**Balance Equations**

At the beginning of the Thermodynamics folder, we set up some conservation laws, or rather, balance equations. First we set up the macroscopic case, and then later the microscopic case. I’d like to do the microscopic case here too, from the starting point of the distribution function. We’ll find excellent agreement with our prior analysis. So let’s analyze some conservation and non-conservation laws. First the former.

**Collisional Invariants associated with 2-particle interaction**

Now before we get to conservation laws, want to talk about collisional invariants. These are quantities A(r,k) which, when integrated against the collision integral, ∫d3k A(r,k) give zero, regardless of the form of f, i.e., (leaving off the NV that goes on the collision integral for two-particle interaction)



(obviously specializing to the two-particle interaction case) What are some of these? We can work out an equation that the A’s must satisfy via steps similar to those above apropos ln(f). First we’ll write k as k2 and k´ as k´2.



Now switch k1 and k2. Since they’re dummy variables, we get the same thing:



Adding two together, and dividing by two, we get:



Then switch primed and unprimed variables:



Adding this to the previous guy and dividing by two we have:



So if we’re to have = 0, then we must have:



Now we know the sort of things that are the same before and after a collision: any constant, momentum, and kinetic energy. And all of these could be added to a function of purely position too, so we could say any single particle energy is a collisional invariant as well.

**Collisional Invariants associated with random impurity potential**

So now we want to consider quantities of the form,



switching primes we have:



which follows from time reversal symmetry, if present. And then,



And adding to first expression and dividing by two:



So any quantity that is the same before and after the collision is invariant. Of course any pure function of position A(**r**,**k**) = A(**r**) will be therefore. Also kinetic energy A(r,**k**) = k2/2m will be, since the magnitude of **k** and **k**´ are identical. But we’ll note that **k** itself certainly is not.

**Conservation Equations**

Now let’s say we have some colliding particles within some random impurity potential subject to some force F, part of which is conservative and part not we’ll say. Then the Boltzman equation would read:



(Those two W’s not same, of course). And now let’s see what it has to say about the time-development of the density, momentum, and energy.

**Continuity equation**

The density and current density are:



We can/will also define an average (entropic) velocity as:



And if we multiply by N and integrate both sides of the Boltzman equation over d3k we’ll get:



Now from our analysis above, we know we get zero for the RHS. So we’re left with:



And in terms of the average velocity defined above, we have:



**Newton’s 2nd Law**

Average momentum, and momentum transfer are:



Note that according to our definition above, we have that:



We can simplify the **j**p guy. Before we do, I think it’s worthwhile to point out a common approximation, which is to replace the **k**2/m term by its average,



If we do this, then we can pull the average out, and write,



The <k2/m> term is proportional to the diffusion tensor – see Diffusivity file. If it’s known, and we usually assume it is approximately known, then that will make the continuity equation and N2L self-consistent, meaning they’re all we need to solve for stuff. So that’s a nice advantage of this approach. But otherwise….it’s conventional to write k as the average velocity + deviation from.



But the middle terms are zero. For instance,



And similarly for the other one. So we have:



The last guy is called the pressure tensor,



So then altogether we may write:



So ℘u is the convective momentum current, and **π** is the pressure tensor. It seems to model both the diffusive momentum current and/or the momentum transfer via reflection off of boundaries between compartments, if there are any. And so it seems to capture the effect of collisions with particles in adjacent compartments, in a way, even though that’s technically got zero contribution according to the collision integral. Now let’s look at N2L. We can obtain this by using the Boltzman equation, multiplying everything by N**k**, and integrating w/r to d3k. So…



We know that the two-particle collision integral gives us zero. But the impurity guy does not. Anyway, if we just call this contribution, -int, then we have, going to just components, and using Einstein summation notation:



where in the penultimate line we assume that the forces are not dependent upon velocity – an assumption which was tacitly made above since we wrote **F**(**r**,t) – and we write the force in terms of the force density. Inserting the definition of jp in terms of the other two things, we have:



To be more explicity, that divergence operator should be contracting with the **u**. This compares nicely with the continuum thermodynamics file stuff I guess.

