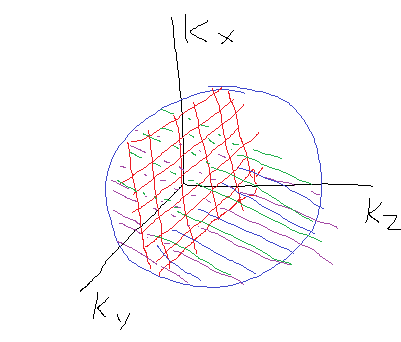
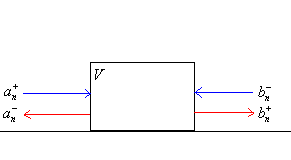
**Q1D Scattering Matrix**

To start we have a sample placed between two leads of same width as the sample. We have clamped boundary conditions so there are N channels at the Fermi-energy N ~ (kFW)d-1, where W is the width (we’re assuming a box geometry) of the sample, and L is its length. Can visualize channels in k-space:



Well this is supposed to represent the channels in the kx – ky plane which constitutes a square, inscribed in the Fermi sphere, and their ancillary kz values which bring the total energy up to the surface of the Fermi sphere at radius kF. The kz values go forward and backward of course, and these are continuous. The kx, ky values are discrete, but note that they may not have the same discretization lengths if the sample is not a square cross-section.



On either side we have wavefunctions:



where we put the wavefunctions in terms of the current amplitude in each channel, like we did in 1D, as the S-matrix relates current amplitudes, not particle density amplitudes. The a’s and b’s may be spinors if spin interactions are present. The total current on the left would be:



(assuming the φ’s are real, though this isn’t critical). Now to get the current, as opposed to current density, we would integrate over the transverse x,y region. And this would fix m = n:



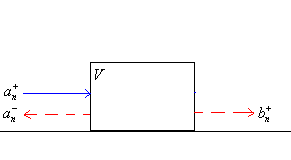
The last line happens because the last two terms combine to give a purely imaginary number. Similarly, if we calculate the current on the right, averaged over space, we will get:



So the coefficients of the wavefunction are written so that the a’s, b’s give the currents themselves. Further we can clearly identify the +’s as forward proceeding currents, while the –‘s are backwards proceeding currents. We could observe that if the coefficients am+ and am- are equal/opposite, then we get no net current on that side. And this is sensible b/c then the exponential terms would combine into a standing wave.

**Transmission and reflection matrices**

These coefficients are related via the transmission and reflection matrices, t, r. These are defined via the following experiment. We send a beam of particles towards the sample from the left hand side (defining the a+ coefficients). These either transmit (defining the b+) or reflect back (defining the a- coefficients). And b- = 0 in this experiment.



So these three sets of coefficients are related via (this is a matrix equation):



Alternatively, if we send a beam in from the right then we have (again, matrix equation):



where a+ would equal 0 in this experiment. So this t is the transmission matrix in the Landauer formula.

**Current Conservation**

In the first situation, current conservation requires:



The only way this can hold is if the middle is 1 identically. So then we have:



Performing the same analysis on the other side, we would conclude that:



as well. We can interpret |tnm|2 as the probability for an electron in channel m to scatter into channel n. We can see this as follows. Let the incident current have unit magnitude and be directed along channel m. Then the reflected and transmitted wavefunctions will be scattered into the other channels, as described by the following wavefunctions:



This is so because the b’s would be given by:



and it follows naturally that |tnm|2 is fraction of current being transmitted from m to n, while |rnm|2 is fraction being reflected from m to n. I suppose we can generalize a little to say that even if there is some spread of currents incident on the left, that |tnm|2 is the fraction of current incident on channel m that emerges into channel n. Likewise |rnm|2 would be the fraction of current incident on channel m that is reflected into channel n. We can think of the matrices t and r as unitary operators that map the incident amplitude ‘a’ onto a transmitted and reflected amplitude ‘ta’, ‘ra’. Now suppose we have unit current in channel m, then it will be transmitted through the other side and populate some of the channels, and it will be reflected into the channels (on same side). The sum total transmission and reflection probabilities must add up to 1. So we must have:



which we know is true from the general current conservation relations (highlighted) above. This affords the interpretation that (t†t)mm and (r†r)mm are the total probability of transmission and reflection respectively *of* channel m. These are usually defined as follows:



and in the other direction we have:



What is the total transmission *into* channel *n* and reflection *into* channel *n*? This would be:



and similarly,



It might help to remember that the † is on the side where the current is bunched up into a single channel. Note that:



So these are not equal. **Going back to the situation where we have current on both sides**…One can argue that the total current being transmitted through channel must have come from either transmission through the left side or reflection from the right side, which gives rise to the identity, in a symmetric scattering situation (see below):



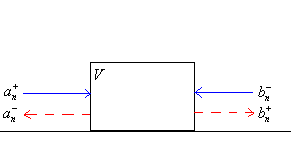
which works out to the following matrix identities:



As a mnemonic, (tt†)mm means current incident anywhere on left and emerging into right side channel m. And (t†t)mm is current incident in channel m on the left, and coming out anywhere on the right. So the current is focused through the side the † is on. And for reflection, (rr†)mm is incident current on left everywhere, reflected into channel m. (r†r)mm is current incident in channel m and reflected anywhere.

**Scattering matrix**

Both of these situations can be concisely encapsulated in the following matrix relation. Suppose we have sent incoming beams from both sides. The set up looks like this:



Then the outgoing beams would follow from solving the Schrodinger equation. Then it follows that the incoming flux can be related to the outgoing flux via the so-called scattering matrix:



This is consistent with the above two sets of equations. If we let the flux come from the left, then b+ ought to be 0, and the matrix relation reduces to the first set of equations above. And likewise if the flux comes from the right and we set a+ = 0. So these t’s, and r’s are the same as those from above.

**Current Conservation**

The current conservation requirement is the same as the condition of unitarity of the S matrix. Consider:



which brings us to the statement S†S = 1. On the other hand, it must also be true that SS† = 1, because S†S = 1 → SS†SS† = SS† → SS†(SS† - 1) = 0 → SS† = 0, 1. We’ll assume that it isn’t 0. Since both are true we can say that S and S† are inverses of each other. So we can say:



As aside, we can work out the determinant of S…



Anyway, going backwards, we can see that the consequence of this statement is the current conservation law:



which implies that,



The first two identities we’re familiar with. The third is interesting….Writing the statement the other way we have:



This then implies that,



The second line implies that:



and this would imply that the sum of the probabilities to transmit into channel n or reflect into channel n equal 1. I guess this sort of expresses the fact that all current which emerges from channel n on the right must have either transmitted from the left side or reflected from the right side. We can also express these statements as:



**Time Reversal Symmetry**

Another symmetry we can glean information from is time-reversal symmetry, should it be present. This implies, if ψ(x,t) is a solution then ψ(x,-t)\* is also a solution. Let’s construct the wavefunction.



Comparing the coefficients, and noting that the S matrix relation between coefficients holds for all wavefunctions, we see that we should have, for both cases respectively:



We can turn the last equation into the form of the first by multiplying both sides by S† and taking the complex conjugate…



Now compare to the original expression and we see that



The consequence of this is:



and so:



These identities make the above two current conservation equations identical.

**Spin-Rotation Symmetry**

In general the elements of S and M are quaternions, if spin interactions are present, so:



a, b, c, d can be complex - that is, the most general quaternion. Apparently, S (and M?) are self-dual if SRS is present. This would mean that:



Therefore self-duality would require that

.

It seems that the dual is a cross between the transpose and the dagger. It transposes, but it doesn’t complex conjugate everything, just the i’s in front of the possibly complex coefficients of the quaternions. The dagger transposes and complex conjugates everything. Of course, the quaternions - **1**, and **σ** - are treated as numbers here, not as matrices, and they don’t get transposed or anything like that. Is it the same for M?

**Parity Symmetry**

What if there were parity symmetry as well? This implies that if ψ(x) is a solution, then ψ(-x) is as well. Note that this doesn’t mean the two wavefunctions are the same. It does mean that the *individual* *eigenfunctions* can be diagonalized by the parity operator, but that they will not all have the *same* parity. So anyway, let’s compare the two wavefunctions.



The scattering matrix describing these two wavefunctions would be:



Again, we can turn the latter into the form of the first via some manipulations:



and so we see that:



which would have the consequence:



which implies:



which would seem obvious in retrospect.

