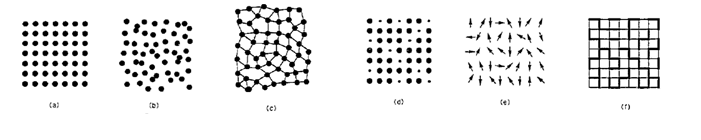
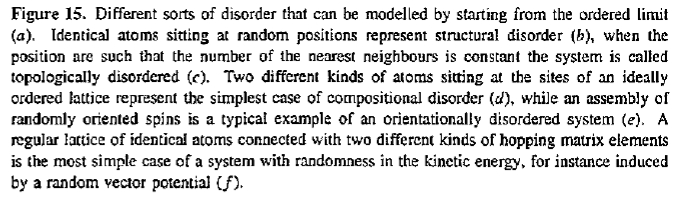
**Electron-Impurity Interaction**

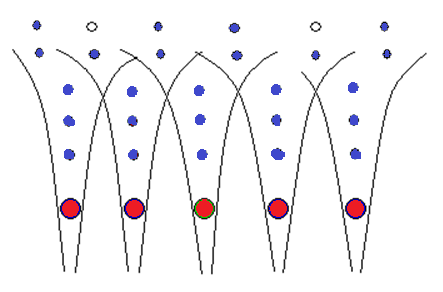
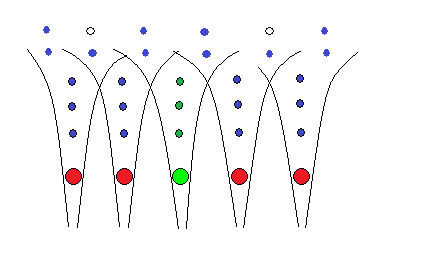
First of all, there are different types of disorder that are usful to rewiew. Took this diagram from a book somewhere…



with commentary….



We’re going to focus on disorder coming from doping, i.e., replacing host atoms in the crystal lattice with impurities. Undoped metals look like this on the left, basically – can see unfilled conduction band on top. But a doped metal might look like this on the right,

The impurity disrupts the periodic crystal lattice by altering the local electric potential, at least. But I guess we can consider the net potential to be the periodic potential plus some difference, which we’ll call the disorder potential. We can imagine periodic potential to come from the imaginary lattice w/o impurities. And the random disorder potential to come from what’s left: basically the potential coming from impurities minus the potential coming from those host atoms whose sites the impurities are technically occupying instead. The impurities might do more than just alter the potential landscape. They could contribute extra electrons to the conduction band, and they could subtract electrons from the conduction band. And they could commensurately open up states, possibly magnetic, for the conduction electrons to jump into or out of. But these extra possibilities we’ll ignore for now – see Magnetic impurities, and Semiconductors for more on that.

So anyway, we’ll consider a bunch of electrons situated within a positive crystal ionic lattice. And add a non-periodic one-particle potential, Vdis(r), from these randomly placed impurity atoms in an otherwise periodic system.



[Since the high temperature phonon correction to the conductivity has the same form as a random impurity, can high temperature ph. – e. interactions be treated under this rubric?] We’ll treat the ee interaction as a constant, and the lattice ions as immobile, which makes the ion-ion potential energy constant and neglectable. So then we have:



We’ll simplify further, and presume all the crystal potential does is renormalize the mass m → m\* (but will still call it m). And so we’ll have:



The disorder potential is:



and results from the impurity potentials Vi(r-Rj) stemming from the N impurity sites Rj, j = 1…N. The corresponding second quantized many particle Hamiltonian can be written in the momentum basis as:



where



because (see that Fourrier Transform file and 2nd quantization file which defines these creation/annihilation operators):

 Diagram

Description automatically generated

Or done out explicitly, using,



we get:



which is the same, once we rename k´ → k. We’ll be interested in thermally averaged GF’s, so we will refer back to the TA GF file in Statistical Mechanics.