**1st Law of Thermodynamics**

As usual, we can obtain this from the Boltzman equation as well. First we’ll define the energy and energy current,



The former simplifies to the following:



We can further break k into the average convective velocity and fluctuation about,



So the first term is kind of the bulk kinetic energy, and the second is the internal energy, comprised of internal kinetic energy κε and potential energy φ, which together I’ll call εint. So:



and so finally,



Might note that κε(r,t) is the trace of (1/2)**π**(**r**,t). We can simplify the **j**ε guy just as we did **j**p. We write k as the average velocity + deviation from.



where we use the earlier definition of **u**(**r**,t). Like before we’ll find it useful to split the kinetic energy up into a convective and diffusive term, leaving off (**r**,t) arguments in **u**.



Three terms are crossed out; thanks to definition of **u** these guys are zero. The red terms are convective transport of bulk kinetic energy and internal kinetic energy. The blue terms are related to pressure tensor. And the green guy is heat current. So,



And defining, as we said, the heat current:



And recalling the definition of the energy density and pressure tensor, we finally have:



With these definitions out of the way, we’ll finally get to the energy conservation equation. We’ll just multiply both sides of the equation by: ε = (1/2)mv2 + φ(**r**), and integrate both sides over d3k. So then…



Of course the RHS is zero. And for the left (Einstein summation notation),



Two integration by parts and we get:



Now the surface term is zero, since the distribution must go to 0 at those ends, and the other terms turn out to:



where **F**(nc) is the (non-conservative) force Fnc = F + ∇φ. And then,

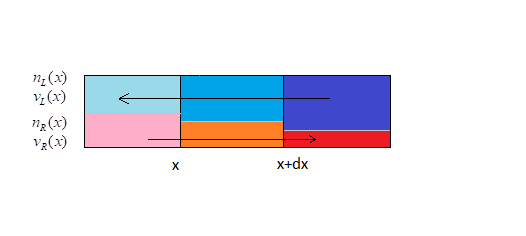


Filling in those definitions pertaining to **j** and **j**ε we have:



**Rudimentary Model of Energy Current**

I’d like to work out a rudimentary model of the energy equation, just to understand it better. So consider a compartment between x and x+dx.



Let the distribution function describe two sets of particles per compartment: one set moving to right all at the same speed, and other to left all at the same speed. I’m going to say the density moving right is nR(x) and left is nL(x). And I’ll say their velocities are vL(x) and vR(x). For simplicity, I’m going to have it that the whole thing amounts to constant net density, so that nL(x) + nR(x) = n, and that the whole thing amounts to moving to the right with speed v. So that jR(x) + jL(x) = j(x) = nu. Also going to make u constant, for simplicity. In my picture above I have vL,R(x) decreasing,increasing to the right. And this means that nL,R(x) is increasing,decreasing to the right. We can write the distribution function as:



where kL,R(x) = mvL,R(x). But let’s write in terms of fluctuations about mean velocity, so let’s say:



According to the conditions above, we have:



This just confirms that the particle flux within each compartment is zero, net. Now the pressure is, leaving off x-dependencies:



This makes sense (see blue term) as the force exerted on the left wall. The force ought to be just the rate at which momentum of particles hitting the wall changes. This is minus the rate at which we are losing leftward momentum plus the rate at which we are gaining rightward momentum. It’s easiest to evaluate this in a comoving reference frame (velocity u), as force is invariant w/r to Galilean transformation anyway. So then,



Now consider the heat current. This is:



This makes sense (see blue term) as minus the rate rate at which energy is vanishing when it hits the left wall (the left current) + the rate at which energy is being ‘created’ as it leaves the left wall. In my picture, the particles are just being reflected off of the wall, so they’re not really ‘vanishing’ or ‘being created’, just being reflected, but yeah. Can see, by the way, that if we had R = L, then jq would be zero. Also, if R = L, we’d have nR = nL, by earlier stipulations. And the vanishing of the heat current makes sense because then our compartment would be in ‘equilibrium’ of sorts, whereby we have equal numbers of particles moving left as are moving right (and equal speeds too). And we should only have a heat current when out of thermodynamic equilibrium. The energy density would be:



which makes sense of course. Let’s look at the entire energy current now,



And we can see that jε = εu + πu + jq, since,



And,



And,



Cool. Going back to jq, we can see that we’ll have a heat current when our distribution is skew, like the one we used above on the left, or more realistically the one on the right, say.

