

Relativistic Electron in Solid Phase

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*“For more than 150 years we have used electrons for practical purposes. Yet they were only discovered in 1897. Early models described electrons in a metal as a gas. In 1956 the Russian physicist Lev Landau (Nobel Prize 1962) explained why electrons in a metal behave like nearly independent particles. Landau provided a model which can predict how electrons behave in increasingly sophisticated electronic applications. The whole microelectronics industry is based upon knowledge of how electrons move. **First practice, then theory, then practice again in constant interplay.** This is the stuff that science is made of”,*

Courtesy: <https://www.nobelprize.org/prizes/physics/1998/9580-practice-and-theory/>

Abstract:

This article presents a discussion on some of the important scientific events that has shaped our understanding of the behaviour of electron in solid materials. By looking at the history, one can appreciate how pure theoretical equations have led to new discoveries, and how investigations of materials under various external and internal stimuli have broadened the knowledge.

1. INTRODUCTION:

Schrödinger’s equation[1], the fundamental equation in quantum mechanics, provides complete description of quantum mechanical systems that are described by complex wave functions. Application of Schrödinger’s equation have led to profound understanding of the behaviour of electrons (many-body system) in the condensed matter systems. Schrodinger’s equation resembles the equation $\frac{p^2}{2m} + V = E$ if the momentum \vec{p} and energy E are written in quantum mechanical linear operator form and operated over the wave function Ψ . In similar line, for *relativistic particles*, if one starts from the relativistic energy-momentum relationship, $E^2 - p^2c^2 = m^2c^4$ or the four vector for $p^\mu p_\mu - m^2c^2 = 0$, by utilizing the relativistic four momentum operator $p^\mu = i\hbar\partial_\mu$, the Klein-Gordon equation is obtained [2, 3]. However, the equation applies to only spin 0 particles, hence not applicable for the behaviour of electron. The relativistic wave equation for electron was formulated by P.A.M. Dirac and published in his paper ‘the quantum theory of electron’ in 1928 where the wave functions are written as bispinors i.e., a column vector with four components [4]. It is a fundamental equation in quantum field theory which is compatible with both theory of

relativity and quantum mechanics of single particle. In the upcoming year of 1933, Schrodinger (1887-1961) and Dirac (1902-1984) shared the Nobel Prize in Physics for the discovery of new productive forms of atomic theory.

In 1929, Hermann Weyl published his seminal paper in which he wrote the electronic wave function as two component spinors with defined chirality [5]. Weyl equation is used to describe *massless* spin- $\frac{1}{2}$ fermion and Dirac spinor can be decomposed to two Weyl spinors in the zero mass limit [6]. In other words, the massless solution of Dirac equation corresponds to a pair of particles called Weyl fermions that have opposite chirality. This equation is compatible with relativistic theory but does not respect parity conservation. Hence, Pauli had initially expressed doubt on it. Eventually, it was understood that parity conservation is not sacred in all sorts of interactions and the validity of Weyl equation was regained. Regarding observation of relativistic particle, it was usual to think that they can be observed in high energy experiments. But the signature of relativistic electron happened to be a pleasant and useful surprise that has widened the horizon of the scientific community in terms of fundamental understanding, technological reach and experimental probe. In the following sections a historical picture depicting the important ideas and discoveries are presented.

2. GRAPHENE AND 2D ELECTRON SYSTEM:

2.1. Graphene

In Dirac's word "A great deal of my work is just playing with equations and seeing what they give". Dirac equation predicted the existence of antiparticles and antimatter and discussed the nature of relativistic electrons. Fast forward to the beginning of 21st century, graphene, that can be visualised as monolayer extracted from graphite, was isolated and electrical measurements were carried out [7, 8]. This allotrope of simple carbon in 2D form with crystalline honeycomb structure gave rise to ample of exotic properties. Graphene is transparent in optical region yet highly dense and possess high stability despite being atomically thin. It is stronger than steel, stretchable and has high mobility. Further, it shows fixed zero point conductivity that remains constant in temperature range of 4K to 100K [8]. The charge carriers in graphene were governed by Dirac equation rather than the Schrodinger's equation. They mimic the behaviour of relativistic particle with zero rest mass and a constant electronic speed (c^*) which was thought to be a property of massless photon and nearly massless neutrino (though two order smaller in magnitude). Accordingly,

graphene does show a linear dispersion relation $E = pc^* = \hbar kc^*$ near to the Fermi level. ($\because m = 0$) and the conduction and valence band meet at the Fermi level forming cones known as Dirac cones as shown in Fig. 1[8].

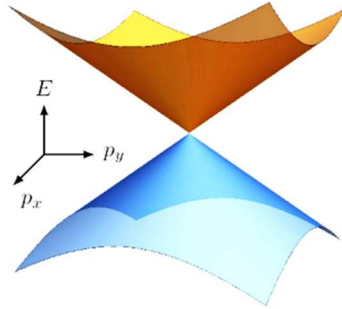


Figure 1: Conduction and valence band touching each other forming a Dirac cone. The dispersion relation is linear near the Fermi level.

