Quantum Mechanics II Notes

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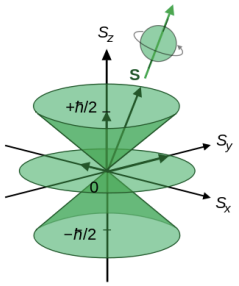
Contents

1 Semiclassical Vector Addition

This is an attempt at unpacking a few concepts about angular momentum addition from Ch. 3.8 (2nd ed, that's 3.7 in 1st ed) of Sakurai. This came up when discussing the interaction between the proton spin and the electron spin, that gives rise to hyperfine structure and the 21 cm spectral line.

1.1 General comments

The semiclassical picture is wildly untrustworthy when the uncertainty is on the order of the mean value. This is the point of the somewhat unwieldy "cone" picture,



where the direction of a spin pointing in the z direction is very uncertain in the xy plane. The z component of that spin is $\pm\hbar/2$, but because it's pointing along a cone (which turns out to have 45 degrees opening angle, if you plug in the numbers), the length of this "semiclassical vector", which of course includes the x and y components, needs to be more than $\hbar/2$. In other words, although the uncertainty relation tells you that you can't know the x and y components if you know the z component, you can know the combination $S_x^2 + S_y^2$, because it's $\mathbf{S}^2 - S_z^2$, and $\mathbf{S}^2$ and S_z commute.

(Contrast uncertainties of x and p, that can have mean values $\langle x\rangle$ and $\langle p\rangle$, the ones we interpret semiclassically as position and momentum, that are enormous by atomic proportions, compared to their uncertainties $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$ and $\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$. Think of a normal distribution: there is nothing wrong with having a big mean and a small spread, or a spread that's comparable to the mean, they're just different.)

1.2 Warmup: eigenvalues for a single spin

Let us use the standard z-direction basis $|m_s\rangle$ (if you want you can write $|s, m_s\rangle$, but for a single spin the s is superfluous, since $s = 1/2$ both for up and down, more about this later), i.e. $m_s = +1/2$, $m_s = -1/2$ for spin 1/2, which can be written as $|+\rangle$, $|-\rangle$. Acting on these states, the x-direction spin S_x has no eigenvalue at all (i.e. it's much worse than being zero, it cannot be defined), because $|\pm\rangle$ are not eigenstates of S_x. Let's remind ourselves of this in a few different ways. To act with S_x on e.g. $|+\rangle$, you can either rewrite the state, or the operator. In other words, you could a) rewrite the eigenstates in an S_x basis, or b) rewrite S_x in the z basis. To do the latter, we could use either a matrix representation of S_x, or writing it in terms of ket-bra pieces like $|+\rangle\langle -|$ (which is equivalent, and can be written on a single line, but is kind of hard to read).

From eq. (3.2.1) we have

$$S_x = \frac{\hbar}{2}(|+\rangle\langle -| + |-\rangle\langle +|) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{1}$$

in the z basis. (In the first equality you see the "hard to read" comment from earlier, or if you don't think it's hard to read, congratulations!) So acting with this operator on spin up we have

$$S_x|+\rangle = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2}|-\rangle \tag{2}$$

For completeness let's also do S_y:

$$S_y|+\rangle = \frac{i\hbar}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{i\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{i\hbar}{2}|-\rangle \tag{3}$$

Since both S_x and S_y flip the spin, the spins are not eigenstates of S_x and S_y so those operators cannot be ascribed any eigenvalue at all in the z basis.

Now let us consider the complex linear combinations $S_\pm = S_x \pm iS_y$, from the previous calculations we see that $S_\pm|+\rangle = (\hbar/2)(1 \pm i^2)|-\rangle$, and similarly on the "spin down" state there's an extra minus sign in (3), leading to $S_\pm|-\rangle = (\hbar/2)(1 \mp i^2)|+\rangle$, so $S_\pm$ act like

$$S_+|+\rangle = 0 \quad \text{and} \quad S_-|+\rangle = \hbar|-\rangle \tag{4}$$

$$S_-|-\rangle = 0 \quad \text{and} \quad S_+|-\rangle = \hbar|+\rangle \tag{5}$$

Let's pause to interpret these equations. This goes back to the Schwinger oscillator model of angular momentum (Ch. 3.9), where you think of S_+ as "creating one unit of angular momentum", like the creation operator $a^\dagger$ in the harmonic oscillator, and S_- as "annihilating one unit of angular momentum". Applying this logic, since there is already a spin sitting in e.g. $|+\rangle$ state, annihilating one unit of angular momentum by S_- leads you to the spin down state, but trying to add another one by S_+ actually annihilates the state. (This last part is special to half-integer spin — in the harmonic oscillator, you can just keep adding oscillators, but here there are only two possible states, so it could either stay the same, go to the "other one" or disappear.) Turning this around, $S_+|+\rangle = 0$ was actually the key point (3.5.17) that led us to the result $m = -j, \ldots, j$ in the first place.

Finally we get to the square of the operator and we have, using $S_x = (1/2)(S_+ + S_-)$,

$$S_x^2|+\rangle = \left(\frac{1}{2}(S_+ + S_-)\right)^2|+\rangle = \frac{1}{4}\left(S_-^2 + S_+S_- + S_-S_+ + S_+^2\right)|+\rangle \tag{6}$$

$$= \frac{1}{4}S_+S_-|+\rangle \tag{7}$$

$$= \frac{1}{4}S_+(\hbar|-\rangle) = \frac{\hbar^2}{4}|+\rangle \tag{8}$$

where I used (4) to go from (6) to (7).

Quick exercise 1: Make sure you follow this step!

Or, we can use the matrix representation

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \Rightarrow \quad S_x^2 = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{9}$$

to also see that $S_x^2|+\rangle = \frac{\hbar^2}{4}|+\rangle$. So actually the z direction spins *are* eigenstates of S_x^2 and S_y^2, which is what lets us construct $S_x^2 + S_y^2 = \mathbf{S}^2 - S_z^2$ simultaneously. In fact we see that

$$\mathbf{S}^2|+\rangle = (S_x^2 + S_y^2 + S_z^2)|+\rangle = 3 \cdot \frac{\hbar^2}{4}|+\rangle \tag{10}$$

which is consistent with

$$\mathbf{S}^2|+\rangle = s(s+1)\hbar^2|+\rangle = \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2|+\rangle = \frac{3\hbar^2}{4}|+\rangle\ . \tag{11}$$

So we have seen that we can speak of lengths and z component consistently, but we need to avoid talking of a z direction spin having a specific S_x eigenvalue.

To prevent any further confusion from this, let us also compute the S_x *expectation value* (as opposed to eigenvalue) in for example the $|+\rangle$ state:

$$\langle S_x\rangle_+ = \langle +|S_x|+\rangle = \langle +|\frac{1}{2}(S_+ + S_-)|+\rangle \tag{12}$$

Quick exercise 2: finish this.

Also note the equation Sakurai (3.2.8):

$$\langle S_x\rangle \to \langle S_x\rangle \cos\phi - \langle S_y\rangle \sin\phi \tag{13}$$

under rotation *around the z axis*. If you were picturing the spin as a little vector pointing straight up, you should have been confused about this, because it should not transform at all if we rotate it around the axis it's pointing along!

1.3 Adding spins

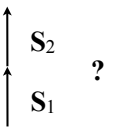
Generically Sakurai writes the angular momenta he's adding as $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$. The most prominent special cases (though there are others) are

- $\mathbf{J} = \mathbf{L} + \mathbf{S}$, where we're specifying ℓ for a given state, it is is integer and $s = 1/2$ always. The complication here is that there can be many states (for large ℓ), so many CG coefficients, but there is a nice semiclassical limit for $\mathbf{L}$ when ℓ is big: $\ell(\ell+1) \approx \ell^2$.
- $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ where $s_1 = 1/2$ and $s_2 = 1/2$. The simplicity of this special case is that in a certain sense (see below) there are only two possible total states — spins opposite or not — but the complication is that the semiclassical picture is completely untrustworthy in the details.

I will pick the second case $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ but what I'm saying here applies conceptually to the addition of any two angular momenta.

First about labelling. The most obvious idea is to label states by spin up or spin down: $|++\rangle$, $|+-\rangle$, $|-+\rangle$, $|--\rangle$ (the m_1, m_2 representation, Sakurai eq. (3.8.13)). But we could also label them by "in the same direction" or "in the opposite direction" (the s, m_s representation, Sakurai eq. (3.8.14)). What is most useful depends on the problem and in particular on rotational symmetry. If there is an external magnetic field pointing up, it *does* matter if both spins are up or both are down — the total energy will be lower if they are both along the field. If, on the other hand we specifically focus on spin-spin coupling (as in the example of the hyperfine structure due to the proton and electron spins), then we could at least temporarily ignore any external magnetic field, and in fact we could use rotational symmetry to rotate "both up" to "both down" so those three $s = 1$ states should be degenerate: hyperfine splitting only depends on "equal or opposite".

Let's say the spins are both up, i.e. the total state is $|++\rangle$. There is a strong temptation to draw a semiclassical picture of vector addition of two up spins like this:



We would then conclude (note the convention is that the total angular momentum has no subscript, in other words $\mathbf{S}_{\text{tot}} = \mathbf{S}$):

$$\text{total length} \stackrel{?}{=} s_{1z} + s_{2z} = \frac{\hbar}{2} + \frac{\hbar}{2} = \hbar \qquad \text{(Attempt 1, wrong)} \tag{14}$$

But we know this is wrong since the length of the "vector" $\mathbf{S}_1$ is

$$\text{length of } \mathbf{S}_1 = |\mathbf{S}_1| = \sqrt{(\mathbf{S}_1)^2} \tag{15}$$

and the eigenvalue of $\mathbf{S}_1^2$ is always $s_1(s_1+1)\hbar^2 = \frac{1}{2}(\frac{1}{2}+1)\hbar^2 = \frac{3}{4}\hbar^2$. so the eigenvalue of $|\mathbf{S}_1|$ is $\frac{\sqrt{3}}{2}\hbar$, not $\frac{\hbar}{2}$, i.e. the vector is not pointing purely in the z direction. The eigenvalue of $|\mathbf{S}_1|$ is what should properly be called the "length" of the semiclassical vector. (The quantum number s_1 itself is sometimes called the "length" in the sense that it is positive and related to the actual length as $\sqrt{s_1(s_1+1)}\hbar$, so s_1 becomes indistinguishable from the length for large quantum number. The problem with trying to interpret that terminology too literally is of course that here $s_1 = 1/2$, which is not exactly large.) So we know both lengths, could we just add them instead of the z components, i.e. the same picture as before but now with the new lengths?

$$\text{total length } \stackrel{?}{=} \sqrt{s_1(s_1+1)}\,\hbar + \sqrt{s_2(s_2+1)}\,\hbar = \frac{\sqrt{3}}{2}\hbar + \frac{\sqrt{3}}{2}\hbar = \sqrt{3}\hbar \qquad \text{(Attempt 2, wrong)} \tag{16}$$

The earlier calculation underestimated the length by only considering the z component, and this calculation overestimates it, by assuming that the full vectors are pointing in the same direction. But at least we learned that the correct value should be somewhere in between $\hbar$ and $\sqrt{3}\hbar$.

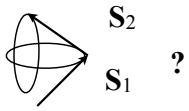
So which direction *are* they pointing in? That's this "cone" business. For $\mathbf{S}^2 = \mathbf{S}_1^2 + \mathbf{S}_2^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2$, in our hyperfine calculation we actually computed the dot product:

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2}(\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2) = \begin{cases} \frac{1}{4} & (\text{"parallel"}) \\ -\frac{3}{4} & (\text{"antiparallel"}) \end{cases} \tag{17}$$

So the angle between them, if there is such a thing, is in any case neither zero nor ninety degrees, but can only be $\arccos(1/4)$ or $\arccos(-3/4)$. Notice that this makes the notion of parallel and antiparallel fuzzy as well, so Sakurai consistently avoids this by calling them singlet $s = 0$ and triplet $s = 1$. To get the dot product above I used the actual calculation: the *quantum numbers* add, $s = s_1 + s_2 = 1/2 + 1/2 = 1$, so we should have

$$\text{total length} = \sqrt{s(s+1)}\,\hbar = \sqrt{1 \cdot (1+1)}\,\hbar = \sqrt{2}\,\hbar \qquad \text{(Correct)} \tag{18}$$

so the $\mathbf{S}^2$ eigenvalue we needed for hyperfine is $2\hbar^2$, and the picture we are left with, which I'd still put a question mark next to, is:



2 Spherical Harmonics and Wigner-Eckart

This tries to give alternative explanations of Sakurai Ch. 3.11, Tensor Operators, assuming that you've at some point tried to read through it and got stuck (as everyone does). Now try to do Problem 3.32 (Prob. 3.28 in 1st ed). Probably you won't completely get it. Then read this. Then go back and read Ch. 3.11.

In quantum-mechanical perturbation theory where the unperturbed problem has spherical symmetry (such as hydrogen-like atoms), it is useful to be able to think of the perturbation as a "spherical tensor", which is closely related to decomposing the perturbation in spherical harmonics. Doing this decomposition helps us decide which integrals we need to calculate (out of a potentially large number, like 45 integrals for the linear Stark effect at level $n = 3$), and is closely related to using the Wigner-Eckart theorem, as I'll try to explain below.

2.1 General remarks on products of vectors

When we teach undergraduates how to multiply two vectors $\mathbf{U}$ and $\mathbf{V}$ in three dimensions, we say there are two options: scalar product and cross product. But let's try to just naively multiply the components U_i and V_j together, for $i, j = 1, 2, 3$ we should get $3 \times 3 = 9$ components. The scalar product is one number, the cross product is a vector so it contains three numbers, so there should be 5 numbers left:

$$3 \times 3 = \underbrace{1}_{\mathbf{U}\cdot\mathbf{V}} + \underbrace{3}_{\mathbf{U}\times\mathbf{V}} + 5 \tag{19}$$

We can think of the cross product $\mathbf{U} \times \mathbf{V}$ as an antisymmetric 3×3 matrix in the following sense:

$$U_iV_j - V_jV_i = \begin{pmatrix} 0 & U_1V_2 - U_2V_1 & U_1V_3 - U_3V_1 \\ -(U_1V_2 - U_2V_1) & 0 & U_2V_3 - U_3V_2 \\ -(U_1V_3 - U_3V_1) & -(U_2V_3 - U_3V_2) & 0 \end{pmatrix} \tag{20}$$

So can express the general product U_iV_j as scalar product + cross product + other:

$$U_iV_j = c_1(\mathbf{U} \cdot \mathbf{V})\delta_{ij} + c_2(U_iV_j - V_jV_i) + c_3 \cdot (\text{whatever remains}) \tag{21}$$

The "whatever remains" is an object you've probably encountered, a *traceless symmetric tensor*. It can be defined as literally whatever is left:

$$S_{ij} = \frac{U_iV_j + U_jV_i}{2} - \frac{(\mathbf{U} \cdot \mathbf{V})}{3}\delta_{ij} \tag{22}$$

meaning apart from the antisymmetric combination in the vector product, we can also make the symmetric combination $U_iV_j + U_jV_i$, which gives the $3 \cdot 2 = 6$ independent components of a symmetric matrix. And if you write out that matrix, its trace will be the scalar product (up to a factor) so we have to subtract that out to avoid double counting. That leaves $6 - 1 = 5$ independent components of the traceless symmetric matrix S_{ij}.

