

## Bird of Passage at Four Universities

Student Days of Rudolph Peierls

*G Baskaran*

A glimpse into the student life of Rudolph Peierls, when he was 18–22 years old, gives us a flavor of happenings during the birth of quantum mechanics and how one started understanding properties of matter such as a metal and a semiconductor, using the newly found quantum mechanics. It also shows how a bright young mind could get nurtured and shaped when placed in a proper environment. Peierls, during his college days, had the opportunity to work closely with three great physicists, Sommerfeld, Heisenberg and Pauli, in succession spending one year with each. This experience had its effect – Peierls’s discovery of *hole theory* of electrical conduction in solids, formulation of the theory of thermal conduction in solids, analysis of anharmonic interactions and discovery of Umklapp process. It is also interesting that the *academic load* was far from a burden and was filled with weekend activities and summer vacations involving sailing, skiing, hiking and concerts.

Peierls was born in 1907 at Berlin in Germany. His schooling and most of his university education was in Germany. On finishing school he was keen on becoming an engineer. However, there was a general discouragement from his family. His father’s friend and a famous chemist, Fritz Haber, advised Peierls to take up experimental physics. But circumstances led him to choose theoretical physics as a career. Peierls stayed as a university student from the winter of 1925 till the summer of 1929. These four years, during the young age 18–22, created a special theoretical physicist, who began



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### Keywords

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Peierls was versatile and had a nose for important things: Peierls theory of hole conduction, Peierls Umklapp process, Landau–Peierls theory of diamagnetism, Peierls substitution, Peierls–Brillouin zone, Bethe–Peierls approximation, Peierls–Nabarro barrier, Peierls stress, Peierls variational principle, Landau–Peierls uncertainty principle, Peierls proof of phase transition in 2D Ising model, Peierls instability, Peierls–Kapur resonance and so on. Peierls was ready to put his mind to any quantitative question in physics. He would start from first principles and work his way up.

At the age of 27, already an established theoretical physicist, Peierls started working on nuclear physics. His first collaborator was Hans Bethe, his student days' friend at Munich University. Peierls' foray into nuclear physics resulted in the historically famous *Frisch–Peierls Memorandum* of 1940, which they sent to the British Government. This led to the Atomic Bomb Project, at first in Britain under the name *Tube Alloys Project* and later in USA as the *Manhattan District Project*. Later Peierls also wrote extensively about matters of public concern, especially to do with nuclear weapons and later the SDI proposals.

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Peierls has written several books: *The Laws of Nature* (1955), *Quantum Theory of Solids* (1956), *Surprises in Theoretical Physics* (1979), *More Surprises in Theoretical Physics* (1992), *Bird of Passage* (1985, memoir) and *Atomic Histories* (1997). There are also 2 volumes, *Sir Rudolf Peierls: Selected Private and Scientific Correspondence*, by Sabine Lee. In his two books on *Surprises in Theoretical Physics*, popular among physicists, Peierls describes several surprises from his personal experience, as a working theoretical physicist. In his biography *Bird of Passage*, the 2nd Chapter, 'The Student



Years' impressed me very much. The present article is my summary and some of my own comments on this chapter.

### I Year – University of Berlin

The university or college system in Germany in those days seems to have been special and different from that in UK or USA. There was maximum emphasis on academic freedom. There was no set syllabus of lecture courses. However, in physics, practical classes were a requirement. Problem solving classes were compulsory in theoretical physics. You could choose to move around different universities in your 3 to 5 years of university education. After this you could submit a thesis and get a PhD (called Dr. Phil). There was a great deal of difference between humanities and science education in universities.

During his 4 years of university education, Peierls spent the first year at Berlin, the second year at Munich, the third year at Leipzig and the fourth year at Zurich in Switzerland. The transfer to different universities happened in a most natural fashion.

Before joining the university of Berlin in the winter of 1925, Peierls got an opportunity to do a summer internship in the Research Department of a telephone company, 'Mix and Genert'. Here Peierls learnt to operate a power drill, a lathe, make small components for automatic circuits and build circuits. In the winter of 1925 he enrolled as a student of physics at the University of Berlin. His course work was 36 hours per week. Because of lack of seats in *practical (experimental) physics* he concentrated on theory and mathematics in his first year.

