Relativistic Quantum Mechanics
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Lecture - 17
Dirac equation structure of low energy graphene states, Relativistic signatures in graphene properties

In the last lecture, I worked out the band structure of Graphene; and it showed that at the corners of the Brillouin zone, there are 0 energy excitations possible. So, this defines essentially the Fermi level for Graphene, where the corners of the Brillouin zone. Actually go exactly through the Fermi level while at a different point anywhere in the Brillouin zone the conduction and the valence band have a non zero separation.

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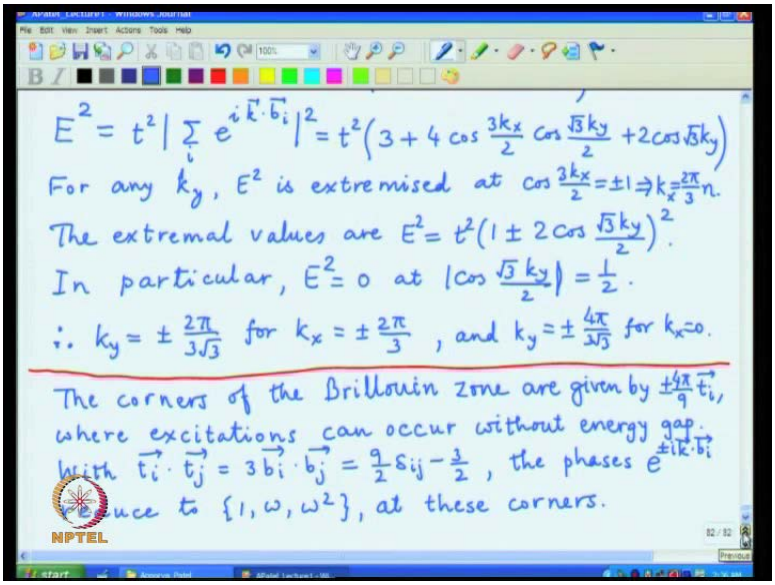

And these points so called 6 corners of the Brillouin zone are given by the vectors explicitly listed here, but they can also be written in terms of the primitive translation vectors; the coordinates are essentially given by 4 pi by 9 t i. And at these points excitations can occur without energy gap or rather e equal to 0 as is dispersion relation shows automatically.

And, now we would like to see the other excitations available at low energy; and for that reason we have to study the neighbourhood of these corners. And there are various identities one can easily workout one is that given these locations; one can easily see

what the phases are. And if you will evaluate these dot products they produce 9 by 2 delta i j minus 3 half. Then the phases which appear in the momentum space Hamiltonian essentially e raise to plus or minus i k dot b i become the 3 cube roots of unity. And that is what defines the Hamiltonian? Of course, when you some over the 3 phase factors as they appear in the Hamiltonian you get 0. And that is why the energy gap is 0 at this particular point. So, in the neighbourhood the phases will now differ slightly from this value 1 omega and omega square. And we can explicitly perform our tailor series expansion to see what these corrections are?

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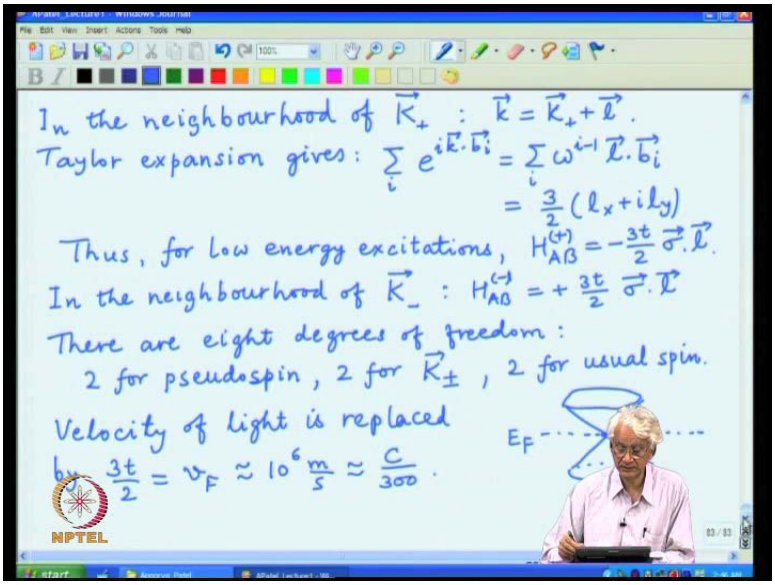