So, S_{ij} is another perfectly OK way to multiply together two vectors $\mathbf{U}$ and $\mathbf{V}$, the only thing that's less familar about it than the scalar and cross products is that it's not written purely in terms of vector algebra. The good news is, there is no other way, we've exhausted the 9 numbers now.

2.2 Spherical tensor, definitions

I advocated using the commutator equation (3.11.25) as definition of spherical tensor, but conceptually (3.11.22b) can also be used as definition:

$$\mathcal{D}(R)T_q^{(k)}\mathcal{D}^\dagger(R) = \sum_{q'=-k}^{k} \mathcal{D}^{(k)}_{q'q}(R)T_{q'}^{(k)} \tag{23}$$

So a spherical tensor of rank k is something that transforms under rotations like this. If it's rank 0, there is only one term on the right, so it's invariant. If the rank $k = 1$, then there are up to three terms on the right, and we like to organize things not in terms of x, y, z but in terms of z, $x_+ = x + iy$ and $x_- = x - iy$, so we label the three components of a rank 1 object as $T_0^{(1)}$ and $T_{\pm1}^{(1)}$, as you see in the sum: for $k = 1$, the index q' runs over $-1, 0$ and $+1$. This also means the Wigner $\mathcal{D}_{q'q}$ matrix is 3×3 so the whole thing is like rotation of a three-dimensional vector, and a generic rotation will mix z, x_+ and x_- components.

Similarly, for a rank 2 spherical tensor you have 5 components: $T_0^{(2)}$, $T_{\pm1}^{(2)}$ and $T_{\pm2}^{(2)}$. These 5 components will mix under rotations, and the $\mathcal{D}^{(2)}_{q'q}$ matrix is 5×5 (this is probably not so familiar, since Sakurai never computed it explicitly).

We start recognizing the 1, 3 and 5 objects from the previous section. A $k = 0$ spherical tensor transforms as a scalar under rotations, a $k = 1$ spherical tensor transforms as a vector, and a $k = 2$ spherical tensor transforms as a traceless symmetric tensor.

2.3 Spherical tensors and spherical harmonics

We're now going to practice Sakurai (3.11.15):

$$T_q^{(k)} = Y_{\ell=k}^{m=q}(\mathbf{V}) \tag{24}$$

If you stare for a while at this equation, you can't say again that you have no idea what the magnetic quantum number q or the rank k is. (You can say you don't have a feeling for them, but not that you have no idea.) But the equation (24) is just an example, not a definition: a completely general spherical tensor could for example have a component that looks like $(U_x + iU_y)(V_x + iV_y)$ (the $q = +2$ component of a spherical tensor of rank 2), which is not captured by equation (24), which only has one vector $\mathbf{V}$ in it.

Exercise: For computing matrix elements in quantum-mechanical perturbation theory, it is useful to be able to decompose for example a) $x^2 - y^2$, b) xy, c) $x^2 + y^2 + z^2$ d) x^2 as spherical

harmonics.
First we're going to need a good table, so let's use Wikipedia:

l = 0[1] [edit]

$$Y_0^0(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{1}{\pi}}$$

l = 1[1] [edit]

$$Y_1^{-1}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\cdot e^{-i\varphi}\cdot\sin\theta \quad = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\cdot\frac{(x-iy)}{r}$$

$$Y_1^{0}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cdot\cos\theta \quad = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cdot\frac{z}{r}$$

$$Y_1^{1}(\theta,\varphi) = \frac{-1}{2}\sqrt{\frac{3}{2\pi}}\cdot e^{i\varphi}\cdot\sin\theta \quad = \frac{-1}{2}\sqrt{\frac{3}{2\pi}}\cdot\frac{(x+iy)}{r}$$

l = 2[1] [edit]

$$Y_2^{-2}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\cdot e^{-2i\varphi}\cdot\sin^2\theta \quad = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\cdot\frac{(x-iy)^2}{r^2}$$

$$Y_2^{-1}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\cdot e^{-i\varphi}\cdot\sin\theta\cdot\cos\theta \quad = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\cdot\frac{(x-iy)z}{r^2}$$

$$Y_2^{0}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\cdot(3\cos^2\theta-1) \quad = \frac{1}{4}\sqrt{\frac{5}{\pi}}\cdot\frac{(2z^2-x^2-y^2)}{r^2}$$

$$Y_2^{1}(\theta,\varphi) = \frac{-1}{2}\sqrt{\frac{15}{2\pi}}\cdot e^{i\varphi}\cdot\sin\theta\cdot\cos\theta \quad = \frac{-1}{2}\sqrt{\frac{15}{2\pi}}\cdot\frac{(x+iy)z}{r^2}$$

$$Y_2^{2}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\cdot e^{2i\varphi}\cdot\sin^2\theta \quad = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\cdot\frac{(x+iy)^2}{r^2}$$

If you're trying to make x^2 from spherical harmonics, a common first reaction is to try to square some $\ell = 1$ spherical harmonic, $(Y_1^m)^2$ for some m. However you're not supposed to multiply any basis functions together when doing a decomposition. Why? It seems we need to back down a little.

2.4 Understanding function decomposition

First two analogies that are useful to keep in mind. It's useful to think about vectors in three-dimensional space. A generic vector $\mathbf{v}$ can be expressed in $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ in the usual way:

$$\mathbf{v} = v_x\hat{\mathbf{x}} + v_y\hat{\mathbf{y}} + v_z\hat{\mathbf{z}} \tag{25}$$

We could call the components v_x, v_y, v_z "expansion coefficients" since we've expanded the vector $\mathbf{v}$ in this basis and v_x, v_y, v_z are the coefficients. If you know the vector $\mathbf{v}$ either geometrically or in some other coordinate system, and wanted to know the components in $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$, we can extract the components by taking scalar products $\mathbf{v}\cdot\hat{\mathbf{x}} = v_x$ and so on. Also note that if you tried to use linearly *dependent* vectors as a basis, for example $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $2\hat{\mathbf{x}}$, you could obviously not expand a generic vector (that may have a $\hat{\mathbf{z}}$ component) in this basis. But as long as you have 3 linearly independent basis vectors, you're fine. Also there is typically no sense to using a bilinear in the basis vectors (like $\hat{\mathbf{x}}\times\hat{\mathbf{y}}$) as another basis vector, because it could itself be expanded in the basis vectors (in fact $\hat{\mathbf{x}}\times\hat{\mathbf{y}} = \hat{\mathbf{z}}$).

It's also useful to think of Fourier decomposition of e.g. a one-dimensional sound wave,

$$f(x) = \sum_n c_n e^{inx} \ . \tag{26}$$

There are an infinite number of frequencies n one could in principle have in a given wave, so there are an infinite number of Fourier coefficients c_n that in principle need to be specified to specify the function $f(x)$. This is not so strange since we can imagine an infinite number of possible periodic functions $f(x)$, so we are trying to span a "space of functions". Function spaces are infinite dimensional, i.e. you need an infinite number of basis functions to expand a given function, as the e^{inx} above for any n. There is now a "scalar (inner) product between functions", defined for example as an overlap integral, and for Fourier modes the orthonormal basis functions are basis waves:[1]

$$\int dx\, e^{inx} e^{imx} = \delta_{mn} \tag{27}$$

This (plus some mathematical fine print) is enough to be able to expand any periodic function $f(x)$ in terms of the basis functions, since we can extract the coefficients by using the overlap integral of $f(x)$ and any basis wave, just like we did for $v_x = \mathbf{v} \cdot \hat{\mathbf{x}}$. For a real sound wave, in practice we only have some reasonably small number that are "excited" (have nonnegligible amplitude c_n). They could be hundreds, but that's still "reasonably small" compared to an infinite number.

What does this have to do with spherical harmonics? They are a basis for scalar functions on the sphere. They are both like basic vectors in 3 dimensions, because you can decompose a generic function on the sphere in terms of them (and only in terms of them). Note in particular you would not use the square of any of them when expanding in them. But they are also like a Fourier basis, because there is an infinite number of them that you would in principle need for a generic function, i.e. we are working with a function space, where the "scalar product between functions" is an integral.

2.5 Restricting to some reasonable number

Above I discussed the rank k of a spherical tensor, which is a generalization of ℓ. The rank k is a useful concept for restricting the number of basis spherical harmonics to a reasonable number. Now x^2 or xy are bilinear $x_i \cdot x_j$ in the coordinates. The maximal rank for a bilinear is $k = 2$, so we won't have to consider any spherical harmonics with $\ell > 2$. Note that in the example in the first section, $\mathbf{U}$ and $\mathbf{V}$ were different, so there were 9 numbers. In the exercise examples above, $\mathbf{U} = \mathbf{V} = \mathbf{x}$, so there are $3! = 6$ combinations. (In fact you can think of this as being the symmetric and scalar part of a product, since the antisymmetric combination of two things that are the same just vanishes.) These 6 combinations are

$$x^2, y^2, z^2, xy, xz, yz \tag{28}$$

[1] Note that you may be able to express e^{inx} in terms of $e^{i(n-1)x}$ using some (possibly nonlinear) trigonometric identities, so the basis functions don't need to be independent in the sense that there exists no functional relationship between them, they only need to be orthonormal in the sense of this overlap integral.

Now, there is one special combination of bilinears. Although x, y and z depend on the angles θ and ϕ, the combination $x^2 + y^2 + z^2 = r^2$ is constant in the angular directions, which means it's proportional to Y_0^0, which is rank $k = 0$. So out of the 6 bilinears, only $6 - 1 = 5$ of them are actually rank 2. This means that any of the 6 combinations above can be expressed in terms of the 5 spherical harmonics Y_2^m plus possibly Y_0^0.

2.6 Systematics

Once we have determined the 6 candidates, we can expand a specific example in them, e.g.

$$x^2 = c_{0,0}Y_0^0 + c_{2,0}Y_2^0 + c_{2,1}Y_2^1 + c_{2,-1}Y_2^{-1} + c_{2,2}Y_2^2 + c_{2,-2}Y_2^{-2} \tag{29}$$

so now instead of an a priori infinite number of expansion coefficients, we have used the "rank" concept to restrict the calculation to only 6 coefficients. One could now explicitly compute the scalar products by using the explicit forms of the Y_ℓ^m:

$$\int d\Omega \; Y_\ell^{m*} x^2 \tag{30}$$

by plugging in x^2 in terms of r, θ, ϕ for each of the 6 spherical harmonics. This would be analogous to computing $v_x = \mathbf{v} \cdot \hat{\mathbf{x}}$ for a three-dimensional vector. But a more efficient way is to use the connection between the spherical harmonic viewed as a spherical tensor that can be expressed in the coordinates themselves, as in the table.

2.7 Solution to Exercise: Decomposing into spherical harmonics

a) $x^2 - y^2$. Looking in the table we see $Y_2^{\pm 1}$ don't look promising because they have an xz. The $Y_2^{\pm 2}$ look better:

$$(x + iy)^2 + (x - iy)^2 = x^2 + 2ixy + (iy)^2 + x^2 - 2ixy + (iy)^2 = 2(x^2 - y^2) \tag{31}$$

so apparently we can expand

$$\begin{aligned} x^2 - y^2 &= \frac{1}{2}\left((x + iy)^2 + (x - iy)^2\right) && (32)\\ &= \frac{1}{2}\left(4\sqrt{\frac{2\pi}{15}}\right)\left(Y_2^2 + Y_2^{-2}\right) && (33)\\ &= 2\sqrt{\frac{2\pi}{15}}\left(Y_2^2 + Y_2^{-2}\right) \; . && (34) \end{aligned}$$

This means in this example, 4 out of the 6 possible coefficients are zero.
b) Following the same pattern we can write the cross term xy as

$$2ixy = (x + iy)^2 - (x - iy)^2 \tag{35}$$

so this is the *difference* $Y_2^2 - Y_2^{-2}$, up to normalization.
c) This one is obviously just Y_0^0.
d) This is a little trickier. We need to get asymmetry between x and y, and Y_2^0 won't do that for us, but the $Y_2^{\pm 2}$ will. With this in mind, we can write an ansatz

$$c_0 x^2 = c_1(x^2 - y^2) + c_2(2z^2 - x^2 - y^2) + c_3(x^2 + y^2 + z^2) \tag{36}$$

and rearranging this, we see that

$$(c_0 - c_1 + c_2 - c_3)x^2 + (c_1 + c_2 - c_3)y^2 + (-2c_2 - c_3)z^2 = 0 \tag{37}$$

which is a linear system for the coefficients, and we find

$$6x^2 = 3(x^2 - y^2) - (2z^2 - x^2 - y^2) + 2(x^2 + y^2 + z^2) \tag{38}$$

so

$$x^2 = \frac{1}{6}\left(3\frac{1}{k_1}(Y_2^2 + Y_2^{-2}) - \frac{1}{k_2}Y_2^0 + 2\frac{1}{k_3}Y_0^0\right) \tag{39}$$

I won't work out the coefficients k_1, k_2, k_3 but you can read them off from the table.

2.8 Matrix element with ground state

Let's say we now wanted to compute the matrix elements of these bilinear operators like $x^2 - y^2$. It's particularly simple if one of the states of the matrix element, e.g. the ket, is the ground state:

$$\int d\Omega\, Y_\ell^{m*} \cdot T \cdot Y_0^0 = \frac{1}{\sqrt{4\pi}} \int d\Omega\, Y_\ell^{m*} \sum_{\ell' m'} c_{\ell' m'} Y_{\ell'}^{m'} = \frac{1}{\sqrt{4\pi}} \sum_{\ell' m'} c_{\ell' m'} \delta_{\ell \ell'} \delta_{m m'} = \frac{1}{\sqrt{4\pi}} \sum_{\ell m} c_{\ell m} \tag{40}$$

so if we have the expansion coefficients $c_{\ell m}$ from above, that's all we need for the angular part of the matrix element. (If it's not zero, we'd still need to do the radial integral.)