Two outstanding physicists of his time, Max Planck and Walther Nernst were his physics teachers at Berlin. Both were Nobel Laureates. Planck was well known

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<sup>1</sup> See *Resonance*, Vol.13, February 2008.

as a founder of modern quantum physics. He discovered, using the concept of *quantum of action*, the famous Planck distribution to describe the spectrum of black body radiation<sup>1</sup>. He introduced what is called the Planck's constant, a most fundamental constant in physics. Planck's course on theoretical physics had a 3-year cycle. When Peierls joined the course Planck was doing optics. Peierls was disappointed by Planck's lecture course, as Planck would only read verbatim from one of his books. The introductory physics course was given by Walther Nernst. Nernst was a physicist and physical chemist, famous for his establishment of the third law of thermodynamics. To the disappointment of Peierls, both these great men were apparently not great teachers.

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While physics courses were somewhat of a disappointment, Peierls seems to have liked his mathematics education at Berlin. It was not because of good teachers or good courses, but because of a unique setup called *Fachschaft*, a sort of club, which allowed students in each subject to organize academic activities of their own. The initiative came mostly from students, the professors approved, and the relations between student and staff were very friendly and informal. For example, in physics and mathematics there was MAPHA (Mathematisch-Physikalische Fachschaft), which organized discussion groups in which the seniormost students would help junior ones who had difficulties with their lectures. Even though physics was covered, the centre of gravity was in mathematics. The society had the usual social functions of a student organization, including arranging Christmas parties and the like. Peierls also remembers an excellent mathematics teacher, Professor Schur, a distinguished algebraist. Even though it was difficult for a beginner, Peierls was fascinated by Schur's lectures and got a taste of modern algebra. Another course, *Introduction to Higher Mathematics* apparently covered vectors,



matrices and orthogonal sets of functions. This must have prepared Peierls well to face the new quantum mechanics that he would encounter in the next 3 years.

Peierls writes, “But even with all these lectures, I did not feel that I was pressed for time. Berlin 1925 was an exciting place, full of intellectual life, theatres, cabarets, lectures on any topic imaginable, and I had time for all of this. I even joined a physical education class run by the university ...” Peierls also started sailing whenever he had time.

## II Year – University of Munich

After 2 semesters at Berlin, Peierls decided to move to Munich, known for Arnold Sommerfeld, the greatest teacher in theoretical physics at that time. There was no difficulty in changing universities, since there was no set syllabus. Peierls was fortunate and joined the beginning of Sommerfeld’s lecture cycle, starting with mechanics, the most basic part of physics. Peierls writes, “Sommerfeld’s introductory lectures were a model of clarity. He never let you forget that physics was an empirical subject, and that, although in doing theoretical work you were concerned with laws that could be expressed in mathematical terms, you always had to be clear about their empirical basis. He was also a master of mathematical techniques and managed to make very sophisticated methods transparent. But his greatest strength lay in the way he could guide research students. He always managed to find problems that were interesting and difficult enough to be of worth a serious effort, yet not too difficult for the student.”

It is a historical fact that Sommerfeld produced many outstanding students. Four among his doctoral students, Werner Heisenberg, Wolfgang Pauli, Peter Debye and Hans Bethe got Nobel Prizes. Two of Sommerfeld’s post graduate students, Linus Pauling and Isidor I Rabi

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When Peierls joined Munich at the age of 19, Sommerfeld was a central figure in quantum theory, well known partly because of ‘Bohr–Sommerfeld’ quantum theory. He was at the peak of his career. Peierls learned in a short time at Munich that there was a big revolution going on in physics. The old physics, based on Newton’s mechanics, Maxwell’s electrodynamics, and the statistical mechanics of Gibbs and Boltzmann, failed in the atomic domain. Many experimental facts involving the interaction of radiation with matter contradicted the established fact that light consisted of waves. Planck introduced the idea of *quantum of action* and Einstein made the bold proposal of light quantum or *photon*. Niels Bohr, inspired by Planck and Einstein tried to explain the behaviour of atoms, by invoking certain special orbits for electrons, defined by a rule in which Planck’s constant appears. Sommerfeld elaborated Bohr’s rules and the Bohr–Sommerfeld quantum theory served to explain many phenomena. But it failed with others, and it contained a number of internal contradictions.