**Summary**

So altogether we have for S:

 (SRS – yes, TRS - yes): S is unitary and symmetric moreover ()

 (SRS – yes, TRS - no): S is unitary

 (SRS – no, TRS - yes): S is unitary and self dual ()

In the β = 1 case, spin is just a spectator – there are no spin terms in H. Additionally, we have TRS, so the transmission coefficient is purely real – only 1 d.o.f. The β = 2 case refers to situations where we might have an L, or p term in H which doesn’t conserve TRS (but not a spin term, presumably). In this case the transmission matrix element can be complex – 2 d.o.f. In the last case, β = 4, we have to explicitly include spin states since we have spin-operators in the Hamiltonian. This gives us 4 d.o.f. in the transmission element since we can have spin up/down for incoming and spin up/down for outgoing.

**Polar decomposition of S**

There is a useful way to write S which separates out the transmission matrix eigenvalues from the rest. From the unitarity property of S, we can write it in polar form.



U and V are unitary matrices, and T is the diagonal matrix of the transmission eigenvalues of tt†. U and V, U′ and V′ have the same symmetries as S in the β = 1, 2, 4 cases. Note how the transmission eigenvalues are degenerate in spin space. This is a consequence of Kramer’s degeneracy. Observe how this form makes sense. On the middle matrix, the left-right diagonal, we just have the reflection eigenvalues (square rooted) which would be r basically. And on the right-left diagonal, we have the square root of the transmission eigenvalues, which is basically t. All we’ve done is separate the transmission/reflection matrices into their magnitudes (middle matrix) and phases (outer matrices). For this reason, its called the polar form – in analogy with the polar representation of a complex number reiφ which separates the complex number into its magnitude times a phase. Now we would like to represent t, t′, r and r′ in terms of this polar decomposition. So we write,



Therefore, we can express the transmission and reflection matrices as



And so then we can say:



Let’s go the other way and determine the U’s and V’s in terms of the r’s, and t’s, setting U = 1 for convenience. Starting from,



we get:



We see that this polar representation separates information about the wavefunction into two parts. U and V contain information about the input phases of the wavefunction. And U′, V′ contain information about the output phases of the wavefunction (the phase shift basically). Notice how this identification makes sense. r is input (U) times reflection coefficient r ~ √(1-T), times the reflection phase U′. t′ is input from left (U) times transmission coefficient, times output phase to right (V′). And similarly for the others. So altogether we see that S contains information about the phase shifts of the wavefunction in the polar matrices, and about the transmission/reflection coefficients in the ‘radial’ matrix.

**Time Reversal Symmetry**

The implications are easiest to see using M. So check out that file. We get:



And so with TRS we can write **S** as:



and this means that the transmission/reflection coefficients would be given by:



**Caveat for spin interactions**

If spin is important, like with SO interaction (which still preserves TRS because both L and S change sign), then we get the slightly weaker symmetry of ‘self-duality’. Parenthetically, having either/and B and SO involved is called a ‘spin-flip’ process. We have instead of:



rather



where the dual operation is defined as:



**A mathematical aside on d.o.f.**

An N×N symmetric complex matrix has N2 + N d.o.f. This is because only the upper or lower triangular part, along with the diagonal are independent entries. The triangular part constitutes (N2 – N)/2 entries and the diagonal N entries. And each carries with themselves 2 d.o.f. (real/imaginary) which equates to 2[(N2 – N)/2 + N] = N2 + N d.o.f.

A Hermitian N×N matrix has N2 d.o.f. because it has the same number as a symmetric matrix, except that the diagonal has to obey the equation Hnn = Hnn\*, which means that the diagonal can only be real. And so that takes away N (imaginary d.o.f.)

A unitary N×N matrix has N2 d.o.f. First, it has 2N2 parameters. The matrix constitutes a set of N mutually orthonormal unit column vectors. Normalizing them all constitutes N conditions (just N b/c magnitude is real). Enforcing orthogonality of first to all those to right constitutes 2(N-1) conditions (factor of 2 is due to real/imaginary). Enforcing orthogonality of second to those on right constitutes 2(N-2) conditions. These orthogonality conditions will add up to a total of 2(N-1) + 2(N-2) + 2(N-3) + … + 2(1) = 2[N(N-1)/2] = N(N-1) conditions. So total number of conditions is N2 – N + N. That leaves N2 total d.o.f. I guess another way to look at it is that a unitary matrix can be written as U = exp(iH), and so it will have the same number of d.o.f. as a Hermitian matrix