2.9 General matrix element

The previous angular integral was for the special case that ground state was one of the states in the matrix element (bra or ket, i.e. either row or column). If they are both general ℓ and m, we have to think just a little more:

$$\int d\Omega\, Y_\ell^{m*} \cdot T \cdot Y_{\ell'}^{m'} = \frac{1}{\sqrt{4\pi}} \int d\Omega\, Y_\ell^{m*} \left(\sum_{\ell'' m''} c_{\ell'' m''} Y_{\ell''}^{m''} \right) \cdot Y_{\ell'}^{m'} \tag{41}$$

where we can't use orthogonality directly since we have *three* spherical harmonics. But now we can expand either Y_ℓ^m or $Y_{\ell'}^{m'}$ in an series using the expansion (3.8.72), to just get two so we can use the orthogonality, which I do explicitly in an example below.

2.10 Seeing the pattern: matrix element with ground state

To take an example, the matrix element of $x^2 - y^2$ with the ground state works out to

$$\int d\Omega\, Y_{\ell'}^{m'} \cdot (x^2 - y^2) \cdot Y_0^0 = \frac{1}{\sqrt{4\pi}} \int d\Omega\, Y_{\ell'}^{m'} \cdot 2\sqrt{\frac{2\pi}{15}} \left(Y_2^2 + Y_2^{-2}\right) = \sqrt{\frac{2}{15}} \left(\delta_{\ell',2}\delta_{m',2} + \delta_{\ell',2}\delta_{m',-2}\right)$$

so the bra ("after") state should better have $\ell' = 2$, $m' = \pm 2$ for the matrix element to be nonzero. On the other hand, $x^2 - y^2$ is a spherical tensor of rank 2 with magnetic quantum number $q = \pm 2$ (to be precise it's the sum of those two componets, as we saw above), so the Wigner-Eckart (WE) theorem says

$$\begin{aligned} \langle n', \ell', m' | T^{(2)}_{\pm 2} | n, \ell, m \rangle &\overset{WE}{=} \langle \ell, k; m, q | \ell, k; \ell' m' \rangle \cdot (n,\ \ell \text{ stuff}) && (42) \\ &= \langle \ell, 2; m, \pm 2 | \ell, 2; \ell' m' \rangle \cdot (n,\ \ell \text{ stuff}) && (43) \end{aligned}$$

Notice in the starting expression, the un-primes are all "before" (bra) and the primes are all "after" (ket), but then when applying the theorem they get a little mixed. Now there are two rules one can use for seeing when the CG coefficient on the right hand side is nonvanishing (this is discussed on p.223 in Sakurai 2nd ed):

$$m' = m + q \quad \text{and} \quad |\ell - k| < \ell' < \ell + k \tag{44}$$

These are easy to remember from semiclassical vector addition: the first one says that the z components of two vectors add, and the second one says that the length of the sum of two vectors has to be somewhere between the sum of the lengths (which occurs if the vectors are parallel) and the difference of the lengths (if the vectors are antiparallel). In particular, for $k = 2$, $q = \pm 2$, the first one gives $m' = m + q = m \pm 2$ and the second one gives $|\ell - 2| \leq \ell' \leq \ell + 2$. For $\ell = 0$ the latter says simply $\ell' = 2$. For $m = 0$ the former gives $m' = \pm 2$. We just get two possible CG coefficients that don't vanish:

$$\langle 0, 2; 0, \pm 2 | 0, 2; 2, \pm 2 \rangle \tag{45}$$

According to the CG tables, if one of the first two j_1, j_2 is zero, the CG coefficient is a Kronecker delta. So which ones are nonzero is consistent with the result above.

Notice the power of the WE theorem was to reduce the calculation to calculating a Clebsch-Gordan (CG) coefficient. Also notice that the theorem itself does not actually tell you anything about what vanishes, but the two CG rules (44) mentioned here are generally useful. Applying the WE theorem *and* knowing something about CG coefficients together produces a "selection rule", a statement about which matrix elements can be nonvanishing.

What about normalization? Cleverly, Sakurai defined the spherical tensors T as including the Y normalization. So the WE result is correct by definition, which means that to relate $x^2 - y^2$ and $T^{(2)}_{\pm 2}$ and use the WE theorem we need to compute the normalization separately. Since in this course we mostly use the theorem to say when something vanishes, this is usually not a big loss.

2.11 Seeing the pattern: matrix element with general state

As mentioned above, Sakurai (3.8.72) says we can expand any two spherical harmonics in a linear combination of single ones:

$$Y_{\ell_1}^{m_1}(\theta,\phi)Y_{\ell_2}^{m_2}(\theta,\phi) = \tag{46}$$
$$\frac{\sqrt{(2\ell_1+1)(2\ell_2+1)}}{4\pi}\sum_{\ell'}\sum_{m'}\langle \ell_1\ell_2; m_1m_2|\ell_1\ell_2;\ell' m'\rangle\langle \ell_1\ell_2; 0\,0|\ell_1\ell_2;\ell'\,0\rangle\sqrt{\frac{4\pi}{2\ell'+1}}Y_{\ell'}^{m'}(\theta,\phi)\ .$$

Let us consider this example, using the decomposition of xy from before:

$$\langle \ell=3, m=2|\, xy\,|\ell=1,m=0\rangle \ \propto\ \int d\Omega\ Y_3^{2*}(Y_2^2 - Y_2^{-2})Y_1^0\ . \tag{47}$$

How do we use the expansion above in this case? Again it boils down to the Clebsch-Gordan coefficient rules in eq. (44). First note that for the upper index, e.g. $Y_2^{+2}\cdot Y_1^0$ requires $m' = 2+0 = 2$. Then for the lower index, $|2-1| \le \ell' \le 2+1$, which means $\ell' = 1,2,3$. So for the two terms we each have three possibilities:

$$Y_2^2\cdot Y_1^0 \text{ can be decomposed into } Y_3^2, Y_2^2, Y_1^2 \tag{48}$$
$$Y_2^{-2}\cdot Y_1^0 \text{ can be decomposed into } Y_3^{-2}, Y_2^{-2}, Y_1^{-2} \tag{49}$$

But this will then be multiplied by Y_3^{2*} and integrated $\int d\Omega$, which by the orthonormality condition gives zero for everything that is not Y_3^2, i.e. $Y_3^{-2}, Y_2^{-2}, Y_1^{-2}$, and Y_3^2, Y_2^2 will all give zero. (Note the orthonormality condition is *with* the complex conjugation). The only nonzero expansion coefficient is that of $Y_2^2\cdot Y_1^0$ into Y_3^2. Which can be read off from a table of Y_ℓ^m, or computed from CG coefficients as above. Explicitly, plugging in $\ell_1=2$, $\ell_2=1$, $m_1=2$, $m_2=0$, $\ell'=3$, $m'=2$ in (46) I find:

$$\frac{\sqrt{(2\cdot 2+1)(2\cdot 1+1)}}{4\pi}\underbrace{\langle 2\ 1; 2\ 0|2\ 1; 3\ 2\rangle}_{\frac{1}{\sqrt{3}}}\underbrace{\langle 2\ 1; 0\ 0|2\ 1; 3\ 0\rangle}_{\frac{\sqrt{3}}{\sqrt{5}}}\sqrt{\frac{4\pi}{2\cdot 3+1}} \tag{50}$$
$$= \quad \frac{\sqrt{5}\sqrt{3}}{4\pi}\cdot\frac{1}{\sqrt{3}}\cdot\frac{\sqrt{3}}{\sqrt{5}}\cdot\sqrt{\frac{4\pi}{7}} = \sqrt{\frac{3}{28\pi}} \tag{51}$$

where I used the CG table from Wikipedia:

j1=2, j2=1 [edit]

m=3 j=

m1, m2=	3
2, 1	1

m=2 j=

m1, m2=	3	2
2, 0	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$
1, 1	$\sqrt{\frac{2}{3}}$	$-\sqrt{\frac{1}{3}}$

m=1 j=

m1, m2=	3	2	1
2, -1	$\sqrt{\frac{1}{15}}$	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{3}{5}}$
1, 0	$\sqrt{\frac{8}{15}}$	$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{3}{10}}$
0, 1	$\sqrt{\frac{2}{5}}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{10}}$

m=0 j=

m1, m2=	3	2	1
1, -1	$\sqrt{\frac{1}{5}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{10}}$
0, 0	$\sqrt{\frac{3}{5}}$	0	$-\sqrt{\frac{2}{5}}$
-1, 1	$\sqrt{\frac{1}{5}}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{10}}$

so the claim is

$$Y_2^2 \cdot Y_1^0 = \sqrt{\frac{3}{28\pi}} Y_3^2 \ . \tag{52}$$

Alternatively, from the table of spherical harmonics we find

$$\begin{aligned} Y_2^2 \cdot Y_1^0 &= \frac{1}{4}\sqrt{\frac{15}{2\pi}} e^{2i\phi} \sin^2\theta \cdot \frac{1}{2}\sqrt{\frac{3}{\pi}} \cos\theta & (53) \\ &= \sqrt{\frac{45}{8 \cdot 16\pi^2}} e^{2i\phi} \sin^2\theta \cos\theta & (54) \end{aligned}$$

and

$$Y_3^2 = \frac{1}{4}\sqrt{\frac{105}{2\pi}} e^{2i\phi} \sin^2\theta \cos\theta = \sqrt{\frac{105}{16 \cdot 2\pi}} e^{2i\phi} \sin^2\theta \cos\theta \tag{55}$$

so indeed

$$\frac{Y_2^2 \cdot Y_1^0}{Y_3^2} = \frac{\sqrt{\frac{45}{8\cdot 16\pi^2}}}{\sqrt{\frac{105}{16\cdot 2\pi}}} = \sqrt{\frac{3}{28\pi}} \ . \tag{56}$$

Either way, I claim that the integral of the three spherical harmonics in our example gives

$$\int d\Omega\, Y_3^{2*}(Y_2^2 - Y_2^{-2})Y_1^0 = \sqrt{\frac{3}{28\pi}}\,. \tag{57}$$

Explicitly, what we have actually shown is that

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\; \tfrac{1}{4}\sqrt{\tfrac{105}{2\pi}}\, e^{-2i\phi} \sin^2\theta\cos\theta \cdot \tfrac{1}{4}\sqrt{\tfrac{15}{2\pi}}\, \left(e^{2i\phi}\sin^2\theta - e^{-2i\phi}\sin^2\theta\right) \cdot \tfrac{1}{2}\sqrt{\tfrac{3}{\pi}}\cos\theta = \sqrt{\frac{3}{28\pi}}\,,$$

which can of course be easily checked with Mathematica or Maple. (As a footnote, one might then wonder why we bother with this at all, if we now have software that can do it for us. I do think excessive repetitive work of calculations by hand ceased to be useful in the last decade, maybe the transition happened when I was in graduate school in the late 90s when we could not rely on commercial software — Mathematica existed but there were webpages collecting mistakes it would make with integrals from standard tables — but part of the *craft* of being a physicist is to be able to compute things, and understanding the inner workings of some of the basics leads to generalization. For example, the general representation theory of Lie algebras, as used in high-energy theory, is a natural generalization of the above. So if all you ever did was plug into Mathematica, you would have no concrete basis to build on for those more general things.)

3 Degenerate Perturbation Theory and Linear Algebra

This is an attempt to give a more elementary example of degenerate perturbation theory than that given in Sakurai, the linear Stark effect. (To be more specific, it is actually essentially the same as the linear Stark effect, but expressed in more elementary and generic terms.)

Consider this matrix

$$H_0 = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} \tag{58}$$

The eigenvalue equation is

$$\begin{vmatrix} E-\lambda & 0 \\ 0 & E-\lambda \end{vmatrix} = 0 \tag{59}$$

that is

$$(\lambda - E)^2 = 0 \quad \Rightarrow \quad \lambda_{1,2} = E \; . \tag{60}$$

We could have read this off right away, since a diagonal matrix has the eigenvalues on the diagonal. This is not called a "degenerate matrix" if we want to be picky, that's one with determinant zero, but it has "degenerate eigenvalues".

The eigenvectors $H_0 v = \lambda v$ are by definition:

$$\begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = E \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \tag{61}$$

which is a linear system

$$\begin{cases} Ev_1 = Ev_1 \\ Ev_2 = Ev_2 \end{cases} \tag{62}$$

that is obviously solved by *any* v_1 and v_2. So we can pick two orthonormal basis vectors

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \; . \tag{63}$$

Now perturb the original matrix by an off-diagonal matrix V:

$$H_0 + V = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} + \begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix} = \begin{pmatrix} E & \epsilon \\ \epsilon & E \end{pmatrix} \tag{64}$$

The eigenvalue equation for $H_0 + V$ is

$$\begin{vmatrix} E-\lambda & \epsilon \\ \epsilon & E-\lambda \end{vmatrix} = 0 \tag{65}$$

that is

$$(\lambda - E)^2 = \epsilon^2 \quad \Rightarrow \quad \lambda_{1,2} = E \pm \epsilon \tag{66}$$

So the eigenvalues are small changes of the original eigenvalues, as we would expect. The eigenvectors are given by

$$\begin{pmatrix} E & \epsilon \\ \epsilon & E \end{pmatrix} \begin{pmatrix} \tilde{v}_1 \\ \tilde{v}_2 \end{pmatrix} = (E \pm \epsilon) \begin{pmatrix} \tilde{v}_1 \\ \tilde{v}_2 \end{pmatrix} \tag{67}$$

which is a linear system

$$\begin{cases} E\tilde{v}_1 + \epsilon\tilde{v_2} = (E \pm \epsilon)\tilde{v}_1 \\ \epsilon\tilde{v}_1 + E\tilde{v}_2 = (E \pm \epsilon)\tilde{v}_2 \end{cases} \tag{68}$$

that is *not* solved by arbitrary $\tilde{v}_1$ and $\tilde{v}_2$. Dividing through by $\tilde{v}_1$ we have

$$\begin{cases} E + \epsilon\frac{\tilde{v}_2}{\tilde{v}_1} = (E \pm \epsilon) \\ \epsilon + E\frac{\tilde{v}_2}{\tilde{v}_1} = (E \pm \epsilon)\frac{\tilde{v}_2}{\tilde{v}_1} \end{cases} \tag{69}$$

that are solved specifically by

$$\frac{\tilde{v}_2}{\tilde{v}_1} = \pm 1 \ . \tag{70}$$

So the two orthonormal basis vectors are

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \ , \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \ . \tag{71}$$

So compared to the original basis this is *not* a small change. Notice also that the new eigenvectors don't contain any ϵ, so this holds for any nonzero ϵ, no matter how small. Since they don't contain ϵ at all, they are *zeroth order* in the perturbation. When we set $\epsilon = 0$ there is a *discontinuous* change in the system, in that the eigenvectors become undetermined.

