**pn Junction**

So now we’ll apply an external potential and see what happens. Let’s go back to our equilibrium pn junction, where we include the ni2/|ΔN| contribution to the carrier densities. The picture doesn’t do the situation complete justice, as ni2/|ΔN| << |ΔN|, while it doesn’t appear quite so in the picture. And as a partial consequence, there are more mobile charges/holes pictured in the depletion zone than there should be.

Diagram

Description automatically generated with medium confidence

It was easier to work out the rough charge density and potential difference, etc., in the previous file, without it. And it doesn’t matter much to the charge density overall. But apparently it matters to the conductivity, since now we’ve opened up P’s conduction band and N’s valence band to the flow of current. If we apply a potential difference ΔV (we’ll presume ΔV << Δφ) to both sides of our pn semiconductor,

Histogram

Description automatically generated with medium confidence

we will be setting up a non-equilibrium situation with a concomittant induced (net positive) flow of charge from left to right. There are a few ‘static’ changes wrought by the application of this potential difference. First note that the ΔV drop will occur almost entirely over the depletion zone. This is because we can think of the depletion zone in the semiconductor as a kind of insulator sandwiched between the pn halves. The zone is an insulator because there are no (or at least very few) mobile charges within it. The rest of the semiconductor outside the depletion zone will have high conductivity by comparison. And as we know from Physics 2, the insulators in an electric circuit will take up most of the applied potential difference. So the effective potential difference across the junction will be reduced to Δφeff = Δφ – ΔV. Plugging this Δφeff into the dp,n formulas in previous file,



we see that the depletion zone will commensurately decrease in length. I tried to reflect this in the drawing above (just made the brackets shorter). Another thing that happens – not obvious yet, but will emerge from math later – is that the carrier density gradients take longer to relax to their homogeneous values. So for instance, w/o the potential, pv will remain Na + ni2/Na roughly all the way from x = -∞ to the depletion zone border at x = -dp. And at this point it will rapidly diminish to ni2/Nd by x = dn, and remain at that value as x → ∞. In contrast, with the applied potential difference ΔV, pv will begin a more gradual diminishment from Na+ ni2/Na, starting in the left diffusion zone, then rapidly and substantially diminish wiithin the depletion zone, and finally gradually diminish to ni2/Nd within the right diffusion zone. A similar thing would happen for the electron density in the conduction bands. It’s important to keep in mind that the charge density is still non-zero basically only within the depletion zone, and this comes from electrons in the n-side diffusing into the p-side. But outside the depletion zone, the charge density is basically zero. The changing carrier density outside the depletion zone is due to changing amounts of electrons being pumped from valence bands into conduction bands. This change in carrier density, i.e., this carrier gradient, gives rise to a diffusive current. And that’s why it’s called the diffusion zone. So ΔV squeezes the depletion zone together, and stretches out carrier density gradients. Here’s some more pictures – a plot of the carrier densities vs. position.

Diagram

Description automatically generated

Not the greatest, but it’s meant to convey slow change in the diffusion zones, and fast change in the depletion zones. The vertical axis isn’t really to scale though.

**Induced Current: First Way**

Now consider the induced current. We’ll use a kind of ad hoc analysis. First, remember that *per* *band*, we can consider current to be carried by electrons or holes, but not both. One way to think about it is this. In general, when we have charged particles in an electric field, E, there will be two parts to the induced current flow. One will be the drift current jdrift ~ σE, where σ ~ ρeτ/m, and the other will be the diffusion current, jdiff ~ -D∇ρ, where ρ is the charge density, and D the diffusion constant, and E is the total electric field. The diffusion current will be present whenever there is a density gradient, regardless of whether a field is present or not.