**Disorder averaged Green’s function (1)**

Now we want to investigate the Feynman rules for the single particle, complex time, GF:



where < > is the thermal average Trfeq.()/Trfeq.. Once we have this, we may calculate energy expectations, other thermal expectations. And certainly we can determine transport properties. Guess we’ll be presuming non-magnetic impurities here. To get the rules, we could, since our perturbation is just a single particle potential, use the differential equation approach. But I’ll stick with the Wick expansion approach rather.

The expression for Vdis(r) above is exact, but it’s specific to a particular set of impurity positions. In practice, we don’t know these positions. However, for a given impurity concentration the macroscopic physical properties turn out to be the same for almost all impurity configurations. For this reason, our best estimate of the physical properties comes from averaging those properties over an ensemble of samples having the same impurity concentration, but all possible distributions of the individual impurities. We define the disorder average of a quantity G to be:



So you integrate over the phase space of the impurities basically – each impurity can range over a volume of V. With this value you can see that the impurity average of a constant is then just the constant, as it should be, and in particular, no one arrangement of impurities is given a higher weight than any other. In any event, we will use the results of the previous section to calculate GC\*(r,rˊ,τ) via its Fourier representations. A useful side-effect of disorder averaging is that translational invariance present in:

,

but broken in



Is restored in



This allows us to write



Where C\*(k,iωn) is the disorder averaged momentum Green’s function. We can see that the disorder averaging will bring us translational invariance again because we will be integrating over all the R’s in Vi(r – R) and so we’ll impose momentum conservation at those vertices, ensuring that no momentum ‘escapes’ from the system. To keep track of the disorder averaging, we work with finite V (volume), and then take V to infinity. And we’ll have:



Or in shorthand notation…



**Let’s calculate the RHS term by term:**

Starting with,

**Order 0:**

Yup,

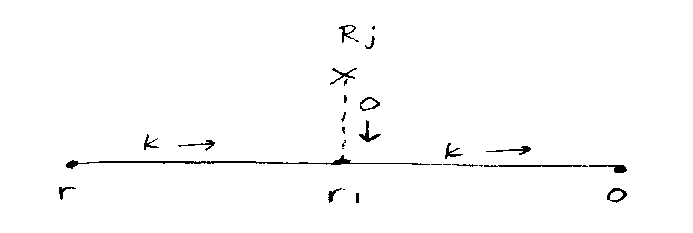


**Order 1:**

Well looks like we got:



We can represent this expression diagrammatically (with reference to the Fourier Transform file),



and then get the following expression



We can effectively set this constant term to zero by measuring our energies from nii(q=0) during our calculation. And so whatever result we get we would then just undo the shift by doing ξk 🡪 ξk + nii(q=0). Or equivalently we could do μ 🡪 μ – nii(q=0). *Another* way to justify the shift is to say that we will absorb this single potential line into the 0th order GF by replacing G0 with the sum of all single potential line graphs. This amounts to:



So there. Now assuming that the shift has been made, we have taken care of/incorporated all V(q=0) terms and are free to effectively set Vi­(q=0) = 0 in the upcoming rest, which means we may ‘say’:



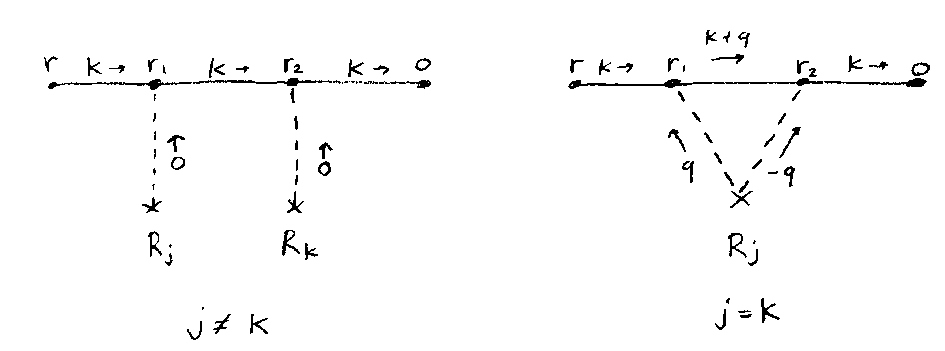
This would’ve also followed from the white noise ensemble procedure mentioned down below. In what follows, we will mostly not explicitly write out the -nii(q=0) term in 0C\*(q). But it will always be implicitly there.

