

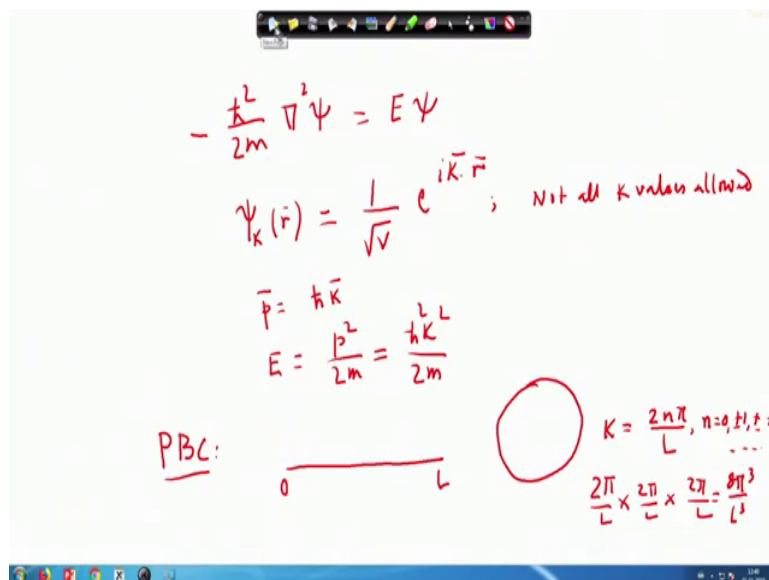
Electronic Theory of Solids
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Lecture - 06
Properties of degenerate Fermi Gas

Hello, what we do today is a continuation of what we were doing and we said in the previous class that, an introduction to the ideas of quantum mechanics particularly Pauli principle; remedies some of the problems that we encountered while fitting classical theory to experimental results.

Now, as we said the first thing that one tries to do in understanding a system of electrons which are basically Fermions which, to treat them as a non interacting quantum gas and then calculate the properties of the electron gas from such a theory. And that theory is of course, a quantum theory and we wrote down the Schrodinger equation. The guiding equation for quantum mechanics is equal to:

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Now, in this equation, look at the equation that we have not put any potential; that means, the electron gas is still non-interacting as in our classical assumption, but the Newton's law is now replaced by Schrodinger equation and whatever comes with it like Pauli principle and so

on for a Fermion. And then what we did was that, we try to identify the number of states, basically the state counting now becomes important because not all values of momentum; so, called momentum k -values, which we wrote down the solution of this as $1/\sqrt{V}$, $e^{i\mathbf{k}\cdot\mathbf{r}}$ and not all k values allowed, ok.

Unlike in classical mechanics where k can be a continuous variable, you can put for any from 0 to infinity and any k value is a possible k value. Then we identified that the momentum is $\hbar k$; this wave function gives you a momentum which is $\hbar k$. The corresponding energy is similarly $E = \hbar^2 k^2 / 2m$.

Now, the important thing was that, we also said that the allowed k values will come from the boundary condition and the boundary condition that we used was; so, called the Periodic Boundary Condition PBC which essentially means in one dimension for example, that you close the two ends of a line, basically identify 0 with L so, that it becomes a circle, ok.

And then consequently, we saw that the k values will be $2n\pi/L$ where n is the integer 0 plus minus 1 and so on and so on. So, that was the essential thing and then we generalized it for two and then the three-dimension. So, the in 3 dimension therefore, every volume 2π by L into 2π by L into 2π by L in k space condense 1 k allowed k value. So, that is $(2\pi)^3 / L^3$ by L^3 . So, this is the amount of volume in k space which gives you 1 k value that is allowed, ok.

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Vol. Ω_k in k -space we have $\frac{\Omega_k}{(2\pi/L)^3} = \frac{\Omega_k V}{8\pi^3}$

$N_L = N_e = \frac{V}{3\pi^2} k_F^3$

$\frac{\hbar^2 k_F^2}{2m} = E_F$; $k_F = \sqrt{\frac{2mE_F}{\hbar^2}}$

$\frac{dN_L}{dE} = \frac{1}{2} \frac{N_L}{E}$; $\frac{dN_e}{dE} = \frac{1}{2} \frac{N_e}{E}$

So, on the basis of that then we said that in a volume Ω_k in k space, we have Ω_k divided by 2π by L cube number of states which is Ω_k times the volume integral space L cube is the volume of the system; so, by $8\pi^3$ cube. So, that was the state counting that we started doing and we do it, because at some point we have to sum over k for calculating all physical quantities and then sum over k if you have to go over all the discrete values of k , then it becomes very difficult to sum. So, one looks for something which is like a region of k between k and k plus dk over which how many states are allowed.