The band structure of Graphene hosts six Dirac cones [9]. Such systems provided prized opportunities for the scientific community for the observation of quantum field theory phenomena in condensed matter in addition to the potential technological applications. Patents on graphene thin film device fabrications were made in 2006 and 2008 by WA DeHeeret *al.*, and for their breakthrough experiments Konstantin Novoselov and Andre Geim at their respective ages of 36 and 52, were awarded Physics Nobel prize 2010.

2.2. Quantum Hall effect:

2.2.1. Experimental discovery and application:

Long before the production of graphene and fabrication of graphene devices, in 1960s the behaviour of 2D electron systems that ought to govern the properties of graphene, were being investigated. Notably, Fowler's et al.'s pioneering work in which they observed Shubnikov–de Haas effect (an oscillation in conductivity at low temperature and strong magnetic field) in a two-dimensional electron gas in the (100) surfaces of p-type silicon implied that when electrons in a conductor are confined to a length of few nm, quantum phenomena can be visualized [10]. In the continued effort towards observation of quantum phenomena in 2D system, on 5th Feb 1980, around 2 A.M., a German physicist K. V. Klitzing (presently 81 year old) during the measurement of Hall voltage in silicon metal-oxide-semiconductor based field-effect transistor observed that the Hall resistance

(R_H) vary in steps when plotted as a function of magnetic field. This effect is called quantum Hall effect (QHE). The plot is presented in Fig. 2. The Hall (transverse) resistance vary in step whereas the longitudinal resistance becomes zero when R_H remains constant in a step. The remarkable thing about the steps was not just the appearance of the steps but the step size. As described in the original paper, the step size was observed to depend on fine structure constant ($\frac{e^2}{4\pi\epsilon_0\hbar c}$) and speed of light(c), the constants that are fundamentally important in quantum electrodynamics [11, 12]. In other words, the values were integral multiple of $\frac{h}{e^2}$ with an accuracy up to 9th decimal place. One of von Klitzing's samples which is a part of an exhibition at the Deutsches Museum in Bonn is shown in Fig.3a.

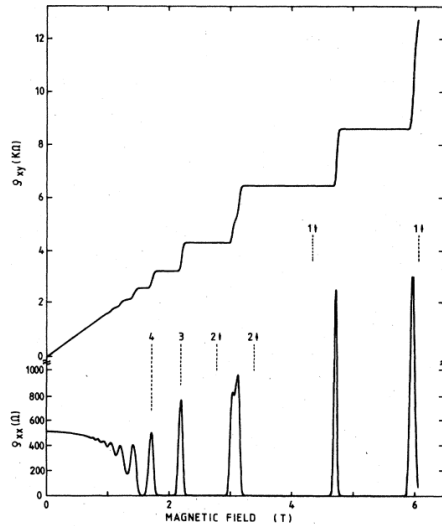


Figure 2: The variation of R_H with magnetic field, when $R_H=R_{xy}$ stays constant in one step, the longitudinal resistance R_{xx} becomes zero [12]

Klitzing et al., in 1985, suggested that in the limit of zero temperature, for an ideal system, the step values are independent of the geometry and material of the device, and other parameters within the experimental uncertainty. With necessary correction in R_H value for real experiment this can be applied in metrology[13]. Now, a new type of universal electrical resistor based on the von Klitzing constant $R_K = \frac{h}{e^2}$ (approximately equal to 25,813 Ω) is established for all 2D electron systems in strong magnetic fields with an uncertainty of less than one part in 10^{10} [14].

2.2.2. Semiclassical and topological understanding of QHE:

In quantum Hall (QH) regime, the behaviour of electron has been discussed and understood from various approaches. The ultraprecision of the step size and the robustness of the system to perturbation is the main objective of such approaches. In a semiclassical picture, for a 2D electron system, in presence of magnetic field, the energies of the cyclotron orbit takes quantized values which are known as Landau levels. In the interior, as shown in Fig. 3b, the electrons complete the full circular path and the Landau levels are fully occupied inhibiting the motion of electron and hence conduction. However, one dimensional and unidirectional (either clockwise or counter-clockwise) path known as QH edge mode is available for the electrons at the edge where the Landau levels are partially occupied. The important implication of such motion is that the electrons at the edge do not backscatter as they are supposed to jump to the other edge to change direction of motion. The edge modes conduct with perfect transmission and the corresponding resistance for such one dimensional current is equal to the Von Klitzing constant.

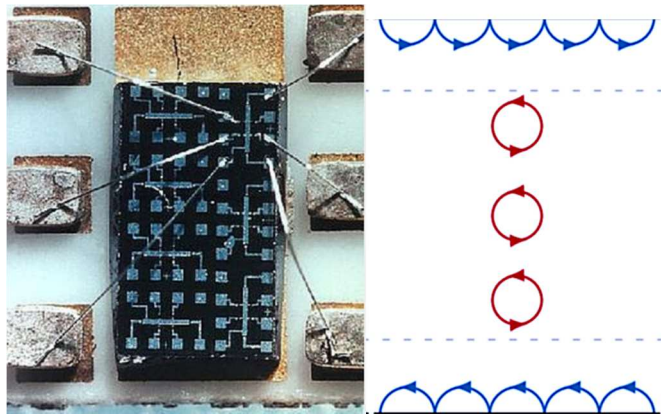


Figure 3: (a) one of the original sample used in the discovery of quantum Hall effect which is now part of an exhibition at the Deutsches Museum in Bonn [15] (b) cyclotron path in the bulk and edge of a 2D electron system.