And, so let us take a particular neighbourhood of the point k plus; and we define the departure as a vector l. And then one can do a Taylor expansion the zeroth order term vanishes. And one has a leading term which is linear in this vector l; and it can be written as omega to the i minus one l dot b i; where these omegas are various roots of unity. And by putting the explicit values one omega and omega square one can do this straight forward linear combination and that equals 3 half l x plus i l y.

And, then for this low energy excitations; we have the effective Hamiltonian in this pseudo spin space not by A and B indices which is sigma dot l. It basically represents l x plus i l y on one side of the diagonal and l x minus i l y on the other side of the diagonal. So, this now becomes the description of the theory for low energy excitation; it is a essentially the structure of the Weyl Hamiltonian or rather Dirac Hamiltonian with mass

equal to 0. And one can work out the other neighbourhood the point k minus. And then one has the same Hamiltonian; but with a opposite sign and that corresponds to the Chirality being opposite at the 2 points k plus and k minus.

So, we have essentially now 4 degrees of freedom described in this low energy theory; 2 degrees of freedom coming from this index of 2 dimensional matrices describing the pseudo spin. Essentially that is where this matrix sigma leaves. And the other 2 possibilities coming from looking at these 2 points k plus and k minus which give the opposite sign of Chirality. And so the total theory does obey the symmetries of a parity and time reversal with both these chiral component being present. But if one specifically concentrates on only one component one can see the unusual feature of the while Hamiltonian corresponding to a single Chirality. So, this is the structure and so there are totally 8 degrees of freedom in the real Graphene system.

And, they correspond to 2 for pseudo spin 2 for choosing either of this k plus or minus points. And the other 2 degrees of freedom which I have not mentioned at all is a usual spin of an electron; that spin essentially remains completely independent of these other degrees of freedom it can be treated as a extra index. And does not play any significant role in the low energy dynamics of graphene. So, this is the system and now we want to study some dynamical consequences; which follow from this particular structure of the Hamiltonian; one can actually represent this structure was a little light cone.

So, one has this point say k plus; where the energy is 0 the Fermi level passes through this point for Undoped Graphene where there is only one pi electron per atom. And one can dope it to move this Fermi level up and down from this conical point. And this cone basically describes the sigma dot l dispersion relation around this particular point. So, it is actually a 2 dimensional system. So, one can actually draw the cone which describes this sigma dot l and the consequences which we have seen for Dirac equation.

Now, follow modulo one particular change and that is that the velocity of light c is now replace by thus number 3 t by 2 and that is quite different. So, the velocity of light is replaced by 3 t by 2 which can be called the Fermi velocity. And experimentally the number corresponding to it is about a million meter per second. And so this is smaller than c by a factor of 300 and this change actually makes this system easily accessible. You do not have to study at very high speeds close to c. The speeds remain whatever is

available in condensed matter systems. And you can still see effects described by Dirac equation; that now can be converted into many of the examples which we have studied before. But I can still point out certain features which are unusual one has this; so called linear dispersion relation instead of the usual quadratic dispersion relation.