So, one multiplies by that quantity, that face value and then one can even integrate. So, will what we did was that, we calculated certain physical quantities. From this and the value of the for example, we calculated the number of levels for example; remember electrons are fermions been half fermions. So, there are two states two levels for each k value. So, when you put an electron in a particular k value, you are allowed to put one more electron with an opposite spin in certain chosen direction of quantization in the same state. So, each k value actually accommodates two electrons.

So, based on that we calculated several things, one of them is these number of levels N_L which is equal to number of electrons in the system, which was V by $3\pi^2$ square into k_F cube. Now, k_F is k_F square by twice m is E_F . So, k_F is E_F . So, this was F

we defined was the Fermi energy. So, Fermi momentum and E_F is the Fermi energy. So, k_F is root over $2mE_F$ by h cross square.

So, that is how one calculates the number of electrons or number of levels in a system. So number of levels is basically twice the number of k values allowed k values. So, this basically gives you the total number of levels within a sphere of radius k_F or a below an energy E_F . So, that is the, that was something that we derived. So, we also derive the dN/dE equal to $3/2 N/L$ by E which is again the same as dN/dE electron number by dE equal to $3/2 N$ by E , ok.

So, given all that, what we wanted to show was that we can actually calculate some physical quantities out of it. For example, we want to calculate the energy.

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$$E = 2 \times \sum_{k \leq k_F} \frac{\hbar^2 k^2}{2m}$$
 one allowed k value in $\frac{8\pi^3}{L^3} = \frac{8\pi^3}{V}$

$$\sum_k F(\vec{k}) = \sum_k F(\vec{k}) \frac{4\pi^3}{(2\pi)^3} V$$

$$\Delta \vec{k} \rightarrow 0 \quad (V \rightarrow \infty)$$

$$\sum_k F(\vec{k}) \frac{4\pi^3}{(2\pi)^3} V = \int_0^{k_F} F(\vec{k}) \frac{4\pi^3}{(2\pi)^3} V k^2 dk$$

$$E = V \cdot 2 \cdot \int_0^{k_F} \frac{d\vec{k}}{8\pi^3} \frac{\hbar^2 k^2}{2m} = \frac{2V\hbar^2}{8\pi^3} \int_0^{k_F} 4\pi k^2 dk k^2$$

$$E = \frac{1}{2\pi^2} \frac{\hbar^2}{m} \int_0^{k_F} k^4 dk = \frac{V\hbar^2}{2\pi^2} \frac{1}{5} \frac{k_F^5}{m} = \frac{V\hbar^2 k_F^5}{10\pi^2 m}$$

$$\frac{E}{V} = \frac{\hbar^2}{10m} k_F^5$$

For example we want to calculate total energy, what we do is we sum over h cross square k square by twice m all the way up to k less than equal to k_F ok. Now, this gives you the number of k your summing over the momentum. So, the energy for a particular k value and then summed over all those k values. But remember each k value allowed k value, you can put two electrons. So, you have to multiply by 2. So, this is the energy of the electron gas, electron in the solid, electronic energy that comes from the solid.

So, and remember that again for one allowed k value in a volume of 8π cube by L cube which is the; so, 8π cube by V , so, in this volume in k space. Now what we do is that we take a. So, convert this any for example, you are summing over a function of k any function F of k , sum over k you can write this as F of k into Δk by 2π cube by V .

So, Δk is the volume in k space and then dividing by this you get the number of k values in it multiply F k by that number and then sum over k . So, that is the same as this. So, this is basically identity and then what we do is that, we take the limit Δk going to 0.

Now, if this volume goes to 0 which happens when V goes to infinity for example so, this Δk is a very small volume. So, we multiply that F k by that value that gives and then by this quantity divide by this quantity that gives me the number of k values their and multiply F k . Assuming that F k is not varying too much within that volume, because the volume is very small and then this identity can now we converted to an integral.

So, what we do is that, now if you remember basically F k Δk , in this limit when Δk goes to 0 is nothing, but integral of $d k$ F of k . This is a very useful quantity because now, I have converted sum over all those discrete states which are allowed discrete states it when into an integral. And, this integral because the states us so, densely packed, there are states at every 2π by L cube; so, every 8π cube L cube. So, then e and that number is extremely small. So, the total number of states in a region is very large so, I can just convert this in sum to an integral.