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In the summer of 1925 Werner Heisenberg introduced his matrix mechanics for the quantum phenomena where orbits did not appear. In 1926 Schrödinger came up with his theory of matter wave and the famous Schrödinger equation. There was a lot of confusion about the meaning and reality of Schrödinger’s wave function and the wave particle duality. Max Born gave a meaning to the wave function in July 1926. Heisenberg developed it further and it resulted in the Heisenberg uncertainty principle. The modern quantum theory of measurement was born. It was at this time that Dirac wrote a paper that proposed a general theory of how measurements should be described in quantum mechanics. Similar work was



also done by P Jordan at Göttingen. These two papers constitute what is called *transformation theory*.

Peierls entered Sommerfeld's group as a young student of 19. Sommerfeld asked Peierls to review the two papers of Dirac and Jordan on transformation theory. Peierls learnt the papers well and presented them. It was apparently a success. However, one member of the audience Professor Wilhelm Wien, well known for *Wien displacement* law was not convinced of these new developments. This is perhaps a representative reaction at that time.

During this period Sommerfeld was trying to understand the behavior of electrons in metals. One of the major problems at that time was that the number of electrons, which are as many as the number of atoms in a metal, should contribute to specific heat, if all of them are moving freely. However, experimentally the electronic specific heat at room and high temperatures was small and was overwhelmed by the lattice contribution. In the context of atomic physics Sommerfeld's former student Pauli had enunciated a profound principle for identical particles in quantum mechanics, namely 'Pauli's exclusion principle'. That is, no two electrons will occupy the same quantum state. Sommerfeld applied this exclusion principle to the behaviour of electrons in a metal, in his free electron theory of metals. It was an instant success! Because of the Pauli principle, the electron waves organize themselves into a filled *Fermi sea* in momentum space. Only electrons in an energy range of  $k_B T$  will contribute to the specific heat, making the specific heat  $C_v \sim T$ . Pauli also used these ideas to discuss paramagnetism of metals, and discovered the famous Pauli paramagnetism.

Sommerfeld's electron theory of metals was written when Peierls was a student. So Peierls learned this very well. A historical side remark: Sommerfeld is supposed to have given a course of lectures at Madras and Calcutta

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on the new quantum mechanics, including application to metals and the idea of a Fermi sea, etc. Subramanyam Chandrasekhar was an attentive BSc student at the Presidency College of Madras. The rest is history – Chandrasekhar was quick to understand this and the result was the balancing of gravitational pull by Pauli pressure of a relativistic electron gas, and the famous Chandrasekhar's mass limit.

In Munich, Peierls met Hans Bethe, one year senior to him. They became collaborators later and life-long friends. Peierls' stay at Munich seems to have been a learning period. He also tried to initiate a MAPHA (Mathematisch-Physikalische Fachschaft) similar to the one he enjoyed at Berlin. The success was only partial as there was not much initiative from others. The society folded up soon after Peierls left Munich. Peierls makes a wise remark, "This taught me that it makes more than good intentions and a reasonable objective to run an organization".

### III Year – Leipzig University

In the spring of 1928 Sommerfeld left Germany to spend a year at the United States. On his advice Peierls left Munich and joined Werner Heisenberg at Leipzig. Heisenberg had at a young age started a school of theoretical physics. According to Peierls, "Where Sommerfeld enjoyed doing mathematics, for Heisenberg it was just a necessary tool. When he was faced with a problem, he would almost always intuitively know what the answer would be, and then look for a mathematical method likely to give him the answer..." When Peierls arrived at Leipzig, Heisenberg had finished his work on the uncertainty principle and was focussing on the theory of ferromagnetism in materials. After several ups and downs Heisenberg came up with the famous Heisenberg exchange interaction, which is a key part of the physics of quantum magnetism.

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Heisenberg was also excited by some spectral lines emitted by canal rays, which were wider than expected. Heisenberg thought that his uncertainty principle was at work. Peierls was asked to look into this problem of canal rays. Peierls wanted to sort out the problem from scratch. He first wanted to decide whether quantum mechanics was important to describe the motion of an object as heavy as an atom in these experiments. He came to the conclusion that quantum mechanics was not important in this context and that the line broadening was not due to Heisenberg's uncertainty principle. Heisenberg was quick to appreciate Peierls finding. Peierls writes, "The time taken for this abortive calculation was not wasted, however. It gave me some experience in setting up an approach to an unfamiliar situation, and, better still, it got me into the habit of never starting an analysis without first working out the orders of magnitude of the relevant effects on the back of an envelope."

