By imitating the approach of [8] a hypothetical model is theorized in $4+1$ dimensions which yields a TRI spin Hall current in $3+1$ dimensions by means of the dimensional reduction. Slightly modifying the approach of [37], a dimensional reduction procedure to $2+1$ dimensions is proposed which provides explicit forms of the gauge field components which take part in the descendant action.

4.1 2+1 Dimensional topological insulator and dimensional reduction to 1+1 dimension

Field theory of electrons interacting with the external Abelian gauge field A_α is given by the Dirac Lagrangian density

$$\mathscr{L}(\psi,\bar{\psi},A)=\bar{\psi}\left[\gamma^\alpha\left(p_\alpha+A_\alpha\right)-m\right]\psi, \tag{4.1}$$

where $\alpha=0,1\cdots d$. By integrating out the fermionic degrees of freedom in the related path integral one formally gets the action of the external fields as

$$S[A]=-i\ln\det[i\gamma^\alpha(\partial_\alpha-iA_\alpha)-m]. \tag{4.2}$$

For $d=2n$ one of the terms which it gives rise to is [38]

$$T[A^{n+1}]=\int[dq_1]\cdots[dq_{n+1}]A^{\alpha_1}(q_1)\cdots A^{\alpha_{n+1}}(q_{n+1})\pi_{\alpha_1\cdots\alpha_{n+1}}(q_1\cdots q_{n+1}).$$

$[dq]$ denotes the integral over the related phase space. At the order of first loop

$$\pi_{\alpha_1\cdots\alpha_{n+1}}(q_1\cdots q_{n+1}) = \int \frac{d^{2n+1}k}{(2\pi)^{2n+1}} \mathrm{tr}\{G(k)\lambda_{\alpha_1}(k,k-q_1)G(k-q_1)\cdots\lambda_{\alpha_{n+1}}(k+q_{n+1},k)\},$$

where $G(k)$ is the one particle Green function of the free Dirac field and λ_α is the photon vertex. $T[A^{n+1}]$ generates the $2n+1$ dimensional Chern-Simons term

$$S^{2n+1}_{eff}[A] = C_n \int d^{2n+1}x \varepsilon^{\alpha_1\cdots\alpha_{2n+1}} A_{\alpha_1}\partial_{\alpha_2}A_{\alpha_3}\cdots\partial_{\alpha_{2n}}A_{\alpha_{2n+1}}, \tag{4.3}$$

which can be taken as the effective topological action in the low energy limit.

In $2+1$ dimensions integration of the massive Dirac fermions in the related path integral with the Lagrangian density (4.1) leads to the effective topological action

$$S^{2+1}_{eff}[A] = C_1 \int d^3x \varepsilon^{\mu\nu\rho} A_\mu \partial_\nu A_\rho, \tag{4.4}$$

where $\mu,\nu,\rho = 0,1,2$.

On the other hand, plugging the field strength (2.38) of the Abelian Berry gauge field (2.34) into (2.40) leads to

$$N_1 = \frac{i}{2\pi}\int d^2k \varepsilon_{ab}\mathrm{tr}\{P\partial_a U \partial_b U^\dagger P\}.$$

Therefore, we conclude that

$$C_1 = \frac{N_1}{4\pi}. \tag{4.5}$$

One can observe that by employing (4.5) in (4.4) the effective topological action of external gauge fields coupled to massive Dirac electrons living in $2+1$ dimensions becomes

$$S^{2+1}_{eff} = \frac{N_1}{4\pi}\int d^3x \varepsilon^{\mu\nu\rho} A_\mu \partial_\nu A_\rho. \tag{4.6}$$

To calculate the related first Chern number (2.40), let us choose the representation $\boldsymbol{\alpha} = (\sigma_x, \sigma_y)$, where σ_a are the Pauli spin matrices. This corresponds to set $\rho_a = (1,-i)$ in (2.37). Thus, the Abelian Berry gauge field can be written as

$$\mathscr{A}_a = \frac{\varepsilon_{ab}k_b}{2E(E+m)}. \tag{4.7}$$

It yields the Berry curvature

$$\mathscr{F}_{12} = \left(\frac{\partial \mathscr{A}_2}{\partial k_1} - \frac{\partial \mathscr{A}_1}{\partial k_2}\right) = -\frac{m}{2E^3}. \tag{4.8}$$

We plug (4.8) into (2.40) and perform the change of variable by (3.41) to express the related first Chern number as

$$N_1 = -\frac{m}{2}\int_D \frac{dE}{E^2}, \tag{4.9}$$

where the domain of integration D will be specified according to the model considered. If it is required to treat the $E>0$ and $E<0$ domains on the same footing, we can deal with

$$N_1 = -\frac{m}{2}\int_{-\infty}^{m} \frac{dE}{E^2} - \frac{m}{2}\int_{-m}^{\infty} \frac{dE}{E^2} = 1. \tag{4.10}$$

4.1.1 A model for $2+1$-dimensional topological insulator

Before presenting the graphene model of [8], let us briefly recall the interconnection between the quantum Hall effect and the Chern-Simons action in $2+1$ dimensions. For electrons moving on a surface in the presence of the external in-plane electric field $\boldsymbol{E} = (E_x, E_y, 0)$ and the perpendicular magnetic field $\mathscr{B} = (0,0,\mathscr{B}_z)$ the Hall current is given by

$$j_a = \sigma_H \varepsilon_{ab} E_b. \tag{4.11}$$

Ignoring the spin of electrons the Hall conductivity is a topological invariant [10, 60]:

$$\sigma_H = \frac{e^2}{\hbar} N_1. \tag{4.12}$$

Here N_1 is the first Chern number resulting from the field strength $\mathscr{F}_{\mathrm{B}}$ of the Berry gauge field obtained from the single particle Bloch wave functions which are solutions of the Schrödinger equation in the presence of the external magnetic field $\mathscr{B}_z$, integrated over the states up to the Fermi level E_F as

$$N_1 = \int^{E_F} \frac{d^2k}{(2\pi)^2} \mathscr{F}_{\mathrm{B}}. \tag{4.13}$$

A field theoretic description is possible in terms of the Chern-Simons action (4.6) with the definition (4.13). In fact, the current obtained from the topological field theory (4.6),

$$j_\mu = \frac{N_1}{2\pi} \varepsilon_{\mu\nu\rho} \partial^\nu A^\rho,$$

gives for $E_a = \partial_a A_0 - \partial_0 A_a$ the Hall current (4.11). It also leads to the charge density $j_0 = \sigma_H B$, where the induced magnetic field is $B = \partial_x A_y - \partial_y A_x$. Note that B would also be generated by the Hall current (4.11) through the current conservation condition $\partial_a j_a = -\partial_t j_0$. We would like to emphasize the fact that the field theory (4.6) is not

aware of the external magnetic field $\mathscr{B}_z$. External magnetic field is responsible of creating the energy spectrum whose consequences are encoded in the calculation of the first Chern number (4.13).