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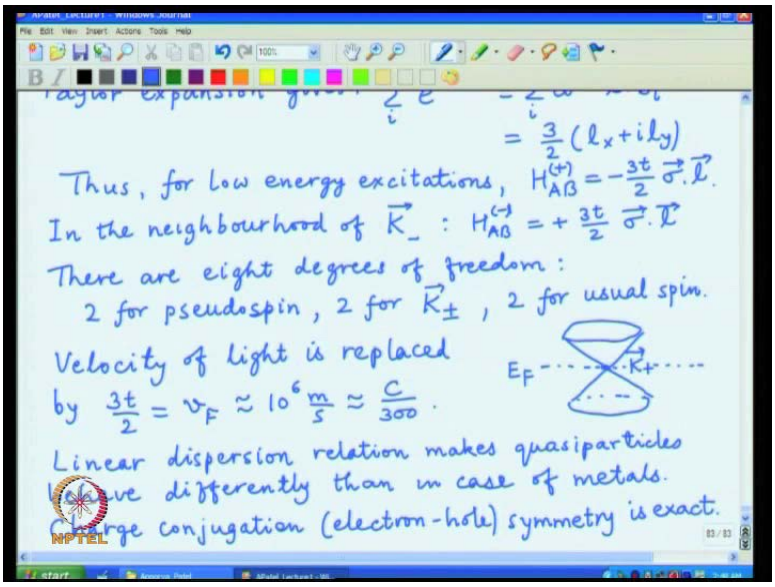

Which describes band structures in many of the metal? In case of metals dispersion case is quadratic. And on top of that we have the charge conjugation symmetry; in other word electron hole symmetry which remains exact for this Dirac equation. So, electron and holes will have the same effective mass and the same mobility; that is also a property different from what is seen in case of metals or semiconductors. So, that is a generic feature those are the consequences of the Dirac equation one can also look at the value of the coupling involved together with this Hamiltonian. That again follows in terms of looking at the electromagnetic modification of this particular Hamiltonian.

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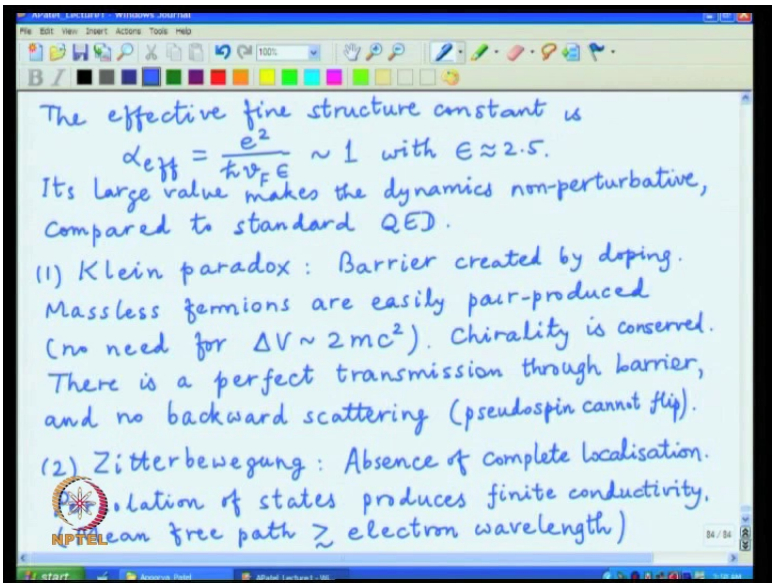

All that happens is that the fine structure constant; now is different. And it can be written in the usual notation with c e d replaced by the Fermi velocity. And to be more precise one has to include a factor corresponding to the dielectric constant of the materials. And this number experimentally turns out to be approximately 1; where the dielectric constant epsilon is about 2.5 in case of Graphene.

You remember in standard electrodynamics alpha was 1 over 137. So, its large value makes the dynamics non perturbative; even though the interaction is just electrodynamics. The standard QED as we study most of the time in high energy physics is perturbative. So, you have to do calculations keeping these large coupling constants in mind. And now I will list some of the well known consequences which follow from this structure of the Hamiltonian; as well as the quite different values of the effective parameters like speed of light and the fine structure constant. So, let me first look at what happens in case of a barrier. And this was a problem which we saw in case of Klein paradox; we can easily create a barrier in case of graphene by doping one can create a gate and put a voltage on it. So, that the electrons feel an extra potential in trying to go through a particular region. And the peculiarity now shows up that we not only have a Dirac Fermion; we have a mass less Dirac Fermion.