In 1982, Thouless, Kohmoto, Nightingale and den Nijs explained QHE with perturbation theory approach and showed the conductivity to vary as an integer which was later termed in literature as TKNN invariant [16, 17]. Eventually, it was established that the TKNN invariant is same as the Chern number encountered in Berry-ology and topological theory, and QHE is a topological phase of matter. Few important terminologies pertaining to topological

theory are described as follows. Topology is a mathematical branch based purely on the geometry of object and their smooth variation. In topological theory, an orange and bottle gourd are topologically in same class whereas the coffee mug and a doughnut are in another class. Here, the defining parameter is the number of hole in the system, called 'genus'. For example, genus is zero for the orange and one for the coffee mug. Analogically, in the topological theory of condensed matter, the classification of materials is based on the shape or geometry of the electronic states or band. The guiding feature of such phases is that the electronic states that can smoothly transform to each other are topologically equivalent. Genus is one example of topological invariant for a particular topological phase, means, this cannot be changed without changing the phase.

In topological study, continuous evolution of a quantum state or the geometrical properties of the quantum wavefunction upon change in external stimulus is discussed in terms of Berry's parameters. Berry *phase* is the phase acquired by the quantum wavefunction when the state traverses a closed path and it can be observed in experiments. Berry *connection* or *potential* $A(k)$ is defined as given in equation 1.

$$A(k) = \langle u_k | i \nabla_k | u_k \rangle \quad (\text{equation 1})$$

Berry's *connection* is analogous to a vector potential and not a physically observable. Berry *curvature* is the curl of connection akin to a magnetic field and the integral of Berry *curvature* over the Brillouin zone gives rise to the Chern number. In QH regime, Chern number gives the number of edge state present in the system.

3. QUANTUM SPIN HALL EFFECT AND 3D TOPOLOGICAL INSULATOR:

With the advancement in the understanding of Quantum hall effect, further discovery of fractional Hall effect with emergent quasiparticles bearing fractional charge (1998 Physics Nobel prize), one more feather was added when a model of quantum spin Hall effect (QSHE) was proposed in 2005 by C. L. Kane and E. J. Mele, originally for graphene [18]. In the proposed model, the external magnetic field is replaced by internal magnetic field arising from the spin-orbit coupling (SOC) leading to a transition from a two-dimensional semimetallic state to a quantum spin Hall insulator. This proposed novel quantum spin Hall state is gapped in the bulk, but supports the transport of spin and charge in gapless edge states. Because of low mass of carbon, the spin-orbit coupling in graphene was not strong enough for a observable QSHE in the 2D system. However, QSHE

generalized to 3D culminated in the discovery of topological insulators (TI). The first topological insulator where the predicted QSHE was discovered was $\text{Bi}_{1-x}\text{Sb}_x$ alloy followed by $\text{HgTe}/(\text{Hg,Cd})\text{Te}$ quantum well, Bi_2Se_3 , and Bi_2Te_3 etc. [19]. TIs are attractive because of the dissipation-less conducting edge state even while being insulator in the bulk. So, in the bulk band structure of TIs, the conduction and valence band do not touch each other whereas the surface states form Dirac cone near exhibiting the relativistic electronic behaviour and because of this sometimes, TIs are loosely described as the 3D analogue of graphene. Nevertheless, graphene can be tuned for an enhanced SOC with heavy atom doping and substrate engineering [20, 21]. In the next section we discuss about a new class of materials in the topological family.

4. TOPOLOGICAL SEMIMETAL:

Followed by the discovery of topological insulators, Dirac semimetals were discovered in which the. After more than eight decades of its theoretical prediction, Weyl fermions were experimentally realised in TaAs for the first time in 2015 and then in the same family materials such as NbAs, TaP and NbP [22, 23]. The particle obeying Weyl equation exhibits linear dispersion relation in three dimension and in its band spectrum two non-degenerate bands meet at points called Weyl nodes [24]. Weyl nodes occur in pair and can be observed experimentally using angle resolved photo electron spectroscopy (ARPES).

5. SUMMARY:

The attempt at writing an relativistic equation for electron predicted the existence of antiparticle and antimatter. Eventually, the antiparticle was experimentally observed, and after more than 70 years, the relativistic behaviour of electron was realised as well in both 2D and 3D materials. Similarly, the effort to understand the observation in quantum Hall effect has now led to a new branch called study of topological materials. Evidently, the interplay of ‘practice and theory’ has helped the human civilization in making important strides both fundamentally, experimentally and technologically.

6. ACKNOWLEDGEMENT:

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