**Order 2:**

So we have:



We can of course represent this diagrammatically too. First we must fix the Rj and Rk that we are going to use. There are Ni2 terms in the above expression. Ni(Ni – 1) of the terms correspond to a situation Rj ≠ Rk, and are illustrated in the first diagram. All of these terms will be 0 because they will contain terms of Vi(q=0), which we have set equal to 0. The other Ni terms will be such that Rj = Rk, and these will be nonzero.



Continuing, we have:



and so,



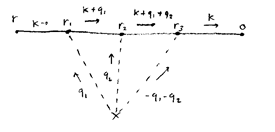
Observe how the white noise ensemble would also force the two external legs to be coincident.

**Order 3:**

And now we have:



Now there are Ni3 terms, corresponding to each of the possible assignments of j, k, and l. However, only the Ni cases where j=k=l will be nonzero, because otherwise we will get the Vi(q=0) term again. This corresponds to the following diagram. And we get the following…

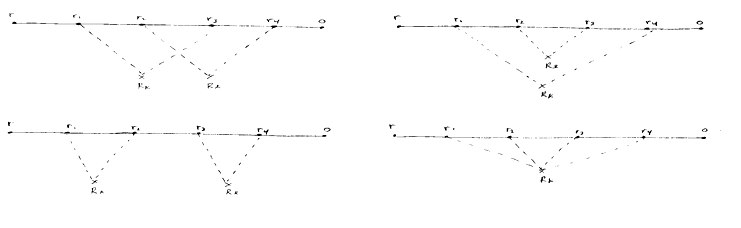


we have:



**Order 4:**

Now there are Ni4 terms, and there are two types of index assignments that will give nonzero results. One is assigning all indices to one value – Rj = Rk = Rℓ = Rm, and results in the familiar Ni number of terms. The other is all possible combinations of assigning just two equal to each other – Rj = Rk, Rℓ = Rm (j≠ℓ). There are 3 distinct ways of choosing which points will be connected to the same impurity. And there are Ni(Ni­ – 1) indistinguishable ways of pairing two impurities. I think that this Ni(Ni – 1) factor is approximated as Ni2. The relevant diagrams are shown below.

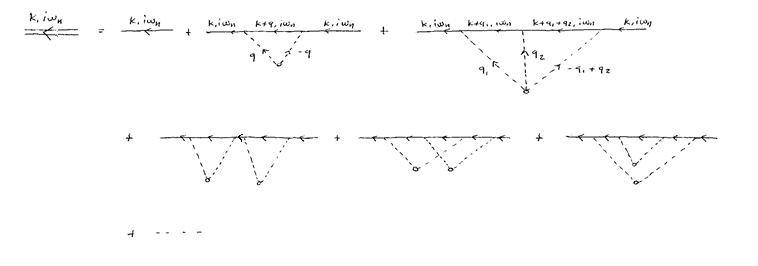


Thus C\*(4)(k,iωn) contains a contribution ~ ni due to quadrupole scattering from the same impurity plus a contribution ~ ni2  due to double scattering at each of two different impurities.

We can base this pattern on reasoning that will be helpful when we encounter disorder averaged current-current correlation functions. Basically, you just expand each Green’s function in the manner we used before disorder averaging, with V1’s at every internal vertex as in the first and third diagrams. Then expand the V1’s as sums over Vi’s coming from all possible impurity sites. You can think visualize this by extending a leg, with an endpoint labeled Rj I suppose. Then realize that when you disorder average, you will get different results depending on whether the Rj, Rk, Rℓ, etc., extending from each impurity potential site are all the same, two the same (which two affects answer as well), none the same...and similarly for all examples with a greater number of impurities. So you have to join the impurity legs in all possible non zero, and distinct ways.