By employing the Berry gauge field derived from the Dirac equation (4.7), we can still get the Hall conductivity as in (4.12) by an appropriate choice of the domain of integration D in (4.9). This construction does not necessitate an external magnetic field. For the first time in [9] Haldane described how to obtain the quantum Hall effect without a magnetic field (vanishing in the average) through a Dirac like theory. To calculate the Hall conductivity following from the Dirac equation we let all the negative energy levels be occupied up to the Fermi level $E_F = m$ in (4.9), so that

$$\sigma_H = \frac{e^2}{h}\left(-\frac{m}{2}\int_{-\infty}^{m}\frac{dE}{E^2}\right) = \frac{e^2}{2h}. \tag{4.14}$$

In [8] Kane and Mele incorporated the spin of electrons into the Haldane model [9] and proposed the following Hamiltonian for graphene

$$H_G = \sigma_x\tau_z k_x + \sigma_y k_y + m\sigma_z\tau_z s_z, \tag{4.15}$$

which leads to a TRI spin current. The mass term is generated by a spin-orbit coupling. The Pauli spin matrices $\sigma_{x,y,z}$ act on the states of sublattices. The matrix $\tau_z = \mathrm{diag}(1,-1)$ denotes the Dirac points $K,\ K'$ which should be interchanged under the time reversal transformation. The other Pauli matrix $s_z = \mathrm{diag}(1,-1)$ describes the third component of the spin of electrons which should also be inverted under time reversal transformation. Thus the time reversal operator is given by $T = UK$ where we can take $U = \tau_y s_y$ and K takes the complex conjugation as well as maps $\boldsymbol{k} \to -\boldsymbol{k}$. Therefore (4.15) is TRI:

$$TH_G T^{-1} = H_G.$$

The Abelian Berry gauge field obtained from the Hamiltonian (4.15) can be written as [34]

$$\mathscr{A}_a = \frac{1}{2E(E+m)}\varepsilon_{ab}k_b 1_\tau s_z, \tag{4.16}$$

where 1_τ is the unit matrix in the τ_z space. The corresponding field strength is

$$\mathscr{F}_{12} \equiv \mathrm{diag}(\mathscr{F}_+^\uparrow, \mathscr{F}_-^\uparrow, \mathscr{F}_+^\downarrow, \mathscr{F}_-^\downarrow) = -\frac{m}{2E^3}1_\tau s_z. \tag{4.17}$$

The indices $\uparrow\downarrow$ and $\pm$ label, respectively, the third component of the spin and τ_z. The spin current defined as

$$\boldsymbol{j}^s = \boldsymbol{j}_+^\uparrow + \boldsymbol{j}_-^\uparrow - \boldsymbol{j}_+^\downarrow - \boldsymbol{j}_-^\downarrow,$$

leads to the spin Hall current

$$j_a^s = \sigma_{SH}\varepsilon_{ab}E_b.$$

The difference of the related first Chern numbers

$$\begin{aligned}\Delta N_1 &= \frac{1}{2\pi}\int_{E=-\infty}^{E=m} d^2k\left[(\mathscr{F}_+^{\uparrow}+\mathscr{F}_-^{\uparrow})-(\mathscr{F}_+^{\downarrow}+\mathscr{F}_-^{\downarrow})\right]\\ &= (\frac{1}{2}+\frac{1}{2})-(-\frac{1}{2}-\frac{1}{2})=2,\end{aligned} \tag{4.18}$$

gives the spin Hall conductivity σ_{SH} as

$$\sigma_{SH} = \frac{e}{4\pi}\Delta N_1 = \frac{e}{2\pi}. \tag{4.19}$$

4.1.2 Dimensional reduction to $1+1$ dimensions

We would like to discuss dimensional reduction from $2+1$ to $1+1$ dimensions by slightly modifying the procedure described in [37]. The dimensionally reduced theory can be defined through the $1+1$ dimensional Lagrangian density

$$\mathscr{L}_{1+1}(\psi,\bar{\psi},A) = \bar{\psi}\left[\gamma^r(p_r+A_r)+\gamma_2\zeta_y - m\right]\psi,$$

where $r=t,x$ and the external field $\zeta_y(t,x)$ is the reminiscent of the gauge field A_y. We define $\zeta_y = k_y+\zeta$, where k_y is a parameter which permits us to deal with one particle Green function of the $2+1$ dimensional theory to derive the effective action of the external fields. In fact, integrating out the spinor fields $\psi,\bar{\psi}$ in the related path integral yields the effective action

$$S_{eff}^{1+1} = G_{1D}(k_y)\int dxdt\,\zeta(x,t)\varepsilon_{rs}\partial_r A_s.$$

The coefficient $G_{1D}(k_y)$ is required to satisfy

$$\int G_{1D}(k_y)dk_y = N_1, \tag{4.20}$$

where the first Chern number N_1 is given by (4.9). Instead of the Cartesian coordinates we prefer to work with the polar coordinates $k,\ \theta$, where $k_x = k\cos\theta,\ k_y = k\sin\theta$. Similar to (4.20) we would like to introduce $G(\theta)$ satisfying

$$\int_0^{2\pi} G(\theta)d\theta = N_1, \tag{4.21}$$

and define the $(1+1)$-dimensional effective action as

$$S_{1+1} = G(\theta)\int dxdt\,\zeta(x,t)\varepsilon_{rs}\partial_r A_s. \tag{4.22}$$

Although it can be deduced directly from the definition (4.21), we can also obtain $G(\theta)$ by writing the components of the Abelian Berry gauge field (4.16) in polar coordinates:

$$\mathscr{A}_\theta = -\frac{k}{2E(E+m)},\ \mathscr{A}_k = 0.$$

The Berry curvature remains the same

$$\mathscr{F}_{k\theta} = \frac{1}{k}\left[\frac{\partial(k\mathscr{A}_\theta)}{\partial k} - \frac{\partial \mathscr{A}_k}{\partial \theta}\right] = -\frac{m}{2E^3},$$

and allows us to calculate explicitly $G(\theta)$ as

$$\begin{aligned} G(\theta) &= \frac{1}{2\pi}\int k dk \mathscr{F}_{k\theta} \\ &= -\frac{m}{4\pi}\int_D \frac{dE}{E^2} = \frac{N_1}{2\pi}. \end{aligned}$$