So could we not have started with these eigenvectors, if the original problem was undetermined? Yes we could, but there would have been no way to find them without doing this analysis. Also, the original eigenvectors might have some simple property that takes advantage of some feature of the unperturbed system, like being parity eigenstates, that would not be guaranteed to be present in the new eigenvectors.

In the linear Stark effect, the V above is the 2×2 matrix where the perturbation is actually nonzero. The new zeroth order eigenvectors are called $|\pm\rangle$ in Sakurai, and they are not parity eigenstates, but they are energy eigenstates of the perturbed system.

Exercise: redo the calculation for a H_0 matrix with values E_1, E_2 on the diagonal, where $E_1 \neq E_2$. How is this nondegenerate case different from the above?

4 Scattering Basics

Again, please *write down* for yourself answers for these problems before you consult the solutions. These should all be much easier than a typical Sakurai problem.

Classical particle scattering

1. Convince yourself by looking in fig. 11.3 that in some generality we can get $d\sigma/d\Omega$ from the more intuitive concepts of impact parameter b and scattering angle θ:

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| \tag{72}$$

Why is this not valid in full generality, i.e. what is the assumption built into equation (72)?

2. Equation (72) can be slightly confusing in that we view b (initial condition) as a function of θ (final outcome) instead of θ as a function of b as we do in question 3 below. What is a sufficient condition on the function $\theta(b)$ that ensures we're free to work with $b(\theta)$ instead, i.e. that the function has a unique inverse?

3. For a hard sphere, the relation between scattering angle θ (final outcome) and impact parameter b (initial condition) in Griffiths eq. (11.2) is

$$\theta = \begin{cases} 2\arccos(b/R) & b \le R \\ 0 & b > R \end{cases} \tag{73}$$

Derive this from elementary geometry (consult fig. 11.2).

4. Now plug in $b(\theta)$ in 1 above, to show that

$$\frac{d\sigma}{d\Omega} = \frac{R^2}{4}\,. \tag{74}$$

Since this hard-sphere scattering cross section is constant as a function of angle θ, it seems we are getting particles scattered also straight in the forward direction $\theta = 0$. But didn't they all bounce backwards off the "front" of the hard sphere?

Electromagnetic scattering

Now instead of a hard sphere we consider the repulsive Coulomb force, and for concreteness pick an alpha particle coming in and a gold nucleus as the scattering center.

5. How is this "Rutherford problem" different from the Kepler problem?

6. Flick through the Wikipedia page `Rutherford_scattering`, or read about it in your favorite book. It writes a differential equation for the trajectory, and solves it to give a formula for the deflection angle (that it calls Θ, I'll keep calling it θ) as function of impact parameter b, analogous to the $\theta(b)$ above:

$$\theta = \arctan b\kappa \tag{75}$$

where $\kappa = Z_1 Z_2 e^2/(4\pi\epsilon_0 m v_0^2 b^2)$ where v_0 is initial velocity. Try to give an interpretation of κ in terms of energies.

7. The incoming alpha particle satisfies Newton's second law $\mathbf{F} = m\mathbf{a} = m\ddot{\mathbf{x}}$, a second order differential equation. Doesn't that mean that for each position, you would have an arbitrary velocity to freely specify, i.e. through each point in space, there is infinite number of possible trajectories passing through? If so, how can we restrict consideration to just hyperbola, parabola, ellipse orbits?

8. Convince yourself that σ_{tot}, the integral over $d\Omega$ of the Rutherford cross section

$$\frac{d\sigma}{d\Omega} \propto \frac{1}{\sin^4(\theta/2)} \tag{76}$$

is infinite. Is there any negative power of $\sin(\theta/2)$ for which σ_{tot} would not have been infinite? Discuss why $\sigma_{\text{tot}} = \infty$ is not surprising, and worry about whether it is a problem.

9. The Rutherford cross section depends on the energy of the incoming particle as

$$\frac{d\sigma}{d\Omega} \propto \frac{1}{E^2} \,. \tag{77}$$

Formulate in words what this means, in terms of how "efficient" the scattering is for high or low energy particles (try to think of a meaning of efficient in this context).

10. For initial velocity of $2 \cdot 10^7$ m and head-on collision, compute the point of closest approach from energy conservation. Is this the radius of the nucleus? By the way, how would you take into account nuclear recoil?

11. The previous problem should show that the scattering cross section in general characterizes how much something interacts, not the physical size of the object causing the scattering (in this sense the hard-sphere example is misleading in general). In particular it is the interaction between the two objects, which may depend on properties of *both* objects. For example the *size of the gold nucleus* bears no direct relation to the size of the "scattering region" which has to do with the electromagnetic force, and is for example proportional to the number of positive electric charges, both in the scattered particle and in the scatterer.

Relate these seemingly abstract statements to the fact that rear fog lights use red rather than white light. To do so, consider the scattering of light off rain droplets in the fog. Does the size of the droplet matter?

5 Bound state scattering (includes solution of Sakurai 6.10)

This is a somewhat more difficult problem than the ones in the homework, but towards the end of your reviewing it would make sense to think about this.

One dimension

Let me first review the situation in one dimension. The transmission coefficient for a square potential *barrier* is Sakurai (B.3.4)

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)} \sinh^2(2a\sqrt{2m(V_0-E)/\hbar^2})} \tag{78}$$

The delta potential *barrier* is the limit $V_0 \to \infty$, $a \to 0$ of the square barrier, but the limit is taken such that the product $V_0 a = \lambda$ (the "area" of the square barrier) is kept fixed in the limit that the barrier is taken to be very thin and very high. Then λ is the constant that ends up in front of the δ function:

$$V = \lambda \delta(x) \tag{79}$$

Note that a δ function barrier should *not* be thought of as an "infinite barrier" in the sense of an infinite square well, as long as λ is finite, since the total energy associated with it is the integral over $V(r)$, which is finite. This can be somewhat surprising, since in classical mechanics nothing can get through an infinitely high barrier *even if* it is arbitrarily thin (i.e. as long as you don't *break* the barrier). In quantum mechanics it's not so much the height that is important as the total energy associated with the barrier.

Either taking a limit of the above expression, or computing it directly, the transmission coefficient for this delta function barrier is

$$T = \frac{1}{1 + \frac{m\lambda^2}{\hbar^2 E}} \ . \tag{80}$$

Three dimensions

Let me consider Sakurai problem 6.10, scattering off of a repulsive spherical delta-function shell:

$$V(r) = \frac{\gamma \hbar^2}{2m} \delta(r - R) \tag{81}$$

with $\gamma > 0$. First, recall from above that a δ function should *not* be thought of as an infinite barrier as long as γ is finite, since the total energy associated with it is the integral over $V(r)$, which is finite. One might think that a positive (repulsive) potential could not trap particles, but if they make it inside, the shell could then repel them from leaving. (This is sometimes used as a "Fermi prepotential" in neutron-nucleus scattering.) The total wavefunction is

$$\psi^{(+)}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \sum i^\ell (2\ell + 1) A_\ell(r) P_\ell(\cos\theta) \tag{82}$$

where we write $A_\ell(r) = u(r)/r$ and u satisfies a one-dimensional-looking radial Schrödinger equation

$$u_\ell'' + \left(k^2 - \frac{2mV(r)}{\hbar^2} - \frac{\ell(\ell+1)}{r^2}\right) u_\ell(r) = 0 \tag{83}$$

Consider $\ell = 0$

$$u_{\ell=0}'' + (k^2 - \gamma\delta(r-R))u_{\ell=0}(r) = 0 \tag{84}$$

This is solved by integrating $\int_{-\epsilon}^{\epsilon} dr$ and taking $\epsilon \to 0$, which gives zero for the smooth contribution from $k^2 u(r)$, leaving us with a jump in the derivative as a matching condition:

$$u'|_{\text{outside}} - u'|_{\text{inside}} = \gamma u \tag{85}$$

Inside ($r < R$) we have $u_0(r) = A \sin kr$ and outside $r > R$ we have $u_0(r) = B\sin(kr + \delta_0)$, with some phase shift δ_0 that is to be determined. Matching u at $r = R$:

$$B\sin(kR + \delta_0) = A \sin kR \tag{86}$$

Matching u' at $r = R$ with the discontinuity from eq. (85):

$$Bk\cos(kR + \delta_0) - Ak\cos kR = \gamma A \sin kR \tag{87}$$

If we divide this equation by the previous one (which means forming the logarithmic derivative u'/u) we get an equation that's free of the normalization constants A and B:

$$k\cot(kR + \delta_0) - k\cot kR = \gamma\ . \tag{88}$$

or

$$\cot(kR + \delta_0) = \cot kR + \frac{\gamma}{k}\ . \tag{89}$$

This determines δ_0. Before solving for it exactly, note that for $\gamma \to \infty$ we have a simple approximate solution: $\cot(kR + \delta_0) \to \infty$, which just means $\sin(kR + \delta_0) \to 0$, so $kR + \delta_0 \approx 0$, or

$$\delta_0 \approx -kR \quad \text{for } \gamma \to \infty \tag{90}$$

like for the hard sphere. Plotting the cross section $\sigma = 4\pi \sin^2\delta_0/k^2$ in this limit we have a $(\sin x/x)^2$ function.

Quick exercise 1: Argue physically why the delta shell phase shift (and therefore cross section) should reduce to the hard sphere in this limit.

There are many ways to solve for δ_0, the most simple-minded is to solve for $\cot\delta_0$ by using the addition formula for $\cot(x+y)$, which reads

$$\cot(kR + \delta_0) = \frac{\cot(kR)\cot(\delta_0) - 1}{\cot(kR) + \cot(\delta_0)} \tag{91}$$

leading to

$$\cot kR \cot \delta_0 - 1 = (\cot kR + \cot \delta_0)(\cot kR + \frac{\gamma}{k}) \quad (92)$$

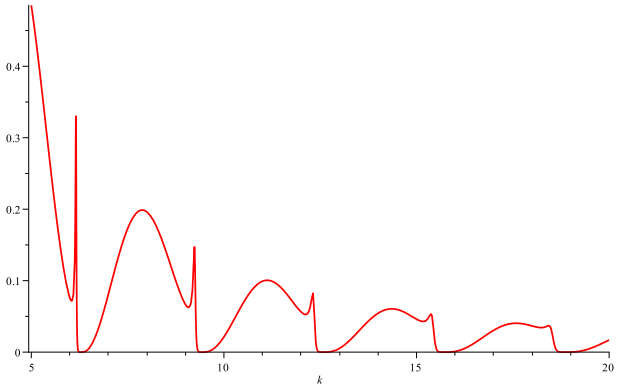
$$= \cot^2 kR + \frac{\gamma}{k} \cot kR + \cot \delta_0 \cot kR + \frac{\gamma}{k} \cot \delta_0 \quad (93)$$

so collecting terms we have

$$\cot \delta_0 = -\frac{k}{\gamma} \left(1 + \cot^2 kR + \frac{\gamma}{k} \cot kR\right) \quad (94)$$

$$= -\frac{k}{\gamma \sin^2 kR} - \cot kR \quad (95)$$

using $1 + \cot^2 x = 1/\sin^2 x$. Plotting the cross section $\sigma = 4\pi|f|^2 = 4\pi/(k^2(1 + \cot \delta_0^2))$ (which is also equal to $4\pi \sin^2 \delta_0/k^2$), we have



We suspect that the spikes are caused by resonances. The resonance condition $\cot \delta_0 \approx 0$ occurs at k values $k = k_r$ for which

$$\frac{k_r}{\gamma \sin^2 k_r R} \approx -\cot k_r R \quad (96)$$

which using $\sin 2x = 2 \sin x \cos x$ is

$$\sin 2k_r R \approx -\frac{2k_r}{\gamma} \quad (97)$$

so $k_r R \approx n\pi - \frac{k_r}{\gamma}$ (we will see below why $(n + 1/2)\pi$ is excluded) or $k_r(R + \frac{1}{\gamma}) = n\pi$, or for the square

$$k_r^2 = \frac{(n\pi)^2}{(R + \frac{1}{\gamma})^2} \approx \frac{(n\pi)^2}{R^2} \left(1 - \frac{2}{R\gamma}\right) \quad (98)$$

and the energy of bound states are $E_r = \frac{\hbar^2 k_r^2}{2m}$ as usual. Comparing to the bound state for infinite spherical well, $E = \hbar^2 k^2/(2m) = \hbar^2 n^2 \pi^2/(2mR^2)$, we have

$$E_r = \left(1 - \frac{2}{R\gamma}\right) E_b \tag{99}$$

so there is an n-independent overall factor. We see that for $\gamma \to \infty$, the energies $E_r \to E_b$.

Recall the formula for the width

$$\Gamma = -2 \left(\frac{d(\cot \delta_0)}{dE}\Big|_{E=E_r} \right)^{-1} \tag{100}$$

For this to make sense we see that $\frac{d(\cot \delta_0)}{dE} < 0$. This is explained in the "Editor's note" as "no unphysical advance", and this prohibits $(n + 1/2)\pi$ above. So

$$\begin{aligned}
\frac{1}{\Gamma} &= -\frac{1}{2}\frac{dk}{dE} \cdot \frac{d}{dk}\left(-\frac{k}{\gamma \sin^2 kR} - \cot kR \right) \quad \text{at } k = k_r & (101)\\
&= \frac{1}{2 \cdot 2\hbar^2 k/(2m)} \cdot \left(\frac{1}{\gamma \sin^2 kR} - \frac{2kR \cos kR}{\gamma \sin^3 kR} - \frac{1}{\sin^2 kR} \right) \quad \text{at } k = k_r & (102)\\
&= \frac{m}{2\hbar^2 k_r} \cdot \frac{1}{\sin^2 kR} \left(\frac{1}{\gamma} - 2kR \cot kR + 1 \right) \quad \text{at } k = k_r & (103)\\
&= \frac{m}{2\hbar^2 k_r} \cdot \frac{1}{\sin^2 k_r R} \left(\frac{1}{\gamma} - 2k_r R(-\frac{k_r}{\gamma \sin^2 k_r R}) + 1 \right) & (104)\\
&= \frac{m}{2\hbar^2 (n\pi/R)} \cdot \frac{1}{(n\pi/(\gamma R))^2} = \frac{mR^3\gamma^2}{2\hbar^2 (n\pi)^3} & (105)
\end{aligned}$$

using the resonance condition and $\sin^2(k_r R) \approx (n\pi/(\gamma R))^2$. We see that the widths $\Gamma \to 0$ as $\gamma \to \infty$, the resonances become very narrow.