So, this Mass less fermions are easily pair produced. In particular we do not have a need for a minimum height of the barrier as in case of Klein paradox; where we need a barrier

height of the order of 2 m c square to see this effect. Here, the effect is seen for any particular potential, because the pair production is very straight forward. And so immediately we see the effect that there will be hole; which will just go through the barrier without any problem. And electron which will be going back. And that phenomena now take a particular form we have a Chirality is conserved; which means the particle which is left handed or in this particular system moving in one particular direction cannot reverse its motion. And the consequence of both those things are together; that there is a perfect transmission through the barrier; one can have a pair production process which is restricted to the domain of the barrier. But on the other side we will get perfect transmission there is no way the Chirality can flip.

And, so there is no backward scattering which is the same thing as saying that the pseudo spin cannot flip with the Hamiltonian structure we have. So, this is an unusual feature that even though you put in a barrier the electrons essentially do not care about it. If you have a incident which is normal to the barrier it will just go through there does occur some reflection; if the incidence is not normal to the barrier that is possible in 2 dimension. But scattering by 180 degree just does not occur. So, this is the analogue of Klein paradox. Another feature which we have seen for Dirac equation is the there was no way to localize the particle perfectly; there was always a Zitterbewegung oscillations; which were of the size of the Compton wavelength of the particular particle.

So, we have absence of complete localization again there is a mass less particle. So, there is no real Compton wavelength. So, the wavelength which matters is actually the one given by the wave vector k and that dictates the scale of the problem. And because of this uncertainty given over the particular wavelength; one can have that what can be called as a percolation of states on neighbouring sites. And that produces non zero conductivity; even though the parameters may have been such that there are no free carriers available. And other way of saying this statement is the mean free path which describes the motion of the electrons in this material it has a lower bound. And that lower bound is just the electron wavelength; we would have an insulator if the mean free path actually become 0, but that is not really possible.

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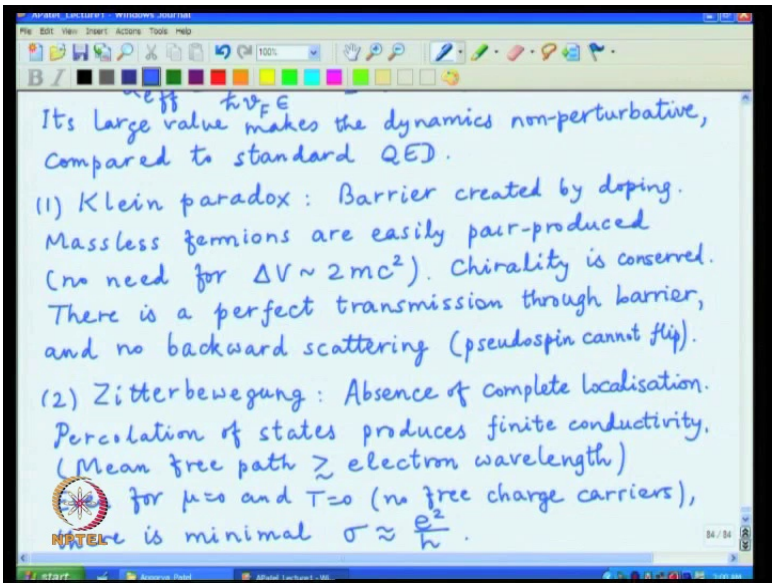

And, so even for 0 chemical potential and 0 temperature; which means there are no free carriers available; there is finite conductivity. And the value of this is specified by the fundamental constants of quantum theory. And which happens to be e square by h. And experimentally again this feature has been observed one can measure conductivity of this particular magnitude; the feature that there is no backward scattering in case of a barrier that also has been experimentally detected.