Let’s look at our semiconductor from left to right. In the p-homogeneous region, the hole carrier density is large, and its gradient is nill. And the electron carrier density is small, and its gradient also nill. So the main contribution to the current will be a hole drift current (σ is proportional to carrier density). In the p-diffusion region, the hole carrier density is still appreciable, as is its gradient. The electron carrier density is small, but its gradient is appreciable. So there will be a hole drift and hole diffusion current, as well as an electron diffusion current. In the depletion zone, the gradients are now quite large for both species, and so their diffusion currents will be large. And while the species’ densities are small, tending to make their drift currents small, the electric field will be quite large here, making the drift current still appreciable. The drift and diffusion currents will be separately much larger than the net current, but in opposite directions, and their slight imbalance will give rise to the net current. Then in the n-diffusion region, the carrier gradients are still fairly large, so each will contribute a diffusion current. But only the electron density is high, so only it will contribute substantially to the drift current. And in the n-homogeneous zone, the electron drift current will be large, due to the electrons’ high carrier density. But the hole drift current will be small, and both diffusion currents will be small, since the carrier densities are roughly constant. Of course, the total current must be the same in all regions.

Anyway, in equilibrium, we have these two opposing currents across the junction. The ‘drift’ current, due to φ, is shuffling holes (in valence band) from N to P, and the ‘diffusion’ current, due to the gradient in hole carrier density (in valence band) has the holes migrating from P to N. These two currents balance and cancel in equilibrium. Likewise the electron (in conduction band) ‘drift’ current would go from P to N and the electron (in conduction band) ‘diffusion’ current would go from N to P. And these also cancel in equilibrium. When we apply an external field in the forward direction, from P to N, this will reduce the potential, φ, to φ – ΔV, and thereby reduce the ‘drift’ currents. So the diffusion currents will predominate. So we’ll get more holes going from P to N and electrons going from N to P. So net current to the right.

We can be more quantitative. This explanation is from Ashcroft and Mermin. So thermal excitations can generate holes in the n-type valence band, by pumping electrons up from the valence band into the donor levels, or conduction band (this is the ni2/|ΔN| contribution to the carrier densities). Once a hole is created, the potential drop Δφeff should promptly shuffle it to the other side. We’ll call this current jgen,



And this current would be analogous to the drift current discussed above. On the p-side, a hole (in the valence band as well) outside the depletion zone could make it to the n-side if it could surmount the potential energy barrier. This is called the recombination current, and is analogous to the diffusion current discussed above. And we’d surmise,



Now when ΔV = 0, these must equal as there is no current. So must have:



This kind of makes sense I guess. Because jgen hole excitations on the n-side would have to jump the gap Eg, which is on the order of Δφ anyway. So can say for the net hole current, that:



And we can make an analogous argument for electrons. So altogether we have:



So when ΔV > 0 we get increasing current for increasing ΔV. I guess this is because larger ΔV means a smaller potential barrier for holes to travel from p to n. Or can think of it as ΔV is giving holes going from p to n (and electrons going from n to p), enough energy to surmount the potential barrier inside the depletion zone. Or can think of it as ΔV is shrinking the size of the depletion zone, and so sort of increasing the carrier density gradient, and so enhancing the diffusion/recombination current. So jrec grows without bound as ΔV is increased, but jgen seems predominantly unaffected. I’m guessing jgen is relatively unaffected because it is the drift current. And the drift current responds to the strength of the net electric field. And as we increase ΔV, the net potential drop over the depletion zone Δφeff = Δφ – ΔV, decreases. But the size of the depletion zone, Δx, also decreases. So *maybe* the electric field at the interface ~ Δφeff /Δx ~ more or less remains the same (maybe *it* is the same *at* the interface, if we do a realistic calculation). Of course what we really require is ρE to be constant.

And when the polarity of ΔV is reversed, this increases the size of the potential barrier, and so jrec shrinks to zero ultimately, while again, jgen is unaffected. So when ΔV < 0, we see the current saturates to a constant value of (2e)Ce-βΔφ.