A Scattering in one dimension: Maple worksheet

This Maple worksheet (which I can give you if you are interested) discusses a few elementary aspects of scattering and transmission in one dimensions that are not immediately evident when staring at expressions.

Elementary quantum scattering

Barrier transmission

restart

$$T := \frac{1}{1 + \frac{V0^2 \sinh(k1a)^2}{4\,E\,(V0 - E)}}$$

$$T := \frac{1}{1 + \frac{1}{4}\,\frac{V0^2 \sinh(k1a)^2}{E\,(V0 - E)}} \tag{1}$$

$$k1a := c\sqrt{1 - \alpha}$$

$$k1a := c\sqrt{1 - \alpha} \tag{2}$$

where E/V0 = alpha, and c = sqrt(2m V0) a /hbar, which is set to 7 in the Wikipedia plot.

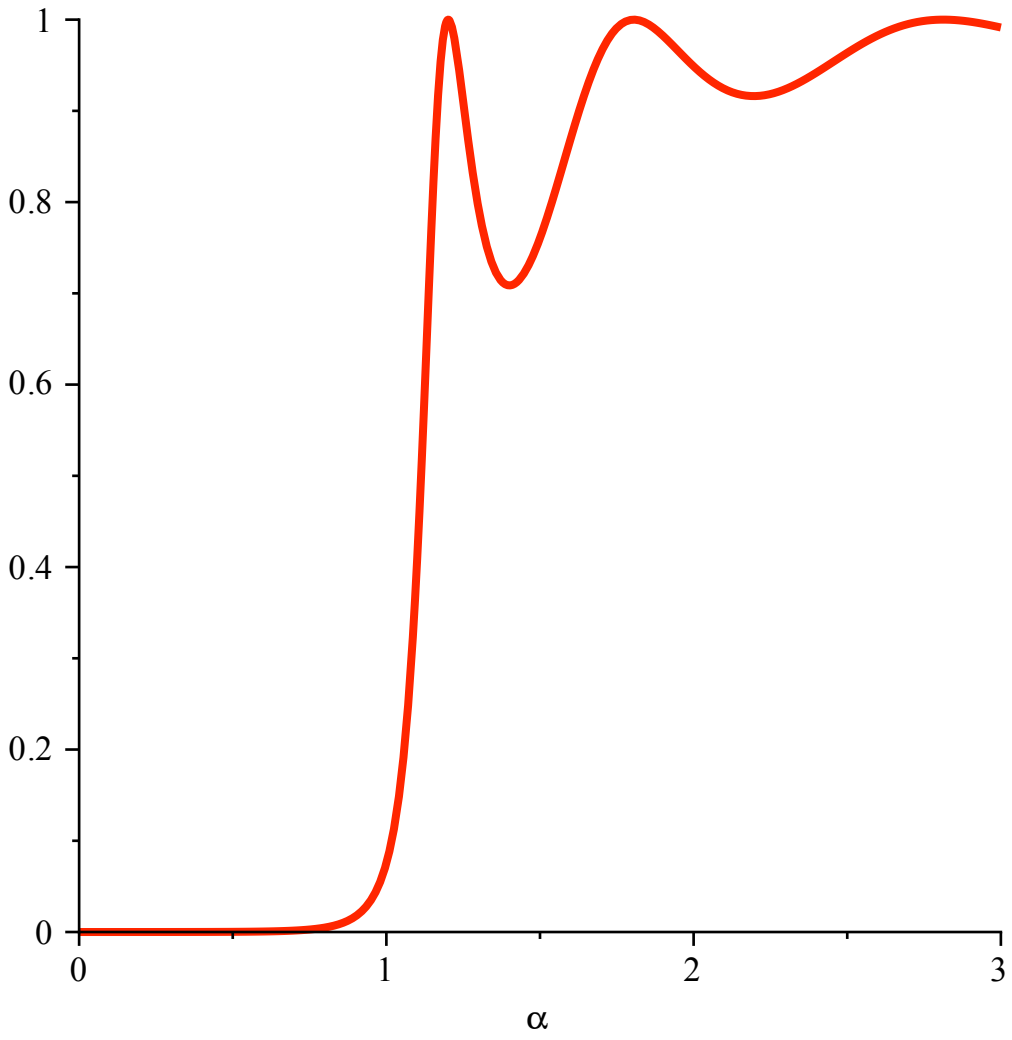
$$cabs := \frac{\sqrt{2\,m\,V0}\,a}{hbar}$$

$$cabs := \frac{\sqrt{2}\,\sqrt{m\,V0}\,a}{hbar} \tag{3}$$

$$Tsimp := simplify(subs(E = V0\,\alpha, T), size)$$

$$Tsimp := -\frac{4\,\alpha\,(-1 + \alpha)}{4\,\alpha - 4\,\alpha^2 + \sinh\left(c\sqrt{1 - \alpha}\right)^2} \tag{4}$$

$$plot(subs(c = 7, Tsimp), \alpha = 0..3, thickness = 3)$$

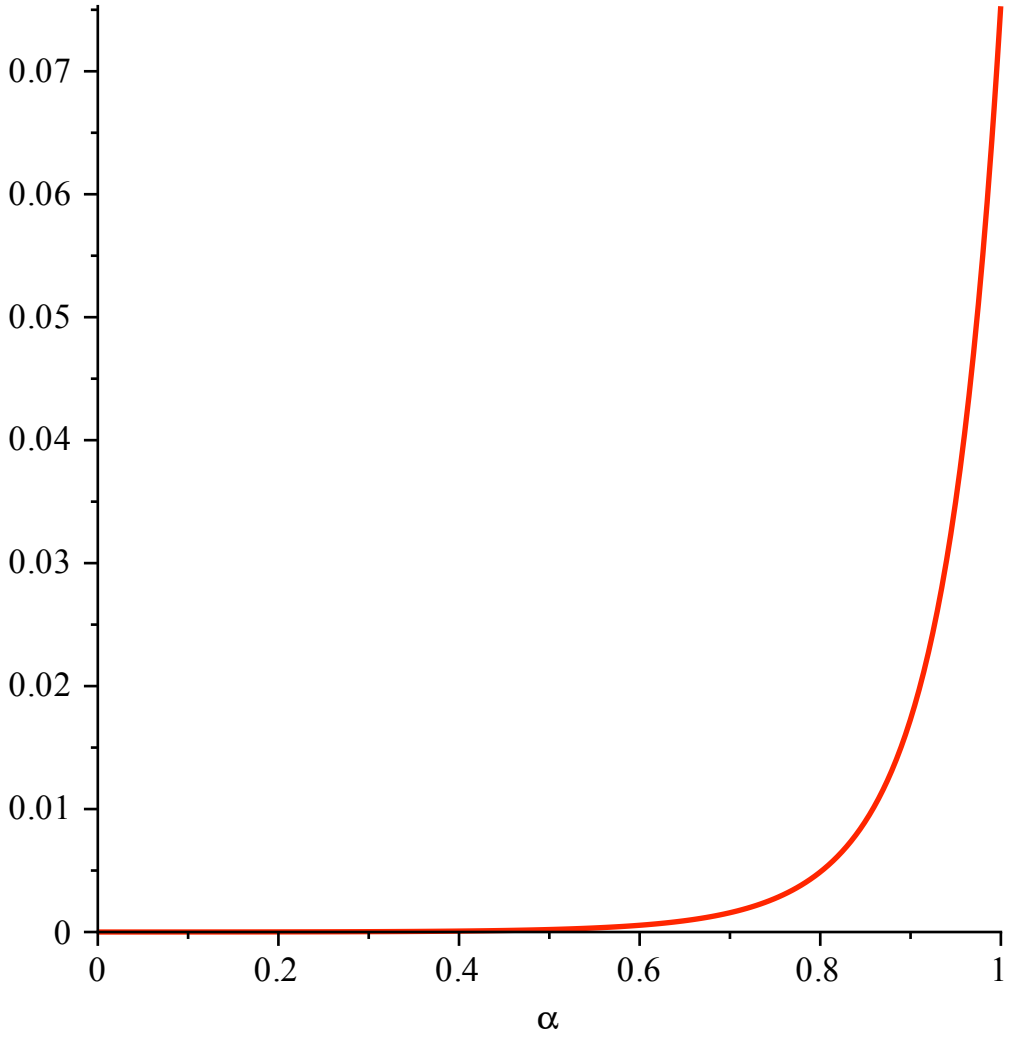


Same as on Wikipedia.

Barrier becomes transparent at some special points (the energies of the infinite square *well*)

If we focus on E $<$ V0, we have

$plot(subs(c = 7, Tsimp), \alpha = 0..1, thickness = 2)$



Well transmission

restart

$$T := \frac{1}{1 + \frac{V0^2 \sin(k1a)^2}{4\,E\,(E - V0)}}$$

$$T := \frac{1}{1 + \frac{1}{4}\,\frac{V0^2 \sin(k1a)^2}{E\,(E - V0)}} \quad \textbf{(5)}$$

Switch k_1 by hand:

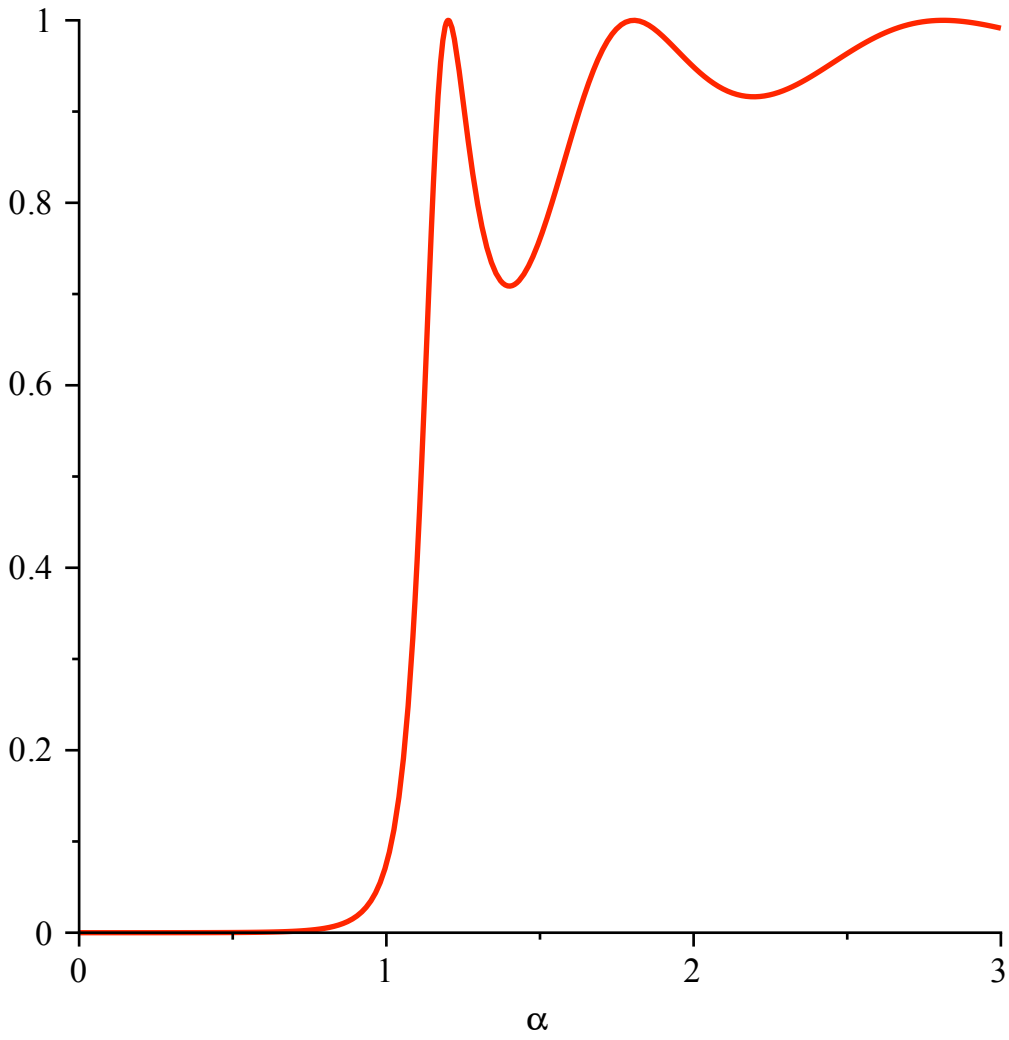
$$k1a := c\sqrt{\alpha - 1}$$

$$k1a := c\sqrt{\alpha - 1} \quad \textbf{(6)}$$

$$Tsimp := simplify(subs(E = V0\,\alpha, T), size)$$

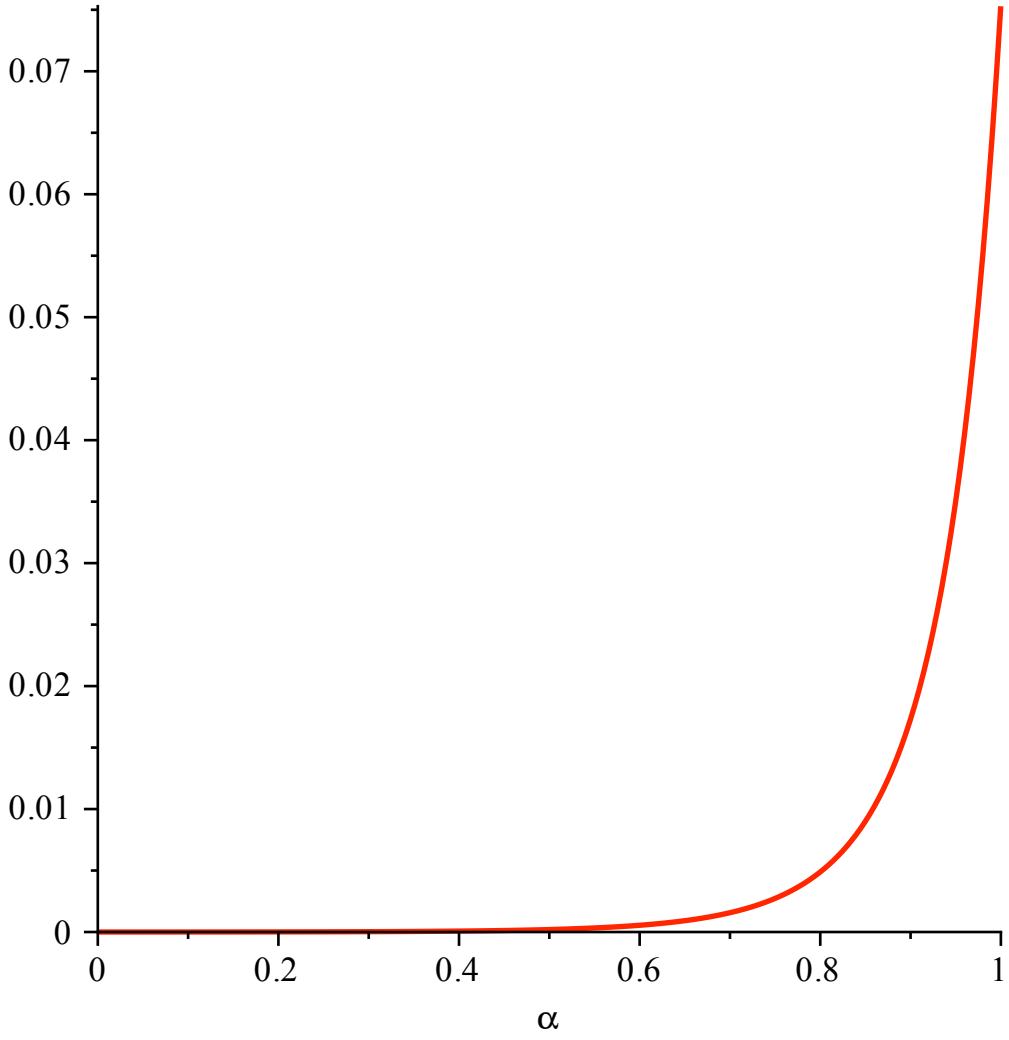
$$Tsimp := \frac{4\,\alpha\,(\alpha - 1)}{4\,\alpha^2 - 4\,\alpha + \sin\left(c\sqrt{\alpha - 1}\right)^2} \quad \textbf{(7)}$$

$plot(subs(c = 7, Tsimp), \alpha = 0..3, thickness = 2)$



Now we focus on E>V0 but |E|<V0, so we get the same looking curve.

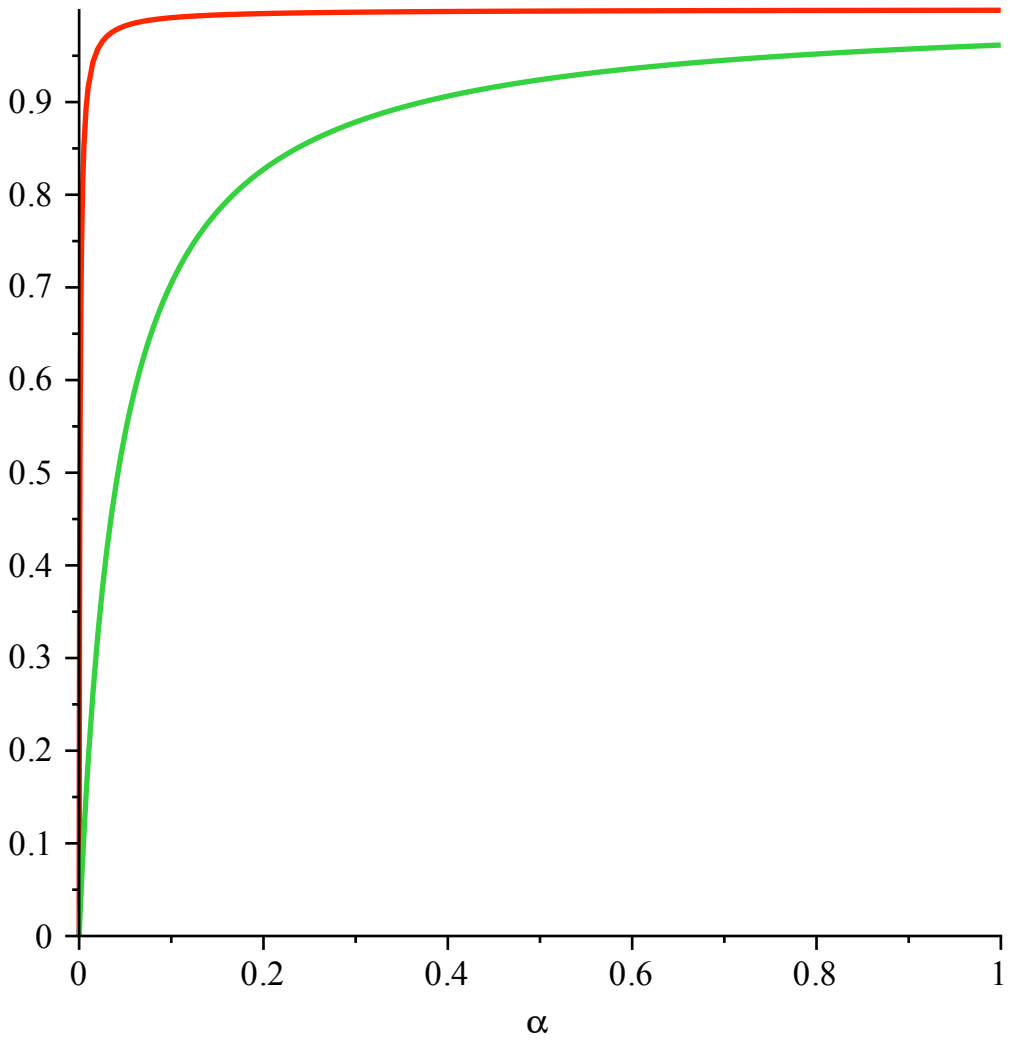
$plot(subs(c = 7, Tsimp), \alpha = 0..1, thickness = 2)$



delta function limit

V0 -> oo, a -> 0 while V0 a = constant.
This means c is small but not negligible

$plot([seq(Tsimp, c = [0.06, 0.4])], \alpha = 0..1, thickness = 2)$



The δ function potential gives

$$Tdelta := \frac{1}{1 + \frac{m\,\lambda^2}{2\,hbar^2\,E}}$$

$$Tdelta := \frac{1}{1 + \frac{1}{2}\,\frac{m\,\lambda^2}{hbar^2\,E}} \tag{8}$$

$series(Tdelta, \lambda, 5)$

$$1 - \frac{1}{2}\,\frac{m}{hbar^2\,E}\,\lambda^2 + \frac{1}{4}\,\frac{m^2}{hbar^4\,E^2}\,\lambda^4 + O(\lambda^6) \tag{9}$$

If we want to compare:

$series(T, c, 3)$

$$1 - \frac{1}{4}\,\frac{V0^2\,(\alpha - 1)}{E\,(E - V0)}\,c^2 + O(c^4) \tag{10}$$

$quad\_term := coeff(series(T, c, 3), c, 2)\,c^2$

$$quad\_term := -\frac{1}{4}\,\frac{V0^2\,(\alpha-1)\,c^2}{E\,(E-V0)} \tag{11}$$

If we set V0 a = λ, we get agreement

$$simplify\left(subs\left(c = cabs,\ \alpha = \frac{E}{V0},\ V0 = \frac{\lambda}{a},\ quad\_term\right)\right)$$

$$-\frac{1}{4}\,\frac{cabs^2\,\lambda}{a\,E} \tag{12}$$

What about the quartic term?

$$quar\_term := coeff\,(series\,(T, c, 5), c, 4)\,c^4$$

$$quar\_term := \left(\frac{1}{12}\,\frac{V0^2\,(\alpha-1)^2}{E\,(E-V0)} + \frac{1}{16}\,\frac{V0^4\,(\alpha-1)^2}{E^2\,(E-V0)^2}\right)c^4 \tag{13}$$

We get agreement from the leading term, this is an expansion for small a, so E*a is negligible

$$expand\left(simplify\left(subs\left(c = cabs,\ \alpha = \frac{E}{V0},\ V0 = \frac{\lambda}{a},\ quar\_term\right)\right)\right)$$

$$\frac{1}{12}\,cabs^4 - \frac{1}{12}\,\frac{cabs^4\,\lambda}{a\,E} + \frac{1}{16}\,\frac{cabs^4\,\lambda^2}{a^2\,E^2} \tag{14}$$

B Two-state time evolution: Maple worksheet

It is easy to sketch two-state time evolution near resonance, but this also includes away from resonance.

Time evolution of two − state system

This is a Maple worksheet that just plots the Rabi expression we discussed in class (and that you derive in Problem 5.30).

```
> restart
```

This is the Rabi formula for the probability |c_2(t)|^2:

```
> c2sq := γ^2 sin(Ω t)^2 / (hbar^2 Ω^2) :
```

where

```
> Ω := ((γ/hbar)^2 + (ω − ω21)^2/4)^(1/2) :
```

If we measure frequences in SI units, omega is a big number which can be inconvenient for numerical analysis. We could use adapted units where e.g. omega is measured in units of 1/hbar, but as we will see, the huge numbers we get are not *too* huge, so let's just use SI.

Let's say gamma is an electron volt, and omega is an electronvolt/hbar.
This is not particularly realistic in any actual system, but I'm just trying to give an illustration.

```
> with(ScientificConstants) : hbar := evalf(Constant(hbar))
```

$$hbar := 1.054571596\ 10^{-34} \tag{1}$$

```
> vals := γ = 1.6 10^-19, ω21 = 1.6 10^-19 / hbar
```

$$vals := \gamma = 1.600000000\ 10^{-19},\ \omega 21 = 1.517203769\ 10^{15} \tag{2}$$

For comparison, the ammonia maser is 24 GHz:

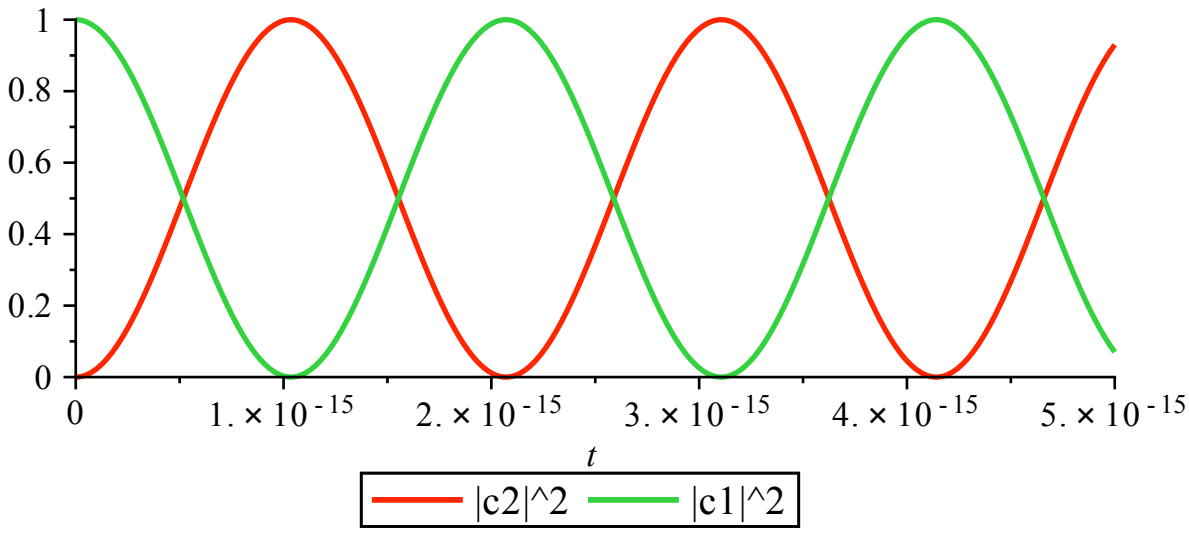
```
> 2.4 10^10 · 2 evalf(π)
```

$$1.507964474\ 10^{11} \tag{3}$$

So the above omega21 is 10 000 times bigger than the 24 GHz of the ammonia maser.