So, these features are qualitative consequences of the Dirac equation. And they have indeed been seen if one literally wants to do detail calculation; one has to solve the problems in presence of this large electromagnetic coupling. And do a non perturbative calculation and that is a technical detail. But the features that we expect are easily seen without doing the complicated algebraic analysis.

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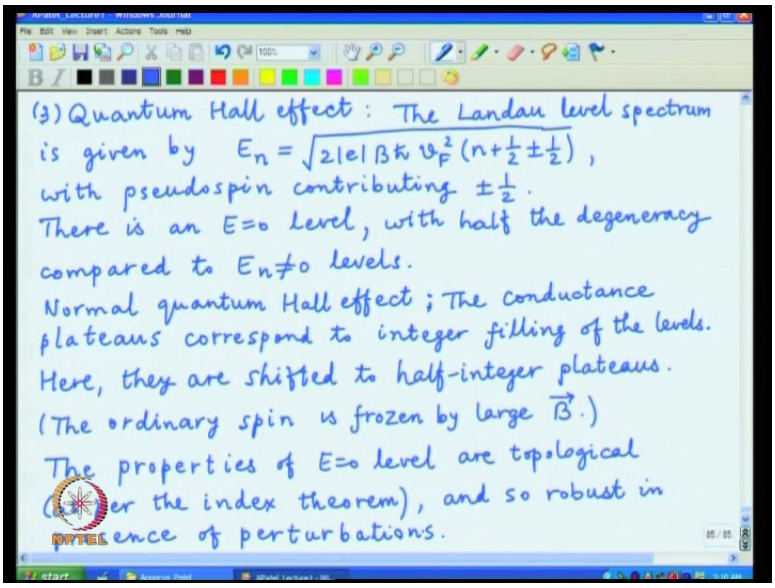

Let us look at yet another feature which is well known in this condensed matter system. And that is quantum hall effect; this is a behaviour of a 2 dimensional gas of electrons subjected to a strong magnetic field. And that results in a particular behaviour of the conductivity. And one sees different features at different; so called filling fraction which describe how many electrons exist in the conduction band compared to a specific density given in terms of landau level physics.

So, that spectrum and that calculation now has to be redone instead of using the Schrodinger equation we have to use the Dirac equation. And its landau level spectrum is now different. It is specified in terms of an integer and going from 0, 1, 2 etcetera. And the result is proportional to square root of B as well as square root of n plus half; and then extra plus or minus half; this arises from solving the equation. And it turns into a harmonic oscillator problem for a electron in a magnetic field.

And, that is where this n plus half combination is coming from the extra plus or minus half is a contribution of the pseudo spin in this Dirac equation. And that is a novelty compared to the result in the case of Schrodinger equation. So, this is a spectrum in particular the smallest value is 0, but there is slightly different dependence on the quantum number n compared to all the other energy levels which are non 0. And that is that any other value for a different integer can be obtained in 2 separate ways.

For example, the one can be obtained by 1 plus half minus half or it can be obtained also as 0 plus half plus half. So, there are 2 ways of reaching this value 1, but there is only one way of reaching the value 0 which has to be 0 plus half and minus half. And for that reason the degeneracy of the E equal to 0 level is half that of the degeneracy of non 0 energy levels. And that give rise to a filling system where one starts with half integers instead of integers. So, in a normal quantum Hall Effect the so called conductance plateaus correspond to integer filling of the levels. But now we have the zeroth level at different degeneracy than all the other ones. And here they are shifted to half integer plateaus because E is equal to 0 level gives half. And then after that all the other ones add integers.

So, we do have a quantum hall effect, but the Dirac structures shifts everything by half compared to the Schrodinger solution. And one can see this in experiment it has indeed been observed; and that is a confirmation of again the Dirac spectrum of this particular system; I should mention that the ordinary spin in this analysis is kind of frozen by large magnetic field. And does not play any role in the analysis of quantum hall effect. And the difference which arising here is coming from this pseudo spin contribution; which is shifting everything by value half.