**Induced Current: Second Way**

I feel like that wasn’t very convincing. We combined equilibrium and non-equilibrium thermodynamics in ways that aren’t really kosher. So let’s look at this a little more closely. Typically, when looking for current, we write down and solve (to first order) the Boltzman equation, or RTA if lazy (yes). I don’t see why we can’t work out such an approach here. The only difference between those previous instances and now is the fact that we have that single particle potential φ(r) in the picture, in addition to the external potential V. But this isn’t a fatal difference. Only problem I can see is that it makes evaluation of the integrals more difficult. Well, actually, there is another issue. We need a result that isn’t just first order in ΔV, because we want to show how the current saturates when its polarity is reversed (which is going to require a non-first order expression ~ eΔV). So that’s why we’re going to use a self-consistent approach – a la Ashcroft and Mermin – that doesn’t require ΔV to be small.

***Electrons***

Let’s go back to the Boltzman equation. And let’s focus on the electrons in the conduction band. Instead of trying to separate the currents into drift and diffusion types, we’ll look at the different scattering mechanisms that have to do with the current. In our setup, there are two relevant mechanisms via which the electrons/holes will relax from a non-equilibrium state back into the local equilibrium state. The first obvious one is scattering off of impurities, disruptions in the crystal potential. Such events shouldn’t make the electron change bands, just change k-states within the band. And the second scattering mechanism is electrons scatttering out of the conduction band and into the valence band (recombination), or scatttering out of the valence band and into the conduction band (generation). Basically the second term just describes electrons jumping into or out of the conduction band. We can include both of these processes in the RHS with generic scattering terms.



Now instead of trying to solve for f itself per se´, we’re going to derive from our equation some balance equations. First let’s look at the current equation. Let’s multiply both sides by N**k**, and integrate over **k**,



Now we should find that the integral over the Sgr term goes away, because the Sgr term conserves momentum (right?). This is the same as how we found that the e-e scattering term also made no contribution to the current (see NESM balance equations). So then we’d have:



And now for simplicity, we’ll presume to model Ssc with a relaxation time approximation.



Now I’ll say τsc is independent of k for simplicity’s sake. Then the integral over fleq will be zero, as fleq is symmetric in k. But the integral over f will not be zero, generally, since we presume the non-equilibrium f will carry some current. Then we can say,



Now ∫d3k N**k**f(r,k) is just the m×(number) current density, **j**(n)(r) = n(r)**u**(r) where n(r) is the local particle density, and **u**(r) is the local average velocity of the particles. Can/will also write this as **j**(n)(r) = **je**(r)/e, where **je**(r) is the electric current coming from electrons. Might check out the balance equations file (Stat Mech folder) for more on this. Now we have:



Gonna do the two integrals component by component, using Einstein summation notation. First guy is:



A common approximation at this point is to replace the ekikjτsc/m2 term by its average <ekikjτsc/m2>. This is called the diffusion constant/tensor,



though I guess it technically could be position-dependent, and even time-dependent, as we really can’t say f is not time-dependent here. But if we approximate D by evaluating it via a local equilibrium distribution, we can say,



Well that’s for 3D; if we are in 1D, then this is:



So same thing. But regardless, then we have:



Guess I’ll just take D to be position independent. And then going back to vectors, we can say,



And the other guy is:



Let’s IBP. Note the boundary term/surface integral that we’d have as part of this will go to zero as f(k) → 0 as k → ∞. So we’ll just ignore that term.



So going back to vectors, we can say,



Filling these in, we have:



So we finally come to our first equation:



Now we’ll go back to our Boltzman equation and just integrate over k,



The Ssc term should be zero now, as scattering off of impurities doesn’t change the local density of particles. But the Sgr term should matter, as when electrons change bands, the local density of electrons in either band will change. So we’ll have:



and now we’ll approximate this term with the relaxation time approximation, and also presume τgre [e superscript is to indicate this scattering time is for electrons, and gr subscript stands for ‘generation, recombination’] to be position/momentum independent,



so our second equation is:



***Holes***

The hole distribution function follows (see Metals/Free Day/Non-equilibrium Properties/Conductivity file – basically everything is the same, but have to realize that **v** = ∂εv/∂k = -**k**/m):



And let’s repeat our manipulations to this guy. Multiplying by sides by N**k**, and integrating over d3k, we’ll find:



Now we should find that the integral over the Sgr term goes away, because the Sgr term conserves momentum (right?). And now for simplicity, we’ll presume to model Ssc with a relaxation time approximation.