Now, one can define the one dimensional charge polarization [52, 53] $P(\theta)$ by

$$\frac{\partial P(\theta)}{\partial \theta} \equiv G(\theta). \tag{4.23}$$

Adopting the first Chern number calculated in (4.10), $N_1 = 1$, we solve (4.23) by

$$P(\theta) = \frac{\theta}{2\pi}. \tag{4.24}$$

The physical observable is not directly the charge polarization given by $P(\theta)$ but the adiabatic change in $P(\theta)$ along a loop, which is equal to

$$\Delta P = P(2\pi) - P(0) = 1.$$

The $(1+1)$-dimensional action (4.22) becomes

$$S_{1+1} = \frac{1}{2\pi}\int dx dt A_r \varepsilon_{rs}\partial_s \zeta(x,t), \tag{4.25}$$

for $N_1 = 1$. The action (4.25) leads to the current

$$j_r = \frac{1}{2\pi}\varepsilon_{rs}\partial_s\zeta(x,t),$$

known as the Goldstone-Wilczek formula [54] and gives the charge

$$Q = \frac{1}{2\pi}\int \frac{\partial\zeta(x,t)}{\partial x}dx = \frac{1}{2\pi}\Delta\zeta.$$

In fact, it corresponds to solitons on polyacetylene with charge $Q = 1/2$ for ζ changing from 0 to π and $Q = 1/3$ for $\Delta\zeta = 2\pi/3$ as it was obtained in [54].

4.2 4+1 Dimensional topological insulator and dimensional reduction to 3+1 and 2+1 dimensions

The topological field theory

$$S^{4+1}_{eff}[A] = \frac{N_2}{24\pi^2}\int d^5x\varepsilon^{ABCDE}A_A\partial_B A_C\partial_D A_E, \tag{4.26}$$

is designated as the effective action of the $4+1$ dimensional TRI topological insulators in [37]. It follows from (4.3). To derive the related second Chern number N_2 we deal with the $4+1$ dimensional realization of the Dirac Hamiltonian (2.30) which is provided by

$$\alpha_{1,2,3} = \begin{pmatrix} 0 & i\sigma_{1,2,3} \\ -i\sigma_{1,2,3} & 0 \end{pmatrix}, \quad \alpha_4 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.27}$$

Observing that $\rho_i = (i\sigma_1, i\sigma_2, i\sigma_3, -1)$, the non-Abelian Berry gauge fields can be obtained from (2.37) as

$$\mathscr{A}_1 = \frac{\sigma_3 k_2 - \sigma_2 k_3 - \sigma_1 k_4}{2E(E+m)}, \quad \mathscr{A}_2 = \frac{-\sigma_3 k_1 + \sigma_1 k_3 - \sigma_2 k_4}{2E(E+m)}, \tag{4.28}$$

$$\mathscr{A}_3 = \frac{\sigma_2 k_1 - \sigma_1 k_2 - \sigma_3 k_4}{2E(E+m)}, \quad \mathscr{A}_4 = \frac{\sigma_1 k_1 + \sigma_2 k_2 + \sigma_3 k_3}{2E(E+m)}. \tag{4.29}$$

By definition the Berry gauge field corresponding to the $4+1$ dimensional Dirac Hamiltonian can also be derived by considering the explicit solutions of the Dirac equation as it was done in [55]. They work in the chiral representation, so that the Berry gauge field components which they obtain differ from (4.28),(4.29).

One can show that the field strength components $\mathscr{F}_{ij} = \partial\mathscr{A}_j/\partial k_i - \partial\mathscr{A}_i/\partial k_j - i[\mathscr{A}_i, \mathscr{A}_j]$, are

$$\begin{aligned}
\mathscr{F}_{12} &= \frac{1}{2E^3(E+m)}\left[\sigma_3(-E(E+m)+k_1^2+k_2^2)+\sigma_2(k_1k_4-k_2k_3)-\sigma_1(k_2k_4+k_1k_3)\right], \\
\mathscr{F}_{13} &= \frac{1}{2E^3(E+m)}\left[\sigma_2(E(E+m)-k_1^2-k_3^2)+\sigma_1(k_1k_2-k_3k_4)+\sigma_3(k_1k_4+k_2k_3)\right], \\
\mathscr{F}_{14} &= \frac{1}{2E^3(E+m)}\left[\sigma_1(E(E+m)-k_1^2-k_4^2)-\sigma_2(k_1k_2+k_3k_4)-\sigma_3(k_1k_3-k_2k_4)\right], \\
\mathscr{F}_{23} &= \frac{1}{2E^3(E+m)}\left[\sigma_1(-E(E+m)+k_2^2+k_3^2)-\sigma_2(k_1k_2+k_3k_4)-\sigma_3(k_1k_3-k_2k_4)\right], \\
\mathscr{F}_{24} &= \frac{1}{2E^3(E+m)}\left[\sigma_2(E(E+m)-k_2^2-k_4^2)-\sigma_1(k_1k_2-k_3k_4)-\sigma_3(k_1k_4+k_2k_3)\right], \\
\mathscr{F}_{34} &= \frac{1}{2E^3(E+m)}\left[\sigma_3(E(E+m)-k_3^2-k_4^2)+\sigma_2(k_1k_4-k_2k_3)-\sigma_1(k_2k_4+k_1k_3)\right].
\end{aligned}$$

Plugging them into (2.41) and taking the trace yield

$$N_2 = \frac{3}{4\pi^2}\int(-\frac{m}{2E^5})d^4k. \tag{4.30}$$

To calculate it explicitly, we would like to deal with the four dimensional polar coordinates given by $k_1 = k\cos\phi_1$, $k_2 = k\sin\phi_1\cos\phi_2$, $k_3 = k\sin\phi_1\sin\phi_2\cos\phi_3$ and $k_4 = k\sin\phi_1\sin\phi_2\sin\phi_3$, where the angles ϕ_1, ϕ_2, ϕ_3, respectively, take values in the intervals $[0,\pi],[0,\pi],[0,2\pi]$. The volume element is $d^4k = k^3\sin^2\phi_1\sin\phi_2 dk d\phi_1 d\phi_2 d\phi_3$. Hence, after the change of variable by (3.41), one can show that (4.30) can be written as

$$N_2 = \frac{3m}{4}\int_D \frac{m^2-E^2}{E^4}dE. \tag{4.31}$$

When D is taken to be an overlap of the $E>0$ and $E<0$ domains, we may deal with

$$N_2 = \frac{3m}{4}\int_{-\infty}^{m}\frac{m^2-E^2}{E^4}dE + \frac{3m}{4}\int_{-m}^{\infty}\frac{m^2-E^2}{E^4}dE = 1. \tag{4.32}$$