And that is very convenient because, I can now calculate the energy for example, as an integral. So, I will ok so, this integral is; that means, a what I have done is that, I have converted this F k into an integral and then. So, I had, remember, into V by 2π cube here. So, I will put that in here V by 2π cube.

So, energy is now simply 2 times. So, V remains 2 times a dk . So, dk is, ok let me write it down again dk by 8π cube h cross square k square by twice m . So, this is my expression for the energy. Remember, these two comes from the spin degeneracy as I said each k value you will put two spins, and this was my sum, this is the sum for any function F k . I can write this

$\int_0^{k_F} k dk$ as integral of at this and I had a multiplication by V by 2π cube. So, this $V \pi^2$ cube just sits outside V by 2π whole cube, ok.

So, that is that is the expression. Now I integrated from 0 to k_F that will give me the total energy. So, how much is this? So, this is $2V$ by 8π cube times, Now this dk is basically $4\pi k^2 dk$ and then I had this \hbar^2 cross square by twice m . So, I write the twice m here 0 to k_F into k^2 . So, this is equal to these gives me 2 k cancels, 4π gives me this 2π square, here V times \hbar^2 cross square into k to the power 4 $d k$ 0 to k_F , ok.

So, this is nothing, but $V \hbar^2$ cross square by 2π square into 1 by 5 k to the power 5 , there is an m is here. So, I will put that k to the power 5 by m . So, this is $V \hbar^2$ cross square by π^2 into k_F to the power 5 by $10m$. This is the expression that you will find in many books and this is a very convenient expression. Because now, I have expressed energy in terms of the total energy of the system in terms of its Fermi momentum and mass and these of just constants.

And then E/N which is the energy per particle energy density E/V which is the energy density is \hbar^2 cross square by π^2 into k_F to the power 5 by $10m$, ok.

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Handwritten mathematical derivations for Fermi gas properties:

$$N = \frac{k_F^3 V}{3\pi^2}; \quad E = \frac{V \hbar^2}{10m} \frac{k_F^5}{\pi^2}$$

$$\frac{E}{N} = \frac{3}{10} \frac{\hbar^2 k_F^2}{m} = \frac{3}{5} E_F \quad E = \frac{3}{5} \frac{\hbar^2 N}{2m} \left\{ \left(\frac{3\pi^2 N}{V} \right)^{2/3} \right\}^2$$

$$P = - \left(\frac{\partial E}{\partial V} \right)_N; \quad E = \alpha V^{-2/3}$$

$$P = + \frac{2}{3} \alpha V^{-2/3-1} = + \frac{2}{3} \frac{\alpha V^{-2/3}}{V}$$

$$\boxed{P = + \frac{2}{3} \frac{E}{V}} \quad \text{Bulk modulus } B = -V \frac{\partial P}{\partial V} = \frac{2}{3} \frac{E}{V}$$

So, once I have that then I also had this expression that N . The total number of electrons is $k_F^3 V / 3\pi^2$. And now I also have E equal to $V h^2 k_F^5 / 10\pi^2 m$.

So, I just divide one by the other and this gives me, $3/10 h^2 k_F^2 / m$. Now, remember $h^2 k_F^2 / 2m$ is the E_F . So, this is $3/5 E_F$. So, this is a very useful expression because, the energy per particle a per electron is on an average is just $3/5$ times the Fermi energy. This expression is very useful in calculating the energy of a system of particles system of electrons.

Now, one even go further. A just by looking at these expressions and a little bit of dimensional ideas, one can be calculate several things. For example, let me just show you that how you can calculate the for example, the pressure exerted by a degenerate Fermi gas, a gas of Fermi on like electrons in a in a solid. So, anything that is field up to a particular region bellow k_F up to k_F this is called a degenerate system of gas because that is the name that stuck this degenerate Fermi gas system exerts a pressure.

Because, if you want to put in another particle an another Fermion it, it will not be able to do at zero temperature. So, all states are field up and so, there is a pressure. So, if you if you want to compress it, so, if you want to change the volume, then the there will be a these levels will come closer and then we will have. So, then be reaction to that and the system like the degenerate Fermi gas will exert a pressure.

So, that pressure can be calculated. So, let us calculate the pressure from this degenerate Fermi gas. So, how do I calculate the pressure? Pressure is basically minus dE/dV the fix number of N . So, what we are trying to do is, basically we are trying to change the volume of the system and the system is opposing it that is how this that is the pressure that we are and why does it opposite? Because there is a change in energy due to this change in value, ok.