**Feynman diagram rules**

Based on the above, we can represent C\*(k,iωn) via a diagrammatic expansion:



The expansion of C\*(k,iωn) includes all topologically distinct diagrams including all numbers of impurity circles q = 1, 2,…,qj. The numbers of dashed lines meeting at circle j is nj ≥ 2. The distinct ways of ordering the p = Σnj scattering lines (equal to the number of intermediate points in the diagram that are integrated over - excluding the impurity positions) , is equal to p!/q!Πnj.

I’ll formulate the expansion in terms of the <Tψψ†>, rather than the GF itself, -<Tψψ†>, ‘cause that’s how I’ve been doing it heretofore, and I’d like to keep everything the same. So each single/double unbroken line represents one factor of -C\*(0)(k,iωn) / -C\*(k,iωn) where k is the labeled wave vector and the line carries an arrow showing (topologically) the direction of the momentum k. The optional frequency label iωn is the same for all lines.

Dotted lines converging on a circle represent scattering from the same impurity. Each dotted line represents one factor of -V­i(q), where q is the labeled wave vector, and the line carries an arrow from the circle to show that the impurity imparts a momentum q. Each circle is associated with one factor of ni, and connects two or more dashed lines

Net momentum is conserved at each vertex (both on the fermion lines and at the circles)

In a diagram with p dotted lines and q circles there remain p-q unconstrained momenta each of which is integrated over with a factor of 1/(2π)3, or equivalently, summed over with a factor of 1/V.

Disclaimer: reasoning straight from a Wick expansion, as we’re doing, we are accustomed to (and we implicitly are) associating a factor of -G and -Vi with each contraction and each impurity potential/line. But as can see above, there will always be an odd number of these, and so we’ll always get an overall (-) sign if we were to do so. Given that the exact GF would also have a negative sign on it, this means that both LHS and RHS will have a net negative sign, and so would cancel. So we could dispense with all negative signs if we wanted to.

**Disorder averaged Green’s Function (2)**

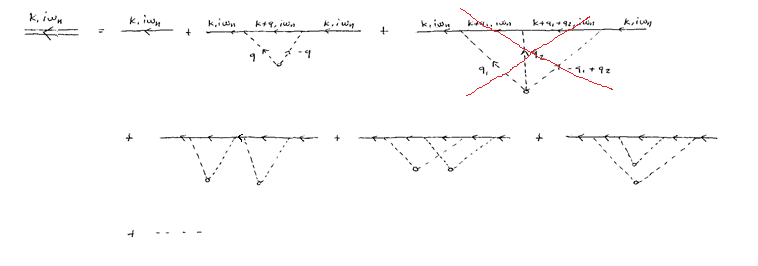
I think a popular alternative procedure is to define the disorder average of V and its correlations in the following manner,



which is the typical white noise distribution, though I’m not sure what γ would be in this case. It would be related to ℓ in some fashion, and hence to the actual diffusion constant D. Then we could carry out the usual FD expansion for a single particle potential (no sum over impurity sites since this is covered by the averages specified above) and at the end, disorder average according to the above. I presume that the disorder average over multiple V’s would break down like a time ordered product or something? It would for Gaussian white noise. If we had used the Gaussian white noise model, then the rules would’ve been similar. The Gaussian weight factor would’ve eliminated the single V contribution as before. And recalling how Gaussian integrals of products works (the Wick expansion – sum of all unique two V correlators), would’ve effectively given us the same rules but each impurity star would have only two impurity lines in it, and we’d have a factor of γ instead of ni.



So the diagrammatic expansion would look like:



These rules give a clearer picture of scattering. The first diagram reads ‘starts at r1ʹ scatters off of r, lands at r2ʹ. And you can see how such a diagram describes essentially classical physics, while the ones with crossed impurity lines describe non-sequential scattering which is inherently wavelike. Anyway, rules would be like above, but each circle would get a factor of γ now.