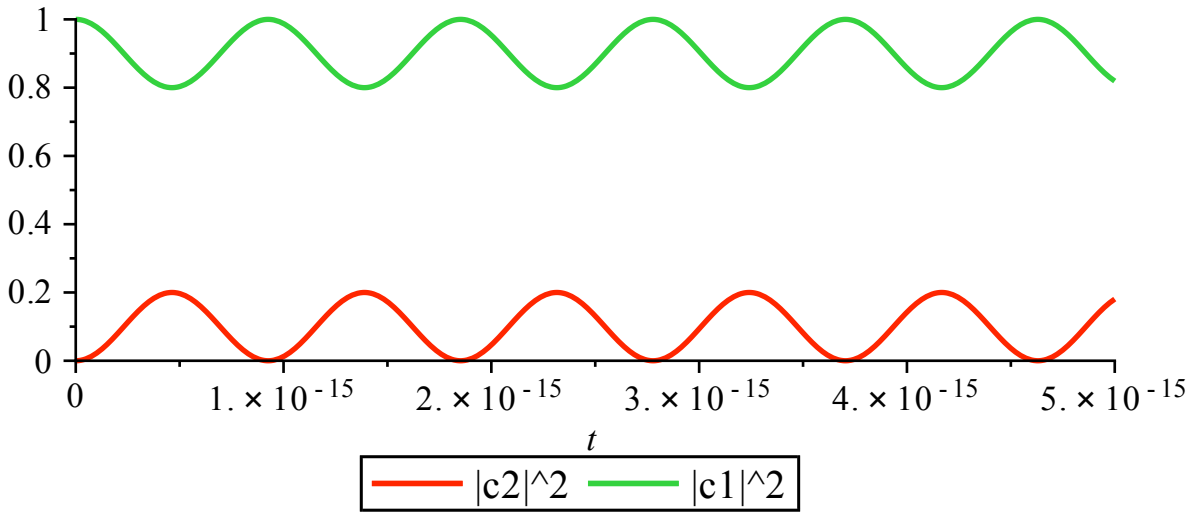
Anyway. First let's plot is as a function of time at resonance:

```
> c2sq_val := simplify(evalf(subs(ω = ω21, vals, c2sq))) :
> plot([c2sq_val, 1 − c2sq_val], t = 0..5. 10^-15, legend = ["|c2|^2", "|c1|^2"], thickness = 2)
```



And off resonance:

```
> c2sq_val := simplify(evalf(subs(ω = 5·ω21, vals, c2sq))) :
> plot([c2sq_val, 1 − c2sq_val], t = 0..5. 10^−15, legend = ["|c2|^2", "|c1|^2"], thickness = 2)
```



The period is:

```
> t1abs := π/(2 Ω) :
> t1 := subs(vals, t1abs) :
> evalf(subs(ω = ω21, vals, t1))
```

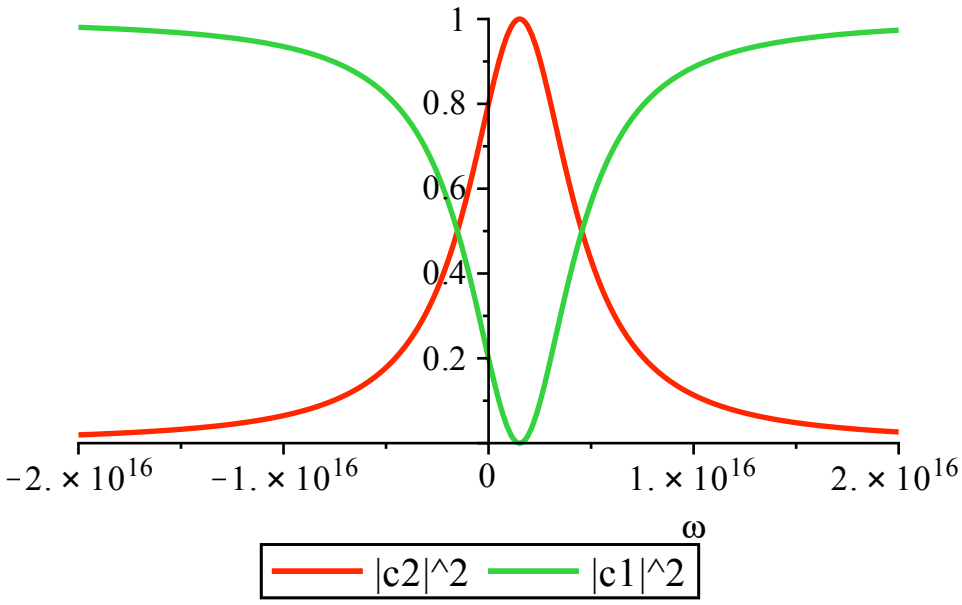
$$1.035323243\ 10^{-15} \tag{4}$$

```
> Then let's plot |c_2(t)|^2 as a function of omega at time t1
> c2sq_val_o := simplify(evalf(subs(t = t1, vals, c2sq)), sin)
```

$$c2sq\_val\_o := \frac{2.301907276\ 10^{30}}{2.301907276\ 10^{30} + 0.2500000000\ (\omega - 1.517203769\ 10^{15})^2} \tag{5}$$

```
> plot([c2sq_val_o, 1 − c2sq_val_o], ω = −2. 10^16..2. 10^16, legend = ["|c2|^2", "|c1|^2"], thickness
```

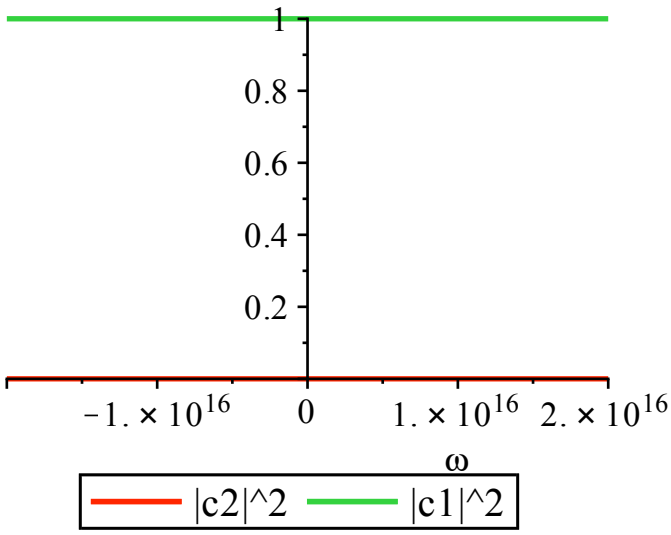
$= 2)$



> *c2sq_val_o* := *simplify*(*evalf*(*subs*(*t* = 2 *t1*, *vals*, *c2sq*)), sin) :

> There is a danger of underflow here, since sin(pi)=0,but the plot is good enough:

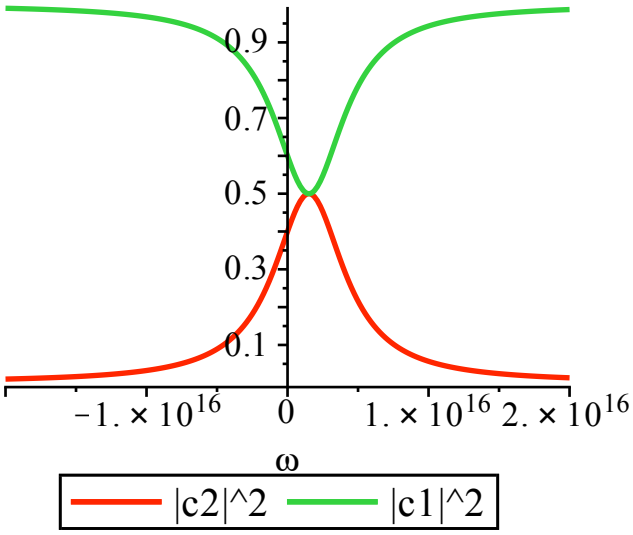
> *plot*([*c2sq_val_o*, 1 − *c2sq_val_o*], ω = −2. 10^{16} ..2. 10^{16}, *legend* = ["|c2|^2", "|c1|^2"], *thickness* $= 2)$



This just says that at t = 2 t1, c2 is always equal to 0.
What about in `between?

> *c2sq_val_o* := *simplify*(*evalf*(*subs*(*t* = 1.5 *t1*, *vals*, *c2sq*)), sin) :

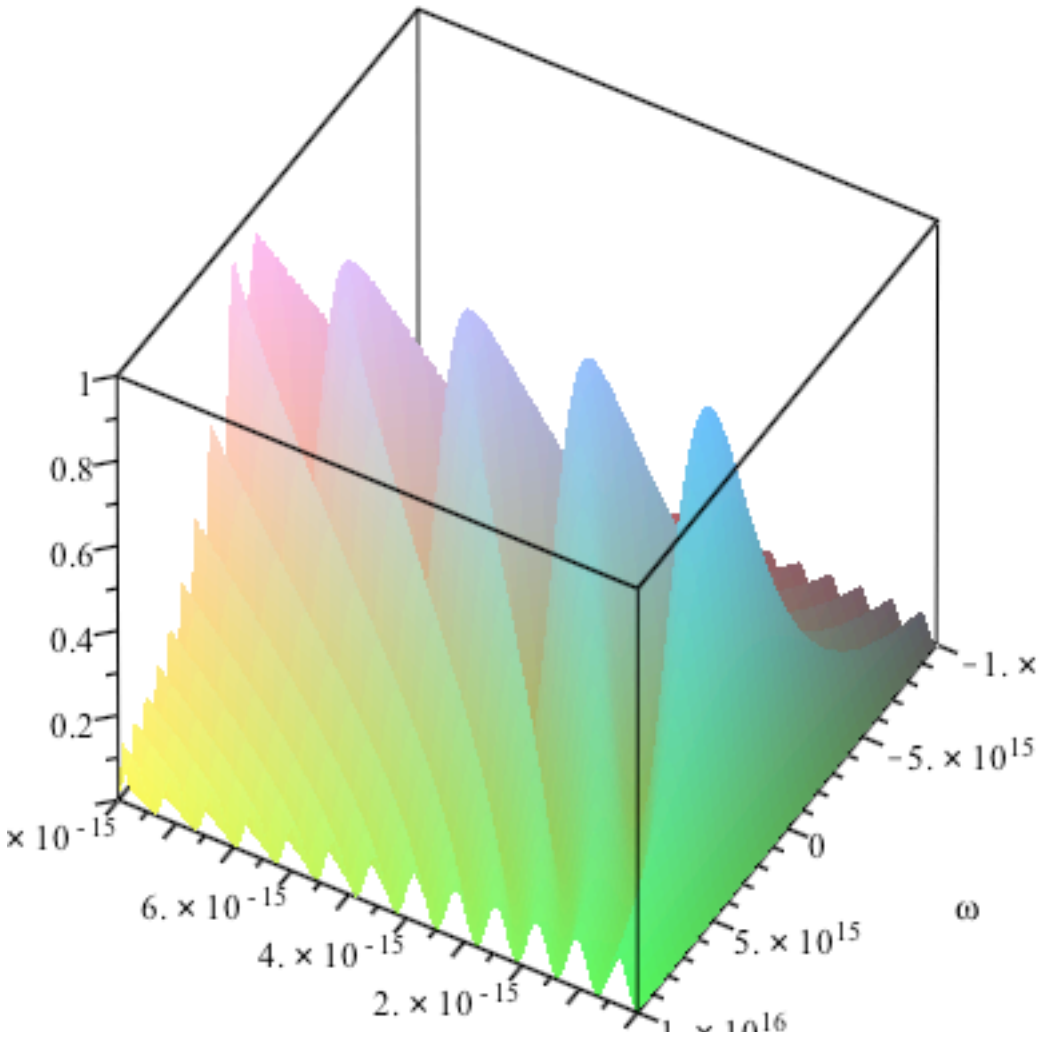
> *plot*([*c2sq_val_o*, 1 − *c2sq_val_o*], ω = −2. 10^{16} ..2. 10^{16}, *legend* = ["|c2|^2", "|c1|^2"], *thickness* $= 2)$



> Now do the 3d plot as a function of both time and frequency:

> $c2sq\_val\_both := simplify(evalf(subs(vals, c2sq)))$:

> $plot3d(c2sq\_val\_both, t = 0..9.\ 10^{-15}, \omega = -1.\ 10^{16}..1.\ 10^{16}, numpoints = 200^2, axes = boxed, style = surface, orientation = [120, 45, 0])$



We see that a given slice at different times can produce quite different plots.

C "Zero-energy" scattering: Maple worksheet

Some of the arguments and plots in the zero energy scattering section seem somewhat mysterious but it is actually quite simple, which this worksheet tries to illustrate. I use a smooth (not just piecewise constant) potential, which turns out to be somewhat important.

Very low energy ("zero-energy") s-wave scattering

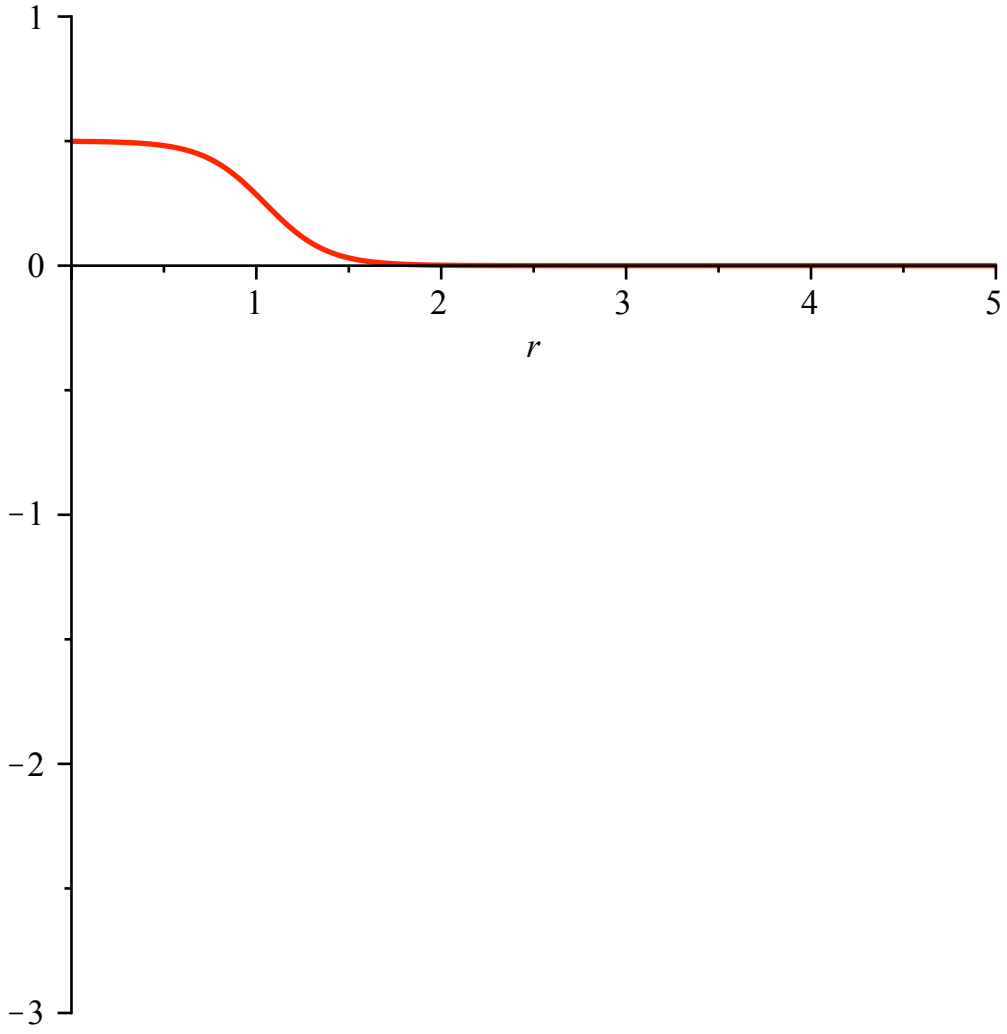
```
> restart
> with(plots) : with(plottools) :
```

Consider the radial Schrödinger equation with angular momentum = 0 (s-wave).
If the original radial wavefunction is A(r), write u(r) = r A(r) as usual for a spherical wave.
I absorb constants into redefinitions of E and V.

```
> SE := diff(u(r), r$2) + (E - V) u(r) :
```