The regular spin does not play any role one can also say one more thing about this 0 energy levels. And which is well known in the analysis of Dirac equations; and how the energy shifts when various levels are crossed. And there is something which is known as a index theorem; which describes how the energy level behave when certain properties change in a smooth way across the value E is equal to 0.

So, the properties of this e equal to 0 level are topological. And this nature made them very easy to see, because it is not easy to perturb them by external disturbances. So, that is the feature of what is seen in quantum hall effect in Graphene; one can ask what are the wave function like the wave functions are not very different. I already say that the solution corresponded to a harmonic oscillator problem. And the scale of that particular problem is as usual.

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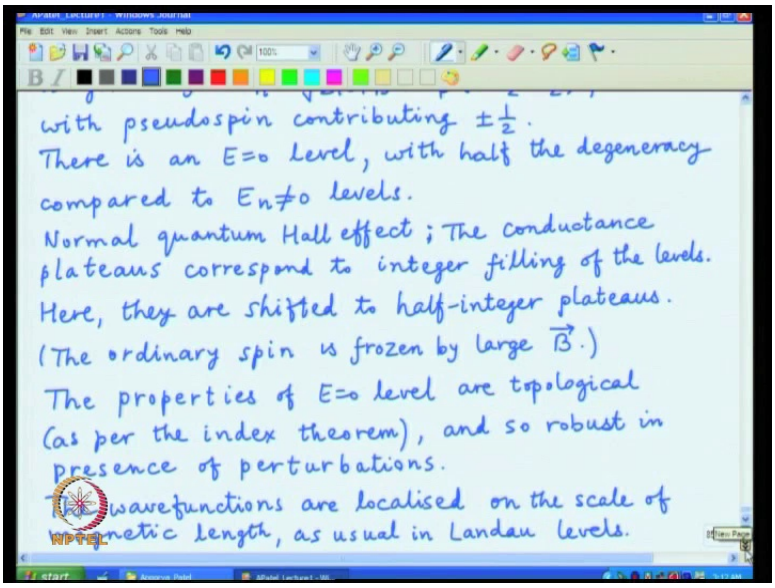

That the wave functions are described on the scale which is the so called magnetic length. And that is the only scale which appears in the case of landau level analysis; even for the Schrodinger equation. So, this is one more feature of the Dirac equation and how it modifies the behaviour.

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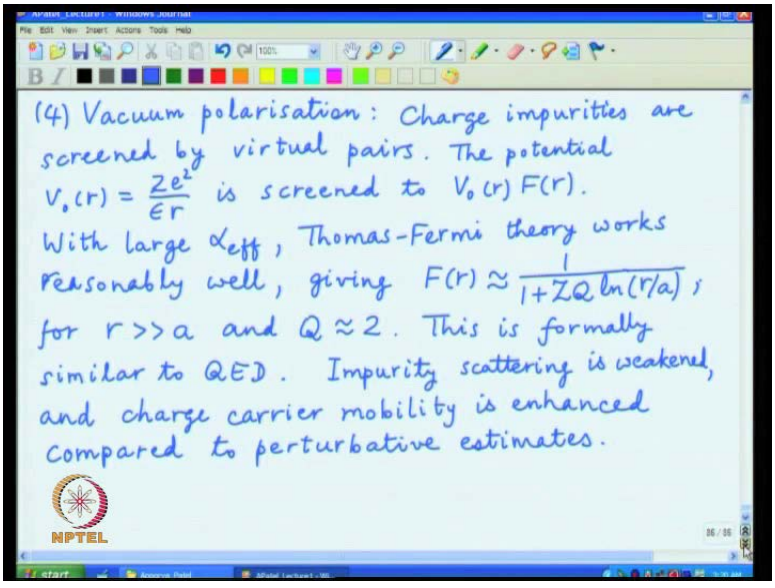

There are still a few more properties I would like to mention one of them is property of quantum field theory; which is known as vacuum polarization; this is an effect of creation and annihilation of virtual particle antiparticle pair. And by producing this

virtual pairs as a cloud the charge basically gets screened. And this the feature which makes that the value of charge you see by an observation from outside depend on how far away you are from that charge many times this feature is also referred to as Debye screening.