4.2.1 Dimensional reduction to $3+1$ dimensions

Dimensional reduction of the $4+1$ dimensional effective action given by (4.1) to $3+1$ dimensions can be described by the Lagrangian density

$$\mathscr{L}_{3+1}[\psi,\bar{\psi},A] = \bar{\psi}\left[\gamma^\alpha(p_\alpha + A_\alpha) + \gamma_4\tilde{\theta} - m\right]\psi, \tag{4.33}$$

where $\alpha = 0,\cdots,3$. The external field $\tilde{\theta}(x_\alpha)$ is the reminiscent of the gauge field A_4. ψ, $\bar{\psi}$ fields can be integrated out through the one particle Green function of $4+1$ dimensional theory introducing the parameter k_4 by setting $\tilde{\theta} = k_4 + \theta(x_\alpha)$. By keeping track of the phase space volume one can obtain the $3+1$ dimensional effective action as

$$S^{3+1}_{eff} = \frac{G_{3D}(k_4)}{4\pi}\int d^4x\theta\varepsilon^{\alpha\beta\gamma\eta}\partial_\alpha A_\beta\partial_\gamma A_\eta, \tag{4.34}$$

where the coefficient is given through the condition

$$\int G_{3D}(k_4)dk_4 = N_2. \tag{4.35}$$

We would like to modify this construction by working with the four dimensional polar coordinates and proposing that the action describing the descendant theory is given by

$$S_{3+1} = \frac{G_3(\phi_3)}{4\pi}\int d^4x\theta\varepsilon^{\alpha\beta\gamma\eta}\partial_\alpha A_\beta\partial_\gamma A_\eta,$$

whose coefficient, like (4.35), is required to satisfy the condition

$$\int_0^{2\pi} G_3(\phi_3)d\phi_3 = N_2.$$

Thus, the coefficient $G_3(\phi_3)$ can be obtained as

$$G_3(\phi_3) = \frac{1}{32\pi^2}\int \varepsilon_{ijkl}\mathrm{tr}(\mathscr{F}_{ij}\mathscr{F}_{kl})k^3\sin^2\phi_1\sin\phi_2 dk d\phi_1 d\phi_2 = \frac{N_2}{2\pi}, \tag{4.36}$$

with the definition (4.31) of the second Chern number N_2.

Similar to the one-dimensional charge polarization (4.23) one can associate the coefficient $G_3(\phi_3)$ to $P_3(\phi_3)$ through the relation [37]

$$\int_0^{2\pi} \frac{\partial P_3(\phi_3)}{\partial\phi_3}d\phi_3 \equiv \int_0^{2\pi} G_3(\phi_3)d\phi_3 = N_2.$$

Hence the “magnetoelectric polarization" can be obtained as

$$P_3(\phi_3) = \frac{N_2}{2\pi}\phi_3. \tag{4.37}$$

Observe that like the one-dimensional case, for $\Delta\phi_3 = 2\pi$ it changes by $\Delta P_3 = 1$ if we choose $N_2 = 1$ as it is calculated in (4.32). $P_3(\phi_3)$ depends linearly on ϕ_3 due to the fact that the second Chern character corresponding to free Dirac particle depends only on k. Interacting Dirac particles may give rise to polarizations which would not be linearly dependent on ϕ_3.

By inserting the definition (4.36) into (4.34) the effective action becomes

$$S_{3+1} = \frac{N_2}{8\pi^2}\int d^4x\theta\varepsilon^{\alpha\beta\gamma\eta}\partial_\alpha A_\beta\partial_\gamma A_\eta. \tag{4.38}$$

It can be written equivalently as

$$S_{3+1} = \frac{1}{4\pi}\int d^4x P_3(\theta)\varepsilon^{\alpha\beta\gamma\eta}\partial_\alpha A_\beta\partial_\gamma A_\eta,$$

where $P_3(\theta) = N_2\theta/2\pi$. This describes the axion electrodynamics which is invariant under the shift $\theta \to \theta + 2\pi$ [3, 56].

4.2.2 A hypothetical model for $3+1$ dimensional topological insulators

In spite of the fact that the underlying topological gauge theory (4.26) is manifestly TRI, the theory given by the descendant action (4.38) is TRB except for the values $\theta = 0, \pi$. Nevertheless, we may deal with the TRB action (4.38) but introduce a TRI hypothetical model generalizing the spin Hall effect for graphene [8]. The current following from the action (4.38) is

$$j^{\alpha} = \frac{N_2}{(2\pi)^2}\varepsilon^{\alpha\beta\gamma\eta}\partial_{\beta}\theta\partial_{\gamma}A_{\eta}.$$

Assuming $\theta = \theta(z)$ and considering the in-plane electric field $E_a(x,y)$; $a = 1,2$, we obtain the current [57]

$$j_a = \frac{N_2}{(2\pi)^2}\partial_z\theta(z)\varepsilon_{ab}E_b(x,y). \tag{4.39}$$

The Hall current can be introduced by integrating (4.39) along the coordinate z as

$$J_a(x,y) \equiv \int j_a dz = \sigma_H\varepsilon_{ab}E_b(x,y). \tag{4.40}$$

It leads to the surface Hall conductivity σ_H [27, 37]

$$\sigma_H = \frac{e^2}{\hbar}\frac{N_2}{(2\pi)^2}\int \partial_z\theta dz = \frac{e^2}{\hbar}\frac{N_2}{(2\pi)^2}\Delta\theta. \tag{4.41}$$

Obviously we defined $\Delta\theta = \theta(\infty) - \theta(-\infty)$, which is non-vanishing for an adequate domain wall or at an interface plane between two samples.

Now we should define the second Chern number (4.31) appropriately. We suppose that all negative energy states are occupied till the Fermi level taken as the first positive energy value $E_F = m$, so that we get

$$N_2 = \frac{3m}{4}\int_{-\infty}^{m}\frac{m^2 - E^2}{E^4}dE = 1/2. \tag{4.42}$$