Now I’ll say τsc is independent of k for simplicity’s sake. Then the integral over fleq(h) will be zero, as fleq(h) is symmetric in k. But the integral over f(h) will not be zero, generally, since we presume the non-equilibrium f(h) will carry some current. Then we can say,



Now ∫d3k N**k** f(r,k) is just the (*negative*) mass × (number) current density. And number current density = **j**(n)(r) = **j**h(r)/(-e), where **j**h(r) is the hole current density. And remember the (*negative*) is because for the hole energy spectrum **v** = -**k**/m, thanks to the concave down spectrum. So now we have:



Recall we did those two middle integrals,



So this comes to:



which differs from the one we got for electrons only in the sign of the **D** term, which we could chalk up to the fact that the -e is the charge of a hole. And let’s get the other equation. So we’ll go back to our Boltzman equation and just integrate over k,



The Ssc term should be zero now, as scattering off of impurities doesn’t change the local density of particles. But the Sgr term should matter, as when hole changes bands, the local density of holes in either band will change. So we’ll have:



and now we’ll approximate this term with the relaxation time approximation, and also presume τgrh to be position/momentum independent (and we’ll use h superscript to remind us of the fact that we’re dealing with holes),



so our second equation is:



**Altogether**

So our complete list of equations is:



and,



where nc is density of electrons in conduction band, pv is density of holes in valence band, and where nc(0), pv(0) are nleq, n(h)leq respectively, and where **j**c,v is the current density in the conduction and valence bands. I guess we should be using different band masses for the electrons and holes too. But oh well. FWIW, the τgr lifetime is much longer than τsc. The former is ~ μs, and the latter ~ ps. And we can take our equilibrium electron and hole densities to be roughly what we found them to be in the last file, i.e., what they are when V = 0.



Of course in the last file, we didn’t consider the presence of the ni2/|ΔN| density contribution to the charge density. But all we’re going to maintain is that the equilibrium electron carrier density goes (left to right) from ni2/Na to Nd + ni2/Nd ≈ Nd, and that the equilibrium hole density goes from (left to right) Na + ni2/Na ≈ Na to ni2/Nd, as sketched out in the V = 0 picture above. Well here,

Diagram

Description automatically generated

Should note there is a constraint on the τgr times. Whenever a hole is created, an electron must be created too, to keep the charge the same. Therefore we need:



So,



Moving on,

**Simplifying the current expression**

Let’s now specialize to time-independence. We’re looking for the steady-state non-equilibrium solution. So, our equations come to (also just going to presume a constant isotropic diffusion tensor):



and,



Before we dive in, let’s try to simplify our considerations. So first, we’ll consider the depletion zone. Here the carrier density is small, and the electric field strong. So the carriers must speed up substantially (by current conservation) across the depletion zone. We’ll presume that their transit time is much smaller than τgrv,c, and so there is negligible generation or recombination in this zone. So across the depletion zone, we can effectively take the last set of equations and set τgrv,c → ∞. This would make jc and jv constant across the depletion zone (assuming we’re working in 1D). And since the total current should be the same everywhere, we can say,



These are convenient points to evaluate the current because jc(-dp) and jv(dn) consist primarily of a diffusion current (as the carrier densities here are small, but the carrier gradient densities are not). So we don’t need to know anything about the electric field per se´ to evaluate the current, just the carrier densities. And we can say,



**Solving for the Carrier Densities**

So to get the currentt, we just need the carrier densities in the diffusion/homogeneous zones. We’ll develop a differential equation for the densities. Now in the difussion region, near x = -dp, since the nc’s drift current is negligible next to its diffusion current, we may take our two Boltzman equations and say,



Plugging the latter into the former, we find:



And we may do the same for pv in the diffusion region near x = dn,



and,



So our two equations, for nc and pv, are:



These are clearly the same equation. And I want to solve them in the diffusion+homogeneous zones. We’ll take nc(0) ≈ ni2/Na, and pv(0) ≈ ni2/Nd, although I feel like these should carry some potential dependence Δφ? Well, I guess that as far as the equilibrium situation goes, the carrier densities will carry Δφ dependence only *inside* the *equilibrium* depletion zone. Our range of concern here is outside the *non-equilibrium* depletion zone. But...the non-equilibrium depletion zone is contracted into the equilibrium depletion zone (see picture above) a little bit. So in our range x ∈ (-∞, -dp) and x ∈ (dn, ∞), it seems there would indeed be a little bit of Δφ and x dependence in nc(0) and pv(0) for x in the vicinity of -dp and dn, though not far away towards x → -∞ and x → ∞. Oh well. This might be a second order effect. For the majority of the range, certainly we can say nc(0) ≈ ni2/Na, and pv(0) ≈ ni2/Nd. Assuming this, the general equation and solution is:



Then we have to match boundary conditions. So for nc(x), we have nc(-∞) = nc(0) = ni2/Na and nc(-dp) = nc(-dp), whatever that is. Of course, now I wonder how appropriate it is to be talking about x = -∞, because we derived our orange-ish equations under the presumption that the diffusive current was larger than the drift current, because this presumption is no longer true for x deep in the homogeneous zones |x| → ∞. Maybe this also is a second order concern. So continuing on, we’ll say:



So,



And for the hole carrier density, we have pv(∞) = pv(0) = ni2/Nd and pv(dn) = pv(dn), whatever that is.



So we have:



Last notational thing. Let’s introduce the diffusion lengths:



These are the same lengths that are referenced in the diagram up above. And altogether,



We can write down two equations for nc and pv at the boundaries of the depletion zone. First, consider that inside the depletion zone, electric charge from n transfers to p, and so inside the zone p or n can have acquired charge or holes from n or p respectively. But outside the depletion there is no charge transfer, and charge or holes come from the native p or n itself. Assuming that in n, all Nd donors go into the conduction band, and in p, all Na acceptor holes go into the valence band, we should always have nc = Nd + pv for n, and pv = Na + nc for p, outside the depletion zone. And so just outside the zone, at the boundary, we can say:



This is one set of equations. Now we need another set of equations. So we claimed up above that inside the depletion zone, the drift and diffusion currents were large, and nearly canceled out – their difference being the net current through the junction. Well if they do nearly cancel, then we can say, from our Boltzman equation:



where φeff = φ + V includes both the intrinsic potential difference induced by charge transfer, φ, and the potential difference induced by the battery. Let’s fill in the diffusion constant (see somewhere above).



So then we have:



And these two guys imply,



So then we have our second set of equations:



And we these four equations, we can get the carrier densities at the borders of the depletion zone. Filling these two into the top two, we have:



And the solutions are:



And these are, filling in Δφeff:



So what is this eeφ/kT factor? Well we can look back in the Thermal Excitations file. And we see,



But then also recall the definition of intrinsic carrier density:



So then we can say,



And then we can say the border charge densities are,



Jeeez. Now we can fill these values into our density expressions:



and,



So that we have, penultimately:



**Back to current**

And finally, we can fill these into our current expression:



So this is our expression for the current,



Might observe that both diffusion constant D depends on τsc and diffusion length, Ln,p depends on τgr. So both scattering mechanisms are present in this expression. And this formula matches the form of our first formula derived/surmised way up above. But now we have an expression for the prefactor C. Reiterating discussion above, so when ΔV > 0 we get increasing current for increasing ΔV. I guess this is because larger ΔV means a smaller potential barrier for holes to travel from p to n. So jrec grows without bound as ΔV is increased, but jgen seems predominantly unaffected. But when the polarity of ΔV is reversed, this increases the size of the potential barrier, and so jrec shrinks to zero ultimately, while again, jgen is unaffected. So when ΔV < 0, we see the current saturates to a constant value as ΔV is increased.