So, we have these charge impurities are screened by virtual particle antiparticle pairs; and that kind of facilitates transmission properties. Because even when you put some impurities into the system you do not see their full strength; how much this modification is requires some calculation. And in this particular case you have to work with a effective fine structure constant which is much larger, but one can make a model of it. And the potential of a charge impurity can be written as V 0 of r has z e square by epsilon r where epsilon is again the dielectric constant. And that is made smaller by a distance dependent function f is less than 1.

But it depends on how far charge you are observing; to calculate F of r explicitly 1 needs to make certain approximations. Because it is a non Perturbative physics. And the one approximation which works reasonably well is the so called Thomas-Fermi model of many body systems in this particular case of electrons. And one get an answer for this function which can be approximately written as 1 plus Z Q log r by a; where a is a typical atomic scale. And this form is valid where one is quite far away from the atomic scale as well as this number Q; which depends on the various parameters of the material being equal to 2 it is related to the alpha effective.

So, this is what one sees and in particular this kind of reduction of the charge; which are logarithmic scale in the denominator is seen in case of standard quantum electrodynamics; in particle physics the only things here are the parameters are different. The consequence is that impurity is not as efficient as a bare charge in terms of scattering the charge is now shielded. And one can see that in terms of mobility of the charge carriers is enhanced. And the full power of this can be seen only by doing this calculation involving the logarithm. Because if you do a standard perturbation theory the logarithm will not appear it is a consequence of so called running coupling in field theory.

And, it is a stronger effect in the sense of summing up the renormalisation group process which modifies this power series expansion or Taylor series descriptions to these logarithms. And the standard power series expansion which if one does they are the so

called Perturbative estimates. And this effect is actually stronger compared to those perturbative estimates; the net result is that the scattering is suppressed. And impurities do not do as much as naively one would have expected.

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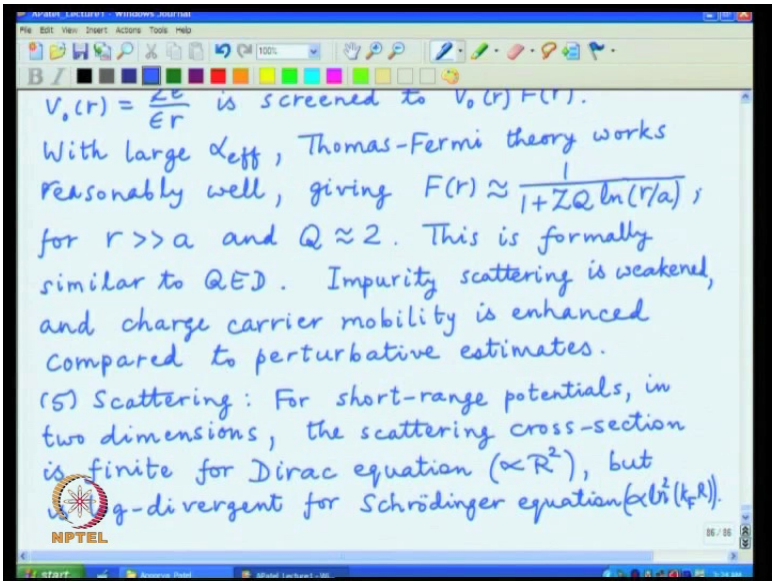

This separation of scattering can be seen again in a slightly different language; and that is just to take the standard quantum mechanic situation. And calculate the cross section for a particular potentials. And in this particular case one can take the simpler model than the full quantum electrodynamics just take so called hard shear repulsive potential or basically a short range barrier. And then one can do the calculations much more easily and what one sees that in 2 dimensions; which is what Graphenes corresponds to the scattering cross section is finite for Dirac equation. In particular it is proportional to R square where R is the range of this particular potential.