His next assignment was a deeper problem of conductivity of metals at low temperatures. Felix Bloch, the first doctoral student of Heisenberg had just finished his quantum theory of conductivity of metals, by going beyond Sommerfeld's theory. Heisenberg was not satisfied with the idea of Sommerfeld and Pauli of the free electron theory of metals. What happens to the strong Coulomb repulsion among electrons? The free electron theory allows an atom to have equal probability to be neutral and positively and negatively charged. Heisenberg suggested that Peierls try the other extreme, namely, each atom always had its correct number of electrons – that is, it remains effectively neutral. This idea was successfully applied to molecules such as  $H_2$  and is called the Heitler–London approach. After some struggle Peierls came to the correct conclusion that this model will not give zero conductivity at low temperatures. To get any current through the system, in this model, it

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will be necessary for all the electrons in a row to jump at the same time, and the chance of this was entirely negligible.

In modern parlance, the situation suggested by Heisenberg, which Peierls analysed, will be called a Mott insulator, where there are no charge fluctuations at low energies. The valence electrons do not move because it costs Coulomb energy to delocalize and form a metallic state. In fact, there are many materials in Nature, such as  $\text{La}_2\text{CuO}_4$ , the parent compound of the famous high temperature cuprate superconductor, which are Mott insulators. In these narrow band materials short-range Coulomb repulsion prevents metalization and the valence electrons effectively stay home.

In a short span of time, Heisenberg suggested a third problem, which turned out to be fruitful. This was related to Hall effect in some conductors. Hall effect is a consequence of the Lorentz force experienced by electrons in an external magnetic field. In the presence of crossed electric and magnetic fields, the trajectory of charged particles deflects in the perpendicular direction, leading to what is called a 'Hall voltage'. The sign of the Hall voltage for a given direction of the electric and magnetic field, according to elementary Lorentz force, depends on the sign of the charge carriers. In some experiments the Hall voltage had a different sign and implied the presence of electric charge carriers with positive charge in some solids. This was the puzzle.

Peierls introduced a fundamental notion of 'hole' in an otherwise filled band, whose group velocity has a direction opposite to the phase velocity.

Peierls was familiar with Bloch's band theory and noticed that an accelerated electron wave packet within an isolated band keeps moving and gets reflected from the top of a band and reverses its velocity. Thinking along these lines he introduced a fundamental notion of 'hole' in an otherwise filled band, whose group velocity has a direction opposite to the phase velocity. Heisenberg was quick to appreciate this discovery of his student and it



resulted in the first two independent papers by Peierls, ‘On the theory of Galvano-magnetic Effects’ and ‘On the theory of Hall Effect’ in 1929. These are classic papers worth reading by students learning the quantum theory of solids. The concept of ‘hole’ is briefly discussed in *Appendix 1*.

While spending a summer vacation in England in 1928, Peierls plucked up courage to contact Dirac at Cambridge. Peierls had met Dirac once, when Dirac went to Leipzig for a talk. Dirac was extremely kind and introduced him to R H Fowler, the senior theorist at Cambridge. Once Fowler learnt that Peierls was from Leipzig, he became eager to learn about Heisenberg’s other student Bloch’s theory of electrical conductivity of metals. He arranged a talk by Peierls on Bloch’s theory in the Kapitza Club. It went well and Peierls also talked about his failed attempt to take care of electron–electron interaction in metallic transport in the extreme Heitler–London approximation. Fowler told Peierls that his student McCrea was trying to do the same. This must have given confidence to young Peierls that the problem that he had been tackling was truly international.

#### IV Year – ETH, Zurich

By the end of his third year in college, Peierls had learned enough mathematics, physics and quantum mechanics and he had also introduced a key notion in the quantum theory of solids, namely *hole* and its manifestation in Hall effect. Now Peierls got a chance to meet and work closely with another great mind. In the spring of 1928 Heisenberg recommended Peierls to go to ETH (Eidgenössische Technische Hochschule, the Federal Institute of Technology) in Zurich, Switzerland to work with Pauli, as Heisenberg would be going to USA for a visit. Peierls found Pauli to be a friendly professor. Peierls had some apprehension at the beginning because of a formidable reputation of Pauli’s sharp tongue.