Considering a plane of interface which yields $\Delta\theta = 2\pi$ the Hall conductivity becomes

$$\sigma_H = \frac{e^2}{2h}.$$

In the representation (4.27) the $4+1$ dimensional Dirac Hamiltonian (2.30) is TRI where the time reversal operator can be taken as $T_{4+1} = \alpha_2\alpha_4 K$. However, the Hamiltonian corresponding to the action (4.33) for $A_{\alpha} = 0$,

$$H_{3+1} = \boldsymbol{\alpha}\cdot\boldsymbol{k} + \alpha_4\tilde{\theta} + m\beta, \tag{4.43}$$

violates time reversal symmetry. We will present a hypothetical model which is time reversal invariant emulating the spin Hall effect for graphene. Let α_i act on sublattices with two Dirac points. Assume that around these points which are interchanged under time reversal transformation, electrons are described by the Hamiltonians as in (4.43). Moreover the third component of the spin given by the Pauli matrix $s_z = \mathrm{diag}(1,-1)$ is included and conserved. Thus, we propose to consider the Hamiltonian

$$\widetilde{H}_{3+1} = \widetilde{\boldsymbol{\alpha}} \cdot \boldsymbol{k} + \widetilde{\alpha}_4 \tilde{\theta} + \tau_z s_z \beta m, \tag{4.44}$$

where $\tau_z = \mathrm{diag}(1,-1)$ and in terms of α_i and β given by (4.27) we defined

$$\widetilde{\alpha}_i = (\alpha_1, \tau_z \alpha_2, \alpha_3, \alpha_4).$$

Now, as in Section 4.1.1, the time reversal operator interchanging the Dirac points and the third components of the spin can be defined by $T = \tau_y s_y K$, so that (4.44) is TRI. Obviously, we can obtain (4.44) through the dimensional reduction from the $4+1$ dimensional action corresponding to the following free Hamiltonian

$$\widetilde{H} = \widetilde{\alpha}_i \cdot k_i + \tau_z s_z \beta m \equiv \mathrm{diag}(\widetilde{H}^{\uparrow +}, \widetilde{H}^{\uparrow -}, \widetilde{H}^{\downarrow +}, \widetilde{H}^{\downarrow -}). \tag{4.45}$$

As we show in Appendix B, the four dimensional Hamiltonians defined by (4.45) correspond to the second Chern numbers

$$N_2^{\uparrow +} = N_2^{\uparrow -} = -N_2^{\downarrow +} = -N_2^{\downarrow -} = N_2,$$

where N_2 is given by (4.31). Repeating the procedure yielding (4.40)-(4.42) in the presence of a domain wall we can obtain the dissipationless spin current as

$$J_a^s = J_a^{\uparrow +} + J_a^{\uparrow -} - J_a^{\downarrow +} - J_a^{\downarrow -} = \sigma_{SH} \varepsilon_{ab} E_b(x,y),$$

with the spin Hall conductivity

$$\sigma_{SH} = \frac{e}{4\pi} \left(N_2^{\uparrow +} + N_2^{\uparrow -} - N_2^{\downarrow +} - N_2^{\downarrow -} \right) = \frac{e}{2\pi}.$$

for $\Delta\theta = 2\pi$. It is equal to the spin Hall conductivity for graphene (4.19).

4.2.3 Dimensional reduction to $2+1$-dimensions

The $2+1$ dimensional Lagrangian density

$$\mathscr{L}_{2+1}[\psi,\bar{\psi},A]=\bar{\psi}\left[\gamma^{\mu}\left(p_{\mu}+A_{\mu}\right)+\gamma_3\zeta_3+\gamma_4\zeta_4-m\right]\psi,$$

describes the dimensionally reduced theory. The fields $\zeta_3(x_\mu),\zeta_4(x_\mu)$ are the reminiscent of the gauge fields A_3,A_4, of the $4+1$ dimensionally theory whose action is given by (4.1) for $d=4$. By setting $\zeta_3(x_\mu)=k_3+\tilde{\phi}(x_\mu)$ and $\zeta_4(x_\mu)=k_4+\tilde{\theta}(x_\mu)$, where k_3,k_4 are parameters playing the role of the momentum components in one particle Green functions. $2+1$ dimensional effective action is derived as as

$$S_{eff}^{2+1}=G_{2D}(k_3,k_4)\int d^3x\varepsilon^{\mu\nu\rho}A_{\mu}\partial_{\nu}\tilde{\phi}\partial_{\rho}\tilde{\theta}.$$

Its coefficient should fulfill the condition

$$\int G_{2D}(k_3,k_4)dk_3dk_4=N_2. \tag{4.46}$$

As in Section 4.2.1, we consider the four dimensional polar coordinates and propose that the action

$$S_{2+1}=G_2(\phi_2,\phi_3)\int d^3x\varepsilon^{\mu\nu\rho}A_{\mu}\partial_{\nu}\tilde{\phi}\partial_{\rho}\tilde{\theta}, \tag{4.47}$$

describes the $2+1$ dimensional descendant theory. Obviously, like (4.46) we pose the condition

$$\int_0^{\pi}\int_0^{2\pi}d\phi_2d\phi_3G_2(\phi_2,\phi_3)=N_2.$$

This can be solved by

$$G_2(\phi_2,\phi_3)=\frac{N_2}{4\pi}\sin\phi_2.$$

Proceeding as in [37] we introduce the vector field

$$\Omega_{\mu}\equiv\Omega_{\theta}\partial_{\mu}\theta+\Omega_{\phi}\partial_{\mu}\phi,$$

however by adopting the definitions

$$\Omega_{\theta}=-\frac{N_2}{4}\cos\phi,\ \Omega_{\phi}=-\frac{N_2}{4}\theta\sin\phi.$$

The field strength of the field Ω_{μ} is

$$\partial_{\mu}\Omega_{\nu}-\partial_{\nu}\Omega_{\mu}=\frac{N_2}{2}\sin\phi\left(\partial_{\nu}\theta\partial_{\mu}\phi-\partial_{\mu}\theta\partial_{\nu}\phi\right).$$

Let us define $\phi = \phi_2 + \tilde{\phi}$ and $\theta = \phi_3 + \tilde{\theta}$ as slowly varying fields, so that at the first order in derivatives we can write $G_2(\phi,\theta)\partial_\mu\theta\partial_\nu\phi \approx G_2(\phi_2,\phi_3)\partial_\mu\tilde{\theta}\partial_\nu\tilde{\phi}$. Therefore, the action (4.47) can be written in the form

$$S_{2+1} = \frac{1}{2\pi}\int d^3x\varepsilon^{\mu\nu\rho}A_\mu\partial_\nu\Omega_\rho. \tag{4.48}$$

The current generated by the field $\Omega_a,\ a = 1,2$, is

$$j^\Omega_a = \frac{e}{2\pi}\varepsilon_{ab}E_b,$$

where the electric field is given by $E_a = \partial_a A_0 - \partial_0 A_a$. It can be interpreted as the spin current yielding the spin Hall conductivity $\sigma_{SH} = e/2\pi$. Hence, by attributing the adequate time reversal transformation properties to the gauge field Ω_μ, the action (4.48) corresponds to the TRI $2+1$ dimensional model of [8] which we discussed in Section 4.1.1,

The action (4.48) generates the electric current

$$j^\mu = \frac{1}{2\pi}\varepsilon^{\mu\nu\rho}\partial_\nu\Omega_\rho.$$

For fields satisfying $\phi = \phi(x),\ \theta = \theta(y)$ it gives the total charge

$$Q = e\frac{N_2}{4\pi}\int dxdy\sin\phi\partial_x\phi\partial_y\theta = e\frac{N_2}{4\pi}\int_0^\pi \sin\phi d\phi\int_0^{2\pi} d\theta = eN_2.$$