And, the difference arises because in case of Schrodinger equation the same scattering cross section is log divergent; in particular it is proportional to log square of the Fermi momentum times the distance scale. And this behaviour is quite distinct the result is that even if you put a short range barriers or impurities inside this material. The separation of conductivity is much less than what one should have expected in case of Schrodinger equation or in other words the resistance which is proportional to the cross section is much smaller for Dirac equation than it is for Schrodinger equation. And one have a material with better transport properties.

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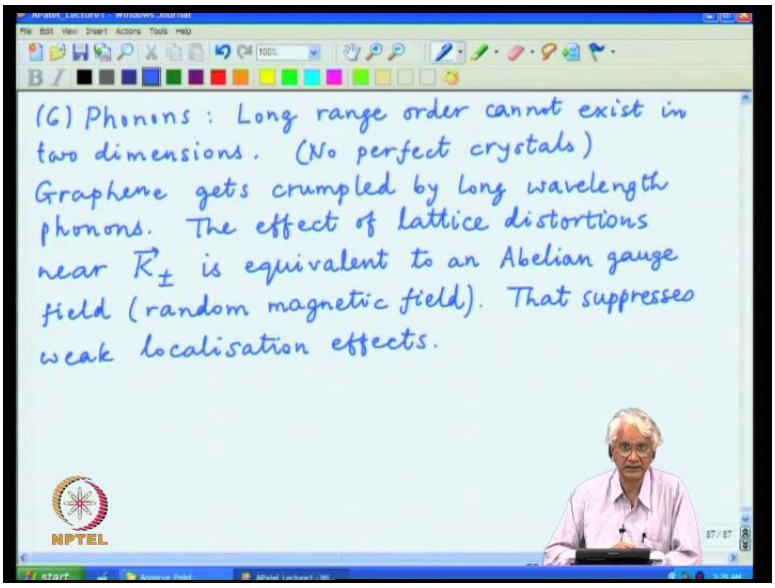

Lastly I one make one more comment about the structure of the graphene has would be seen in a real finite temperatures set up. And there it is impossible to avoid distortions of the structure by the vibrations of the lattice sites. And those are described typically in terms of phonons; the distances are not going to remain equally spaced lattice points there will be certain movements. And they will contribute to the dynamics of the transport properties as well. And there is a strong theorem in case of 2 space dimensions that so called long range order cannot exist in 2 dimensions unlike the situation in 3 dimension. And so one can have crystals which are periodically ordered to long range even infinite range there is no problem, but it is 2 dimension perfect crystals are not possible.

And, because of that the phonons will inevitably leave its effect on structure. There is no way to get rid of them completely even at temperatures going to arbitrarily low values. This general theorem is so called the Mermin Wagner theorem; if you have heard about it. And the consequence of this thing is that the Graphene sheet is crumpled by long wavelength phonons; there will be a cut off on the crumpling at short distance it is provided by the lattice unit itself. But at long distances there will be so called wavy distortions. And this distortion now can be included in the band structure analysis; which I did again as some small perturbations on top of the regular behaviour.

And, we again have to study what happens in the neighbourhood of these 2 particular points k plus or minus. And it turns out that this disturbance is equivalent to a so called Abelian gauge field corresponding to random magnetic field; the distortions are uncontrolled. And that is why the magnetic field does not have specified direction it can occur randomly. But the effect is having this extra random magnetic field at every point on the practice one has its effect on the Brillouin zone.

And, the consequence of this one can now workout more rigorously by treating again this extra Abelian gauge field produced by the phonons. In addition to the gauge field corresponding to the electrodynamics as well and the net result is again these are fluctuation. And they end up suppressing effects which are called weak localizations. And this suppression further give rise to improvement in a transport properties of this particular material.

So, that is a whole list of things which have now opened up to the experiments and theoretical analysis; in case of Graphene there are many features to be understood in terms of detail calculation. But Dirac equation does lead the way in predicting very unusual features compared to the usual behaviour in case of metals.