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At the beginning of his stay in Zurich, Peierls had another project that he began at Leipzig. It was the translation of Louis de Broglie's book on wave mechanics from French into German. It gave him one more chance to learn the then evolving quantum mechanics. Peierls finished this task quickly and settled down to work with Pauli. Pauli suggested to Peierls a problem on anharmonic interaction of lattice vibrations in solids. In the theory of lattice vibrations of solids, starting from Einstein, Born and von Kármán and Debye, the normal modes of vibrations do not interact. For many equilibrium low temperature properties, this is an excellent approximation. However, for issues such as low temperature heat transport or thermal conductivity, interaction among the normal modes becomes important. At the level of classical equations of motion one has a non-linear equation. At the level of quantum mechanics the quantized lattice vibrations start interacting. Pauli realized that the most important elementary anharmonic interactions are three-phonon processes, where one phonon could decay into two phonons conserving total momentum. Pauli had done some calculations. This was the beginning of non-linear quantum field theory, similar to quantum electrodynamics.

Pauli realized that the most important elementary anharmonic interactions are three-phonon processes, where one phonon could decay into two phonons conserving total momentum.

Unlike quantum electrodynamics in free space, the excitations of lattice vibrations, namely phonons, arise in a periodic structure. Peierls recognized that they carry a pseudo-momentum and the momentum conservation is always modulo a reciprocal lattice vector. Physically, the underlying lattice could supply momentum and turn the direction of one phonon into two phonons moving in the opposite direction. This will cause momentum dissipation and hence finite thermal conductivity. Excitations with wave vector close to the reciprocal lattice vector have a high energy. Thus these processes, which Peierls named as *Umklapp* (flip over) processes are less important at low temperatures. At high tem-



peratures they are important, and they are the source of momentum decoherence and finite thermal conductivity. Peierls predicted that the thermal conductivity should go up as one goes to very low temperatures. Peierls' theory of thermal conductivity made significant improvement over Debye's theory, which ignored the lattice structure and the key Umklapp process and also Pauli's theory which had some technical errors. Umklapp process is briefly discussed in *Appendix 2*.

This detailed work on thermal conductivity formed Peierls' DPhil thesis, which was submitted to Leipzig. This was the end of 4 years of Peierls' student life.

### End of Peierls' 4 Years of Student Life

While continuing as an assistant to Pauli, after completing his degree, Peierls developed a theory to explain the origin of oscillations in physical properties of metals as a function of external magnetic field, known as de Haas van Alphen effect. This work was a non-trivial generalization of Landau theory of diamagnetism of metals. It explained successfully the oscillations in metallic bismuth and paved the way for remarkable experimental and theoretical developments.

In his book *Surprises in Theoretical Physics* you will find a nice account of some surprises related to absence of diamagnetism in classical systems (Bohr–van Leeuwen theorem) and how it emerges as Landau diamagnetism in quantum systems. You will find a nice discussion on this in the article by Prof S Dattagupta.

At Zurich, In addition to producing new work, Pauli met Lev Dev Landau, a visitor to Pauli. Landau was 6 months younger to Peierls. They became friends and collaborators and wrote some famous papers. Peierls made extensive tours in Europe and met several outstanding physicists from the former Soviet Union. He also met his future wife, Eugenia Kannegisser.

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I thank Prof. N Mukunda and Dr Rajlakshmi of *Resonance* for inviting me to write this article. This gave me a good opportunity to learn more about this remarkable physicist and his time. I thank Dr G Rajasekaran for bringing to my attention the association of Prof. Rajat Bhaduri, Prof. P Divakaran and his own, with Peierls at Oxford. I thank Professor N Kumar for carefully reading the manuscript.