On the other hand the three dimensional Skyrmion field $\boldsymbol{n}$ coupled to Dirac fermion in $2+1$ dimensions yields the current [58]

$$j^T_\mu = \frac{1}{8\pi}\varepsilon_{\mu\nu\rho}\boldsymbol{n}\cdot\partial^\nu\boldsymbol{n}\times\partial^\rho\boldsymbol{n}.$$

The Skyrmion field configuration discussed in [59] satisfying $\boldsymbol{n}^2 = 1$ possesses the charge $Q^T = 2e$. Hence, if we deal with $N_2 = 1$, the Skyrmion theory can be described for the field configurations satisfying

$$\sin\phi\left(\partial_\nu\theta\partial_\mu\phi - \partial_\mu\theta\partial_\nu\phi\right) = \frac{1}{4}\boldsymbol{n}\cdot\partial_\nu\boldsymbol{n}\times\partial_\mu\boldsymbol{n},$$

which leads to $j^T_\mu = 2j_\mu$. In principle this condition can be solved to obtain $\boldsymbol{n}$ in terms of the fields ϕ and θ.

Observe also that for the field configurations $\phi = \phi(t),\ \theta = \theta(y)$ the net charge flow in x direction is

$$\int dtdy j_x = -N_2. \tag{4.49}$$

Moreover, we can introduce the magnetoelectric polarization in the form given (4.37) by defining it as

$$P_3(\theta) = -\int_0^{\pi} d\phi \Omega_{\phi}/\pi = \frac{N_2}{2\pi}\theta.$$

Then the pumped charge (4.49) can also be written as $\Delta Q = \int dP_3 = N_2$ which gives $\Delta Q = 1/2$ for $N_2 = 1/2$, as it is given for the Hall effect (4.42).

5. CONCLUSIONS

One of the main topics addressed was the consequences of incorporating spin into the semiclassical formalism which is described in Section 3. A differential form formalism was employed. In our semiclassical formalism, acting in the classical phase space where position and momentum are dynamical variables, but spin comes into play in the matrix-valuedness of the symplectic 1-form and the Berry gauge fields. This leads to matrix-valued time evolutions of position and momentum variables. It was demonstrated that our formalism is suitable to calculate the spin Hall conductivity for Dirac-like systems. The spin Hall current, thus the spin Hall conductivity was defined through the time evolutions of position and momentum variables. Dealing with electrons, without loss of generality the third component of spin was considered whose explicit matrix form depends on the details of the underlying Dirac-like Hamiltonian. When the third component of spin is conserved at the quantum level, constructing the spin current is not intriguing. However, the spin Hall effect can persist even if the third component of spin is not conserved. Within the Kane-Mele model of graphene, it was shown in Section 3 that even for the systems where the spin is not a good quantum number, it is always possible to establish the leading contribution to the spin Hall effect in terms of the Berry field strength derived in the appropriate basis. Moreover, it was demonstrated that it is always given in terms of the spin Chern number which is defined to be one half the difference of the Chern numbers of spin-up and spin-down sectors.
To investigate the Kane-Mele model in $2+1$ dimensions and topological insulators in $4+1$ dimensions, we mainly employ the Foldy-Wouthuysen transformation of the Dirac Hamiltonian. The Foldy-Wouthuysen transformation diagonalizes the Dirac Hamiltonian. In order to define the Berry gauge field, the adiabaticity condition dictates that one should operate within either the positive energy eigenstate states or the negative energy eigenstates. Thus, the Foldy-Wouthuysen transformation turns out to be a powerful tool in the investigation of a physical system with topological properties related to a Dirac-like Hamiltonian. Topological properties are characterized through the related Chern numbers: The first Chern number in $2+1$ dimensions and the second

Chern number in $4+1$ dimensions acquired by the Berry field strengths.

In Section 4, we deal with the effective field theory of the $4+1$ dimensional time-reversal invariant topological insulator. The Foldy-Wouthuysen transformation was employed to obtain the Berry gauge fields of Dirac Hamiltonian and the first and second Chern numbers were derived explicitly. In the line of the Kane-Mele model, a hypothetical model was introduced that yields a dissipationless spin current in $3+1$-dimensions. This can be helpful in understanding some aspects of the three dimensional time-reversal invariant topological insulators if its relation to some realistic models can be demonstrated. Moreover, in terms of our explicit constructions one can discuss $\mathbb{Z}_2$ topological classification of time-reversal invariant insulators in a tractable fashion.

In principle our approach can be generalized to the interacting Dirac particles where the related Foldy-Wouthuysen transformation at least perturbatively exists, where the inverse of rest energy of the particle is the perturbation parameter. However, it is also possible to employ $\hbar$ as the perturbation parameter [61]. Recently, the latter approach attracted considerable interest in the kinetic theory of the chiral particles [62, 63]. We believe that it suits well in developing our approach to more complicated interacting Dirac-like systems which can be useful in either condensed matter or high energy systems.

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APPENDICES

APPENDIX A: Kubo Formula Derivation of Spin Hall Conductivity
APPENDIX B: Berry Gauge Field and Curvature in $4+1$ Dimensions
APPENDIX C: Eigenstates of Kane-Mele Hamiltonian in the Presence of Rashba Spin-orbit Coupling

APPENDIX A : Kubo Formula Derivation of Spin Hall Conductivity

Introducing the label $I = (\uparrow+, \uparrow-, \downarrow+, \downarrow-)$ corresponding to each of the two dimensional Dirac-like Hamiltonians given in (3.27), (3.28),

$|p^I\rangle$ and $|a^I\rangle$ denote, respectively, the positive energy $E = \sqrt{v_F^2\hbar^2k^2 + \Delta_{SO}^2}$ and the negative energy $-E$ eigenspinors of the related Dirac-like Hamiltonians. For instance, let us consider the Hamiltonian for the spin up carriers in the K valley, $H^{\uparrow+}$, whose eigenspinors can be written in the chiral basis as

$$|p^{\uparrow+}\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2})e^{i\phi} \end{pmatrix}, \tag{A.1}$$

$$|a^{\uparrow+}\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ -\cos(\frac{\theta}{2})e^{i\phi} \end{pmatrix}, \tag{A.2}$$

where $\cos\theta = \frac{\Delta_{SO}}{E}$ and $\tan\phi = \frac{k_y}{k_x}$. When the Fermi level of graphene is in the gap generated by the spin orbit interaction we should set $\boldsymbol{k} = 0$, hence $\cos\theta = 1$

we need to consider their eigenspinors. In fact, for the spin up carriers in the K' valley described with $H^{\uparrow-}$ the eigenspinors are

$$|p^{\uparrow-}\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ -\cos(\frac{\theta}{2})e^{-i\phi} \end{pmatrix}, \tag{A.3}$$

$$|a^{\uparrow-}\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2})e^{-i\phi} \end{pmatrix}. \tag{A.4}$$