Now, let us start from here see this is; so, let me just remove all the I will remove all the constant. So, $3/5 \cdot 3/5 h^2 k_F^2 / m$ into remember I had these expression for N . So, I am calculating the energy now. So, energy this N I will replace

from here. So, let me go ahead and do it and then; so, this first let me calculate the; so, what I will do it and I will replace k_F from here.

So, let us do $3\pi^2$ let us see N by V . Now k_F is to the power of one third of this, ok. So, this N , this N is here to the power one third times square. So, that is the. So, this E then from here E is now you can see is proportional to V to the power minus two-third. So, I can write this as some all the other things being constant, I can write this as sorry, I can write this as E equal to some constant say αV to the power minus two-third.

Now, I can go back here. So, what I do is that I calculate P equal to minus $\frac{2}{3}$ αV to the power minus $\frac{2}{3}$ minus 1 which is minus $\frac{2}{3}$ αV to the power minus two-third divide by V which is nothing, but minus 2, minus is cancelled because there was a minus sign there. So, I have to put a plus sign here plus two third αV to the power minus $\frac{2}{3}$ itself this αV to the power minus two-third itself is E . So, $\frac{2}{3} E$ by V ; so, that is my P . So, two-third E by V is P I can also calculate the bulk modulus for example.

So, bulk modulus is defined as B equal to minus V del P del V ok. So, this object, is actually inverse of compressibility k is the compressibility.

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$$P = \gamma V^{-5/3}$$

$$-V \frac{\partial P}{\partial V} = +\frac{5}{3} V \gamma V^{-5/3-1}$$

$$\boxed{B = \frac{5}{3} P} = \frac{1}{K}$$

$$B = \frac{5}{3} \times \frac{2}{3} \frac{E}{V} = \frac{10}{9} \frac{E}{V}$$

$$\frac{E}{N} = \frac{3}{5} E_F ; \boxed{B = \frac{2}{3} \frac{N}{V} E_F = \frac{2}{3} n E_F}$$

$$B \sim 10^{10} - 10^{12} \text{ dynes/cm}^2$$

Now, again I go back I just derive the fact that P is some constant times V to the power minus $\frac{5}{3}$. So, V to the power minus there; so, all I have do is to take a derivative of del P del V

times minus V which is minus then becomes plus V times gamma V to the power minus $5/3$ minus 1 times $5/3$.

Again with the same argument that gamma V to the power minus $5/3$ is; so, that V to the power minus 1 and this V will cancel. So, this will become simply $5/3 P$. So, $5/3 P$. $5/3 P$ is my bulk modulus equal to 1 by compressibility. Now, P again I can write as I just did that P is two-third E/V . So, then B is equal to $5/3$ into $2/3 E/V$ which is $10/9 E/V$. These are all relations that are useful when then again u by E/N is $3/5 E/F$ we just calculate in the previous page.

So, that will give me B equal to $2/3 N/V$ into E/F equal to $2/3$ density of electrons times E/F , N/V is the density. So, typically for a metal typical metal the bulk modulus for example, is of the order of 10 to the power 10 to the power 12 dynes per centimeter square its fairly large. And so, the idea of this whole algebra that we did its trivial straight forward algebra is to get the physical quantities that you measure in your experiment that you measure any experiments through some quantity which is actually measurable.

So, I go to the last page. So, as we can see a bulk modulus is a measureable quantity. So, if I measure the bulk modulus, I can get from and the density of electrons I can actually get the Fermi energy or vice versa. If I know the Fermi energy, if I know the density then I can theoretically predict the bulk modulus and then do an experiment and check with the experimental values.

So, these are basically free electron model, but using quantum mechanics and that quantum mechanics puts a lot of restriction on the electron system because you cannot put two state two electrons in the same state. In the same value, you can put two electrons because there is a spin, but; that means, that there is savior restriction on the number of electrons per state, it cannot be more than 2 per k so; that means, you are going up in energy while filling up filling up the states.

So, you are ground state already has a quite a large amount of energy which we found out that its typically $3/5$ average an energy per practical is $3/5 E/F$. E/F is quite a large quantity its between 1 to 10 , 15 electron holds in certain system and; that means, that you had to pay that much of energy even in the ground state to construct the ground state of the

electron degenerate electron gas which is filled up to the Fermi level. And consequently, all the physical quantities like bulk modulus compressibility and so on pressure can be worked out from such.

So, in next class what we will try to do is to show that the effect of this Pauli principle, when you want to supplies of energy into the electron gas degenerate electron gas and specific heat for example, can be calculated and the right temperature dependence is come out of this specific heat from this kind of a calculation which originally was done by Sommerfeld.

Thank you.