**Indian Connections**

Peierls had some good Indian connections. Rajat Bhaduri (McMaster, Canada) was a Research Assistant to Peierls and worked closely with Peierls at Oxford. You will find the Article-in-a-Box (AIB) in this issue contributed by Prof R Bhaduri. G Rajasekaran (Matscience), P P Divakaran (Matscience and CMI), as PhD students of Dalitz, have seen Peierls in action at the Department of Theoretical Physics established and headed by him. Both of them have interesting things to say about Peierls. Ramesh Anishetty (Matscience) has seen Peierls in action at University of Washington, where Peierls was a half-time Professor. Peierls has written important papers with three Indian collaborators, Kundan S Singwi, P L Kapur and A K Das. While at Cambridge, Peierls wrote a paper that removed some technical objections raised by Eddington on the work of S Chandrasekhar dealing with the stability of stars and mass limit. Peierls has also visited India once.

It is amusing to note that it is because of Sommerfeld's long trip abroad, that included visits to Kolkata and Chennai in India, that Sommerfeld sent Peierls to Heisenberg at Leipzig!

**Appendix 1. Peierls's Concept of Hole in a Crystal**

In the Bohr model of an atom, atoms with higher atomic numbers are obtained by filling hydrogen-like orbitals respecting Pauli principle. This prescription, Aufbau principle, works remarkably well, except when one has an open shell. Then one has to invoke Hund's rules. In a confined *finite* system like an atom, energy levels have finite energy spacing, barring degeneracies that arise from symmetry. In a solid containing an Avogadro number of atoms (often approximated as an infinite periodic crystal) one has a periodic array of nuclei. Electrons see this periodic potential and form a different set of quantized orbits, called Bloch waves. The energy eigenvalues of these spatially extended eigenstates of an infinite crystal are no longer discrete. They form a (quasi) continuum. However, there are energy



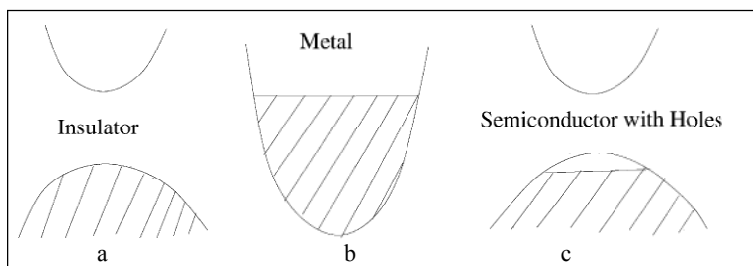


Figure 1.

gaps or forbidden regions, with absence of stationary states. This is analogous to the gaps between two neighboring eigenvalues in a hydrogen atom.

In the elementary theory of electrons in a solid, electrons obeying the Pauli principle fill the Bloch states, giving us a metal or an insulator (*Figures 1a and 1b*), depending on the crystal structure and number of electrons per unit cell. Lithium is a metal and diamond is an insulator. The observation of Hall effect with an anomalous sign is seen in semiconductors. Semiconductors are basically insulators with a small gap. However, defects, such as substitution of a silicon atom in solid Si by a phosphorous atom or Si by a boron atom can result in the addition of an electron at the bottom of the conduction band or removal of an electron from the top of the valence band. When one has a finite density of such impurities called dopants, there will be a finite electrical conductivity coming from doped carriers.

Peierls's remarkable discovery was that if there are missing electrons in a filled band (*Figure 1c*) they will behave differently from electrons in free space. Young Peierls recognized that this follows from the electron energy dispersion (dependence of energy of a Bloch state on wave vector or momentum) close to the top of the filled band. This is something we can do by doing an elementary wave packet analysis. That is we pick a momentum  $k_0$  close to the top of the valence band and build a localized state by superposing nearby plane wave states over an interval  $\Delta k$ . The size of the wave packet is  $\xi \sim \frac{1}{\Delta k}$ . If one follows the dynamics of this wave packet, using the Schrödinger equation, the group velocity (given by the curvature of the energy dispersion curve) will have an opposite sign to that of a wave packet from the bottom of the valence band.

Peierls recognized that the negative group velocity will make missing electrons close to the top of the filled band behave like positive charges in the presence of external electric and magnetic fields. Peierls' first paper, written when he was 21, is a model of clarity and logic. There was the concept of a *hole* in Peierls' paper. However, the name 'hole' appeared only later in the literature.