Similarly, for the spin down carriers in the K valley, we can show that the eigenspinors of the Hamiltonian $H^{\downarrow+}$ are

$$|p^{\downarrow+}\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ \cos(\frac{\theta}{2})e^{i\phi} \end{pmatrix}, \tag{A.5}$$

$$|a^{\downarrow+}\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ -\sin(\frac{\theta}{2})e^{i\phi} \end{pmatrix}. \tag{A.6}$$

The eigenspinors of the Hamiltonian $H^{\downarrow-}$ corresponding to the spin down carriers in the K' valley are

$$|p^{\downarrow-}\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ -\sin(\frac{\theta}{2})e^{-i\phi} \end{pmatrix}, \tag{A.7}$$

$$|a^{\downarrow-}\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ \cos(\frac{\theta}{2})e^{-i\phi} \end{pmatrix}. \tag{A.8}$$

Kubo formula corresponding to the Hamiltonians (3.27), (3.28) can be written in the notation introduced as [10]

$$(\sigma_H^S)^I = \frac{e\hbar^2}{2}\int^{E_F^{(2)}} \frac{d^2k}{(2\pi)^2} \frac{2\mathrm{Im}\left[\langle a^I|\dot{y}|p^I\rangle\langle p^I|\dot{x}|a^I\rangle\right]}{4E^2}, \tag{A.9}$$

where $\dot{x}$, $\dot{y}$ are the related velocity operators which can be read from (**??**) and

$$E_F^{(2)} = \sqrt{v_F^2 \hbar^2 k_F^2 + \Delta_{SO}^2}.$$

For $H^{\uparrow +}$ the velocity operators are $\dot{x} = v_F \sigma_x$, $\dot{y} = v_F \sigma_y$ and the eigenspinors $|p^{\uparrow +}\rangle$ and $|a^{\uparrow +}\rangle$ are given in (**A.1**) and (**A.2**). Employing them in (**A.9**) leads to [**?**]

$$(\sigma_H^S)^{\uparrow +} = -\frac{e}{8\pi} \frac{\Delta_{SO}}{E_F^{(2)}}. \tag{A.10}$$

For the spin up carriers in the K' valley, we set $\dot{x} = -v_F \sigma_x$, $\dot{y} = v_F \sigma_y$ and deal with the eigenspinors (**A.3**),(**A.4**). We obtain the same conductivity

$$(\sigma_H^S)^{\uparrow -} = -\frac{e}{8\pi} \frac{\Delta_{SO}}{E_F^{(2)}}. \tag{A.11}$$

The contributions arising from the spin down carriers in the K and K' valleys are also equal but differ in sign with the spin up contributions:

$$(\sigma_H^S)^{\downarrow +} = (\sigma_H^S)^{\downarrow -} = \frac{e}{8\pi} \frac{\Delta_{SO}}{E_F^{(2)}}. \tag{A.12}$$

To obtain the spin Hall conductivity we should take the difference of the spin up and spin down contributions as

$$\sigma_H^S = ((\sigma_H^S)^{\uparrow +} + (\sigma_H^S)^{\uparrow -}) - ((\sigma_H^S)^{\downarrow +} + (\sigma_H^S)^{\downarrow -}). \tag{A.13}$$

Inserting (**A.10**), (**A.11**) and (**A.12**) into (**A.13**) leads to the spin Hall conductivity

$$\sigma_H^S = -\frac{e}{2\pi} \frac{\Delta_{SO}}{E_F^{(2)}}.$$

This is the same with the result obtained in terms of the Berry phase (3.38).

APPENDIX B : Berry Gauge Field and Curvature in $4+1$ Dimensions

The Hamiltonian (4.45) which comprises τ_z and spin degrees of freedom denoted $\pm$ and $\uparrow\downarrow$, respectively, yields the $4+1$ dimensional Dirac Hamiltonians

$$\widetilde{H}^{\uparrow+} = \alpha_1 k_1 + \alpha_2 k_2 + \alpha_3 k_3 + \alpha_4 k_4 + m\beta, \quad \widetilde{H}^{\uparrow-} = \alpha_1 k_1 - \alpha_2 k_2 + \alpha_3 k_3 + \alpha_4 k_4 - m\beta, \tag{A.14}$$

$$\widetilde{H}^{\downarrow+} = \alpha_1 k_1 + \alpha_2 k_2 + \alpha_3 k_3 + \alpha_4 k_4 - m\beta, \quad \widetilde{H}^{\downarrow-} = \alpha_1 k_1 - \alpha_2 k_2 + \alpha_3 k_3 + \alpha_4 k_4 + m\beta. \tag{A.15}$$

Let us first consider the two spin up Hamiltonians (**A.14**). They yield slightly different non-Abelian Berry gauge fields

$$\mathscr{A}_1^{\uparrow\pm} = \frac{1}{2E(E+m)}(\pm\sigma_3 k_2 - \sigma_2 k_3 \mp \sigma_1 k_4),\ \mathscr{A}_2^{\uparrow\pm} = \frac{1}{2E(E+m)}(\mp\sigma_3 k_1 \pm \sigma_1 k_3 - \sigma_2 k_4),$$
$$\mathscr{A}_3^{\uparrow\pm} = \frac{1}{2E(E+m)}(\sigma_2 k_1 \mp \sigma_1 k_2 \mp \sigma_3 k_4), \quad \mathscr{A}_4^{\uparrow\pm} = \frac{1}{2E(E+m)}(\pm\sigma_1 k_1 + \sigma_2 k_2 \pm \sigma_3 k_3).$$