## Appendix 2. Umklapp Process

In free space, momentum conservation follows from Galilean invariance. In solids, dynamical variables like displacements of atoms from their equilibrium position are described with respect to equilibrium positions of atoms which form a periodic lattice. Young Peierls discovered that the issue of momentum and its conservation is subtle and it has non-trivial consequences. Pauli was trying to apply the quantum theory of lattice vibrations to the issue of heat transport in solids. Pauli and Debye had theories for heat conduction, or in modern terminology, theory of phonon transport in solids. Peierls recognized that there were conceptual and technical problems with the theories of Pauli and Debye. He started, in his characteristic way, working from first principle and asked basic questions.

First he realized that, as there is no net transport of matter during the process of heat conduction in a crystal one can only talk about pseudomomentum. Then he showed, by elementary analysis that in elementary non-linear processes or anharmonic interactions among phonons, the pseudomomentum is not strictly conserved. It is conserved only modulo the reciprocal lattice vector. The mathematics behind this is simple. Let us consider a one-dimensional chain of atoms, having a very simple anharmonic coupling given by the term

$$H_{\text{anh}} = K_3 \sum_n (u_n - u_{n+1})^3. \quad (1)$$

Here  $u_n$  is the displacement of the  $n$ -th atom from its equilibrium position. As we have a periodic crystal we can rewrite this cubic anharmonic term in terms of normal mode variables, lattice Fourier transforms of  $u_n$ 's,  $u_k = \frac{1}{\sqrt{N}} \sum_n e^{ikan} u_n$  as

$$H_{\text{anh}} \sim K_3 \sum_{k_1 k_2 k_3} g(k_1, k_2, k_3) \gamma(k_1 + k_2 + k_3) u_{k_1} u_{k_2} u_{k_3}. \quad (2)$$

Here,  $g(k_1, k_2, k_3)$  is a form factor and  $\gamma(k_1 + k_2 + k_3) \equiv \sum_n e^{i(k_1+k_2+k_3)an}$ . The last sum,  $\gamma$  is a lattice Fourier transform and it is easy to check that it does not reduce to a simple Dirac delta function  $\delta(k_1 + k_2 + k_3)$ . This is because we have a lattice sum, rather than a continuum integral. It is easy to check that the lattice sum reduces to

$$\sum_n e^{i(k_1+k_2+k_3)an} = \sum_{m=0, \pm 1, \pm 2, \pm 3, \dots} \delta(k_1 + k_2 + k_3 - \frac{2\pi m}{a}). \quad (3)$$





That is, momentum is conserved modulo reciprocal vector. That is, the standard momentum conservation equation  $\hbar k_1 + \hbar k_2 + \hbar k_3 = 0$  is replaced by

$$\hbar k_1 + \hbar k_2 + \hbar k_3 = m \frac{\hbar 2\pi}{a}, \quad m = 0, \pm 1, \pm 2, \pm 3, \dots \quad (4)$$

Physically it amounts to saying that the underlying periodic lattice structure can absorb or give a momentum corresponding to any one of the reciprocal lattice vectors  $\frac{2\pi m}{a}$ , through a Bragg reflection. Equation (4) can be also viewed as a Fourier transform of the periodic function on the right-hand side, with respect to the variable  $(k_1 + k_2 + k_3)$  with period  $\frac{2\pi m}{a}$ .

This discovery of Peierls had remarkable implications. Peierls realized that if you have a gas of non-interacting phonons and study non-equilibrium properties, the system will never reach thermal equilibrium. Even the anharmonic interaction that Debye introduced (because of strict momentum conservation) will not lead to an equilibrium state at low temperatures. Peierls Umklapp process found a source of momentum dephasing in a translationally invariant system. This solved some important conceptual questions related to equilibration and irreversibility of heat transport in lattice systems, such as a perfect crystal. Peierls also showed that because of the Umklapp term, the thermal conductivity will increase exponentially with decrease in temperature. The reason was that Umklapp process involves a phonon close to the Brillouin zone boundary. Phonons close to the Brillouin zone boundary have a finite energy. So the probability of this process will be cut off by a Boltzmann factor at low temperatures. Thus Umklapp processes, which are the source of momentum dephasing, will become less important as we go to lower temperatures, leading to an exponential increase of thermal conductivity. Peierls prediction was confirmed in real systems, much later in the 50's, when very pure single crystals were prepared and studied. Actually, the Umklapp process together with other temperature-dependent effects (specific heat) gives an Umklapp peak in thermal conductivity at low temperatures.

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