The corresponding field strengths can be calculated as

$$\begin{aligned}
\mathscr{F}_{12}^{\uparrow\pm} &= \frac{1}{2E^3(E+m)}\left[\mp\sigma_3(E(E+m)-k_1^2-k_2^2)+\sigma_2(k_1k_4-k_2k_3)\mp\sigma_1(k_2k_4+k_1k_3)\right],\\
\mathscr{F}_{13}^{\uparrow\pm} &= \frac{1}{2E^3(E+m)}\left[\sigma_2(E(E+m)-k_1^2-k_3^2)\pm\sigma_1(k_1k_2-k_3k_4)\pm\sigma_3(k_1k_4+k_2k_3)\right],\\
\mathscr{F}_{14}^{\uparrow\pm} &= \frac{1}{2E^3(E+m)}\left[\pm\sigma_1(E(E+m)-k_1^2-k_4^2)-\sigma_2(k_1k_2+k_3k_4)\mp\sigma_3(k_1k_3-k_2k_4)\right],\\
\mathscr{F}_{23}^{\uparrow\pm} &= \frac{1}{2E^3(E+m)}\left[\mp\sigma_1(E(E+m)-k_2^2-k_3^2)-\sigma_2(k_1k_2+k_3k_4)\mp\sigma_3(k_1k_3-k_2k_4)\right],\\
\mathscr{F}_{24}^{\uparrow\pm} &= \frac{1}{2E^3(E+m)}\left[\sigma_2(E(E+m)-k_2^2-k_4^2)\mp\sigma_1(k_1k_2-k_3k_4)\mp\sigma_3(k_1k_4+k_2k_3)\right],\\
\mathscr{F}_{34}^{\uparrow\pm} &= \frac{1}{2E^3(E+m)}\left[\pm\sigma_3(E(E+m)-k_3^2-k_4^2)+\sigma_2(k_1k_4-k_2k_3)\mp\sigma_1(k_2k_4+k_1k_3)\right].
\end{aligned}$$

Although they are different, they generate the same second Chern number equal to (4.30):

$$N_2^{\uparrow\pm} = \frac{1}{32\pi^2}\int d^4k\,\varepsilon_{ijkl}\,\mathrm{tr}\left[\mathscr{F}_{ij}^{\uparrow\pm}\mathscr{F}_{kl}^{\uparrow\pm}\right] = \frac{3}{4\pi^2}\int(-\frac{m}{2E^5})d^4k. \tag{A.16}$$

The non-Abelian Berry gauge fields corresponding to the two spin down Hamiltonians (**A.15**) can be shown to satisfy

$$\mathscr{A}_i^{\downarrow\pm}(k_1,k_2,k_3,k_4) = (-1)^{\delta_{4i}}\mathscr{A}_i^{\uparrow\pm}(k_1,k_2,k_3,-k_4),$$

without summation over the repeated indices. Thus, the components of the related Berry curvature are

$$\mathscr{F}_{ij}^{\downarrow\pm}(k_1,k_2,k_3,k_4) = (-1)^{\delta_{4i}+\delta_{4j}}\mathscr{F}_{ij}^{\uparrow\pm}(k_1,k_2,k_3,-k_4).$$

They yield the same second Chern number which is given by (**A.16**) up to a minus sign: $N_2^{\downarrow\pm} = -N_2^{\uparrow\pm}$.

APPENDIX C : Eigenstates of Kane-Mele Hamiltonian in the Presence of Spin-orbit Coupling

The Hamiltonian for the K subspace is obtained from (3.25) by setting $\tau_z = 1$:

$$H_K = \begin{pmatrix} \Delta_{SO} s_z & \mathbf{1}_s v_F (p_x - i p_y) + \lambda_R (s_y + i s_x) \\ \mathbf{1}_s v_F (p_x + i p_y) + \lambda_R (s_y - i s_x) & -\Delta_{SO} s_z \end{pmatrix}.$$

The eigenstates of H_K corresponding to the energy eigenvalues (3.41) can be shown to be

$$\Phi_1 = N_1 \begin{pmatrix} i\frac{p_x - i p_y}{p_x + i p_y} \\ \frac{E_1 - \Delta_{SO}}{v_F (p_x + i p_y)} \\ -i\frac{E_1 - \Delta_{SO}}{v_F (p_x + i p_y)} \\ 1 \end{pmatrix}, \Phi_2 = N_2 \begin{pmatrix} -i\frac{p_x - i p_y}{p_x + i p_y} \\ \frac{E_2 - \Delta_{SO}}{v_F (p_x + i p_y)} \\ -i\frac{E_2 - \Delta_{SO}}{v_F (p_x + i p_y)} \\ 1 \end{pmatrix},$$

$$\Phi_3 = N_3 \begin{pmatrix} i\frac{p_x - i p_y}{p_x + i p_y} \\ \frac{(E_3 - \Delta_{SO})}{v_F (p_x + i p_y)} \\ -i\frac{(E_3 - \Delta_{SO})}{v_F (p_x + i p_y)} \\ 1 \end{pmatrix}, \Phi_4 = N_4 \begin{pmatrix} -i\frac{p_x - i p_y}{p_x + i p_y} \\ \frac{(E_4 - \Delta_{SO})}{v_F (p_x + i p_y)} \\ i\frac{(E_4 - \Delta_{SO})}{v_F (p_x + i p_y)} \\ 1 \end{pmatrix},$$

where the normalizations are $N_\alpha(p) = \frac{v_F p}{\sqrt{2(v_F^2 p^2 + (E_\alpha - \Delta_{SO})^2)}}$.

When $\tau_z = -1$ is taken in (3.25), the Hamiltonian for the K' valley is obtained:

$$H_{K'} = \begin{pmatrix} -\Delta_{SO} s_z & -\mathbf{1}_s v_F (p_x + i p_y) - \lambda_R (s_y - i s_x) \\ -\mathbf{1}_s v_F (p_x - i p_y) - \lambda_R (s_y + i s_x) & \Delta_{SO} s_z \end{pmatrix}.$$

The eigenstates of $H_{K'}$ are as follows,

$$\Phi_5 = N_1 \begin{pmatrix} -i\frac{E_1 - \Delta_{SO}}{v_F (p_x + i p_y)} \\ 1 \\ i\frac{p_x - i p_y}{p_x + i p_y} \\ -\frac{E_1 - \Delta_{SO}}{v_F (p_x + i p_y)} \end{pmatrix}, \Phi_6 = N_2 \begin{pmatrix} i\frac{E_2 - \Delta_{SO}}{v_F (p_x + i p_y)} \\ 1 \\ -i\frac{p_x - i p_y}{p_x + i p_y} \\ -\frac{E_2 - \Delta_{SO}}{v_F (p_x + i p_y)} \end{pmatrix},$$

$$\Phi_7 = N_3 \begin{pmatrix} -i\frac{E_3 - \Delta_{SO}}{v_F (p_x + i p_y)} \\ 1 \\ i\frac{p_x - i p_y}{p_x + i p_y} \\ -\frac{E_3 - \Delta_{SO}}{v_F (p_x + i p_y)} \end{pmatrix}, \Phi_8 = N_4 \begin{pmatrix} i\frac{E_4 - \Delta_{SO}}{v_F (p_x + i p_y)} \\ 1 \\ -i\frac{p_x - i p_y}{p_x + i p_y} \\ -\frac{E_4 - \Delta_{SO}}{v_F (p_x + i p_y)} \end{pmatrix}.$$

The corresponding energy eigenvalues are given by (3.41) since $E_5 = E_1$, $E_6 = E_2$, $E_7 = E_3$, $E_8 = E_4$.

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