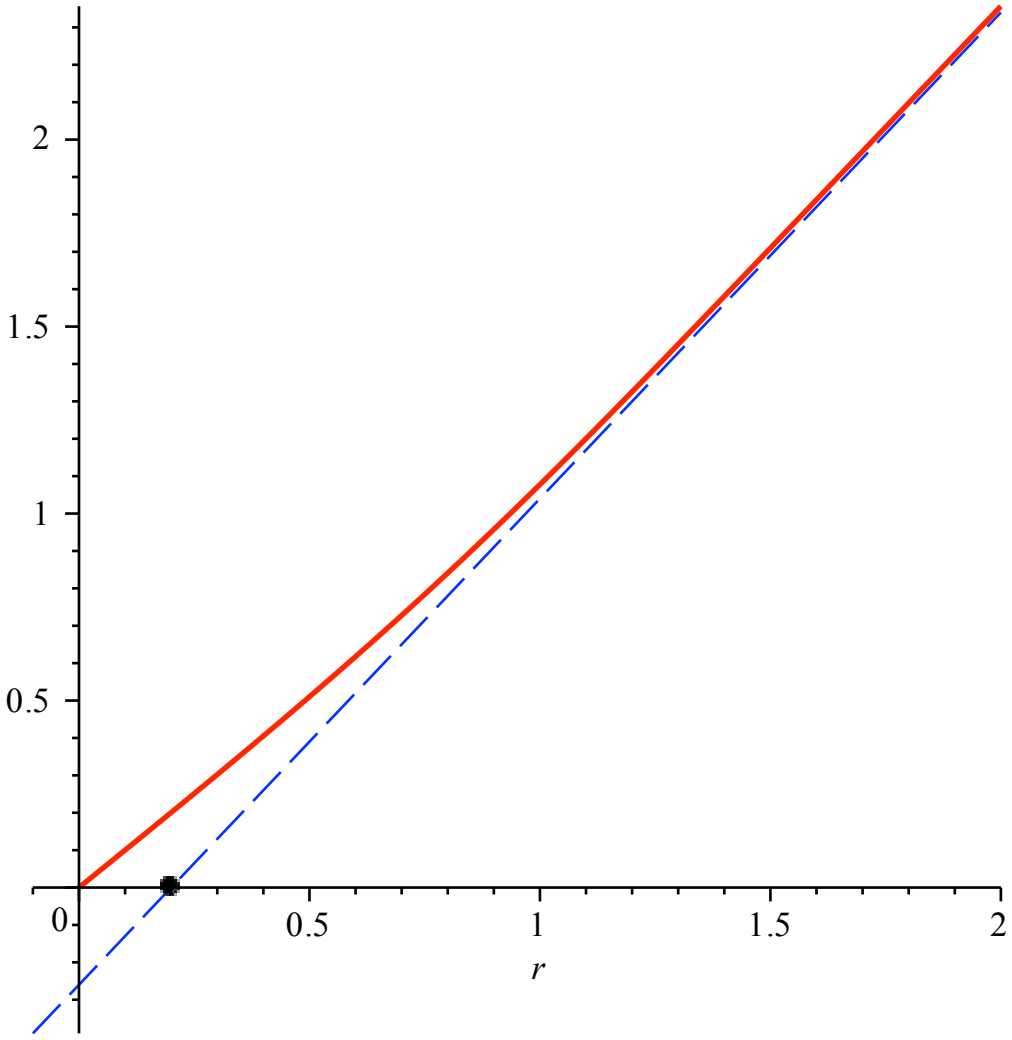
Here's a simple model for a smooth (as opposed to step function) repulsive potential, with R ~ 1.

```
> Vrep := -0.25 (tanh(3 r - π) - 1) :
> plot(Vrep, r = 0..6, view = [0..5, -3..1], thickness = 2)
```



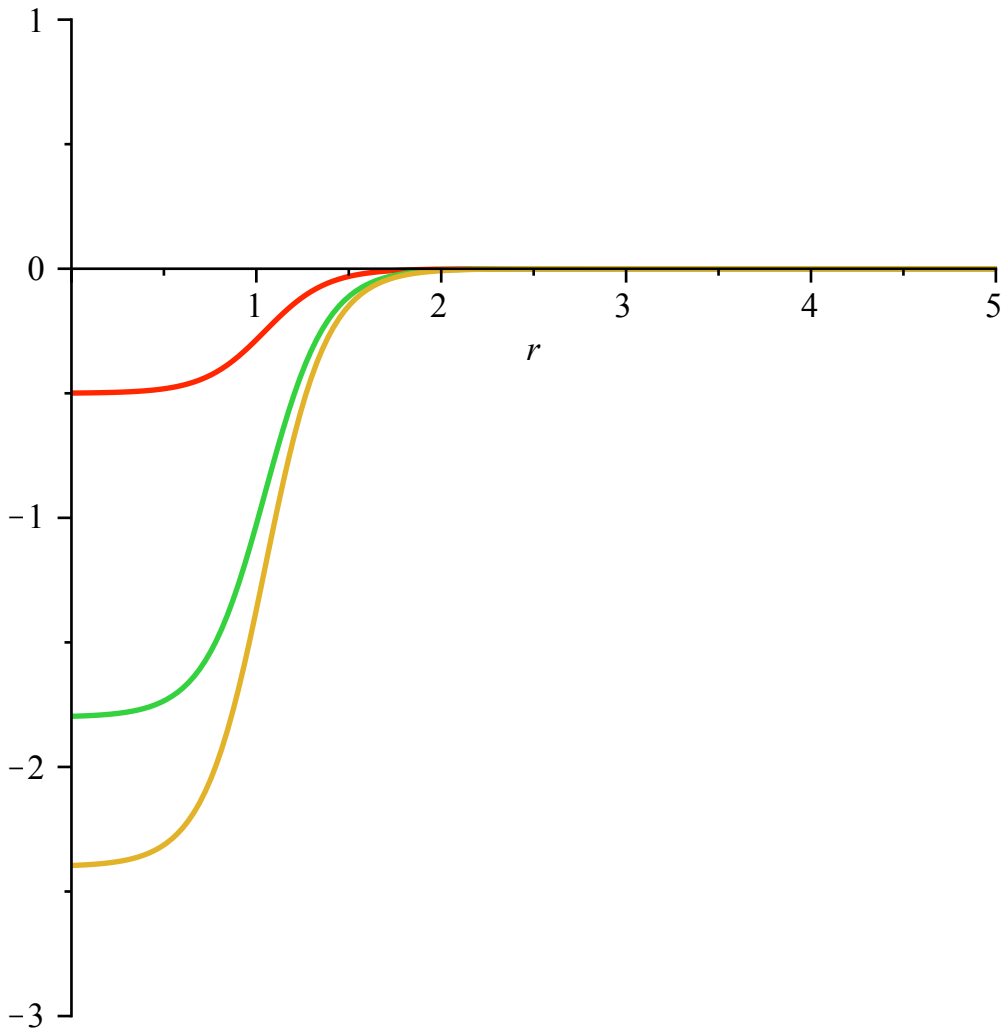
The wavefunction for this repulsive potential (finite smooth barrier) is

```
> V := Vrep :
> sol := dsolve([subs(E = 0.01, SE), u(0) = 0, D(u)(0) = 1], u(r), numeric) :
> display(plot(1.3 (r - 0.20), r = -0.1..2, color = blue, linestyle = dash), point([0.2, 0], symbol
      = solidcircle, symbolsize = 15), odeplot(sol, [r, u(r)], 0..2, thickness = 2))
```



where we read off the scattering length a from the intercept (marked with a black dot).
Note that the linear function is *not* a particularly good approximation to the inside (R<1) solution, we are just extending
it to there to estimate the scattering length *a*, following the discussion in Sakurai.
Now we move on to an attractive potential, still R ~ 1. We consider three potentials of of increasing depth, V1, V2 and V3:

```
> V1 := 0.25 (tanh(3 r − π) − 1) : V2 := 0.9 (tanh(3 r − π) − 1) :
  V3 := 1.2 (tanh(3 r − π) − 1) :
> plot([V1, V2, V3], r = 0 ..6, view = [0 ..5, −3 ..1], thickness = 2)
```

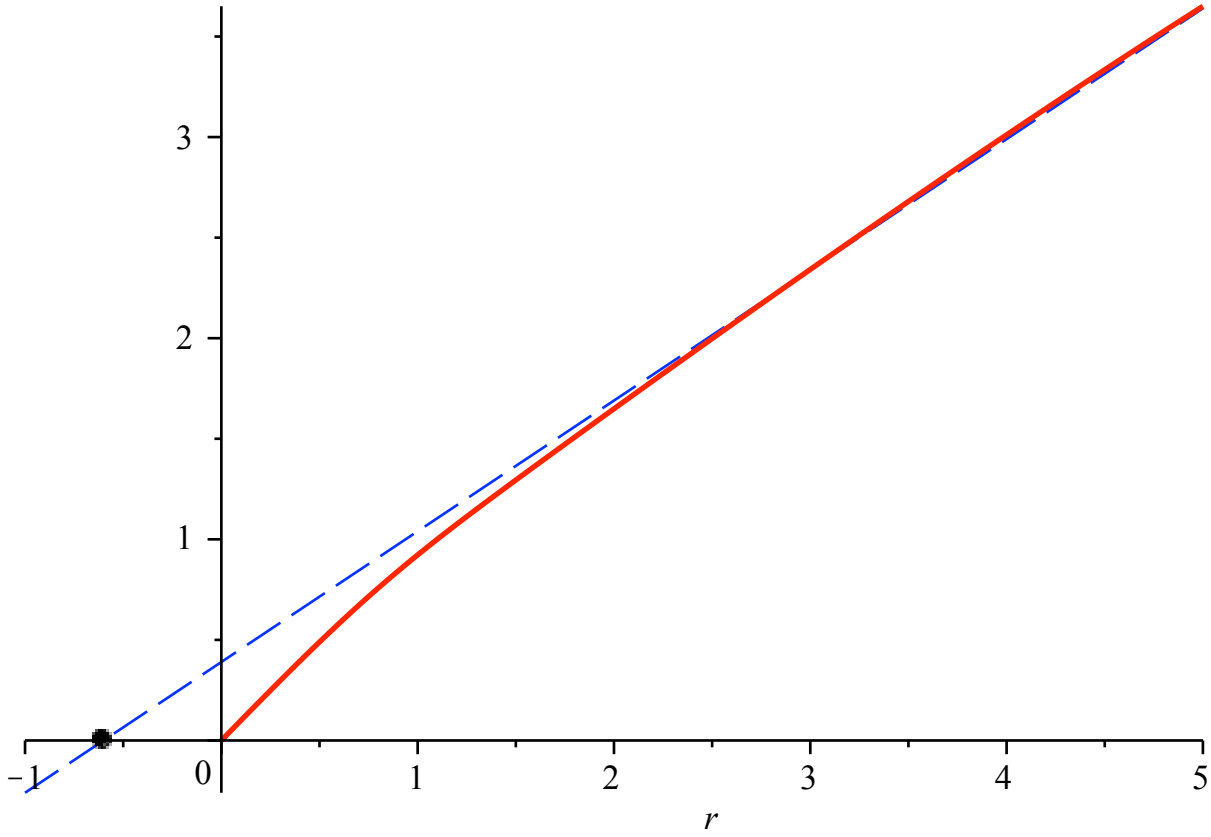


For the most shallow well we have:

```
> V := V1
```

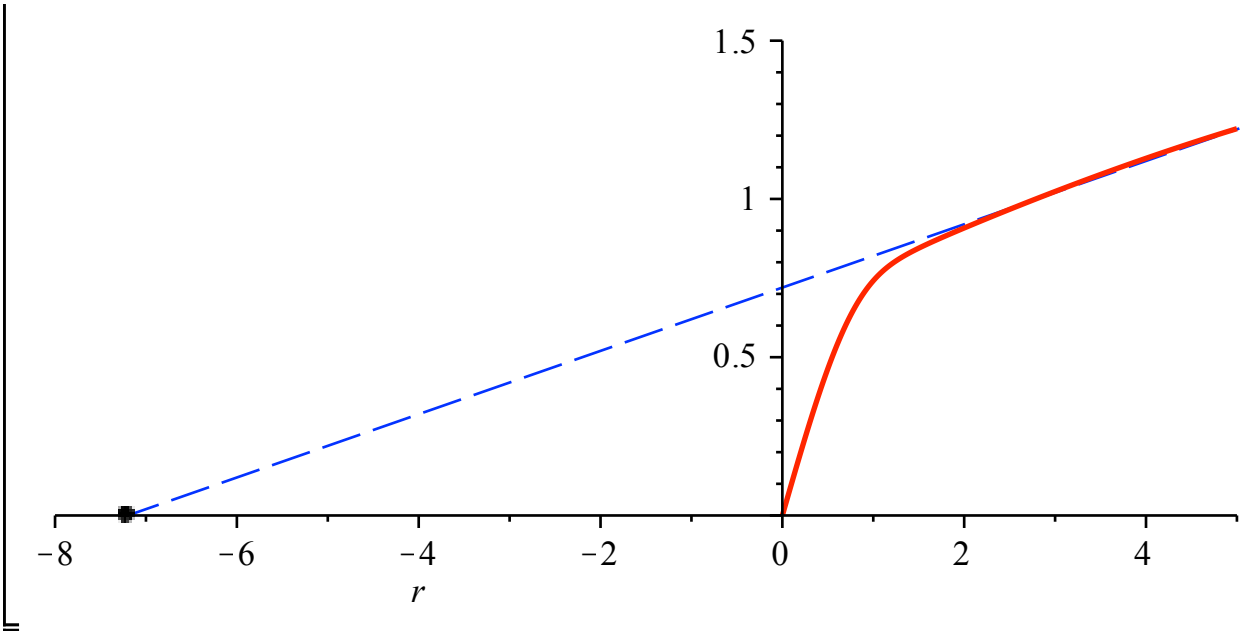
$$V := 0.25 \tanh(3\,r - \pi) - 0.25 \qquad \textbf{(1)}$$

```
> sol := dsolve([subs(E = 0.01, SE), u(0) = 0, D(u)(0) = 1], u(r), numeric) :
> display(plot(0.65 (r + 0.6), r = -1 ..5, color = blue, linestyle = dash), point([-0.6, 0], symbol
      = solidcircle, symbolsize = 15), odeplot(sol, [r, u(r)], 0 ..5, thickness = 2))
```



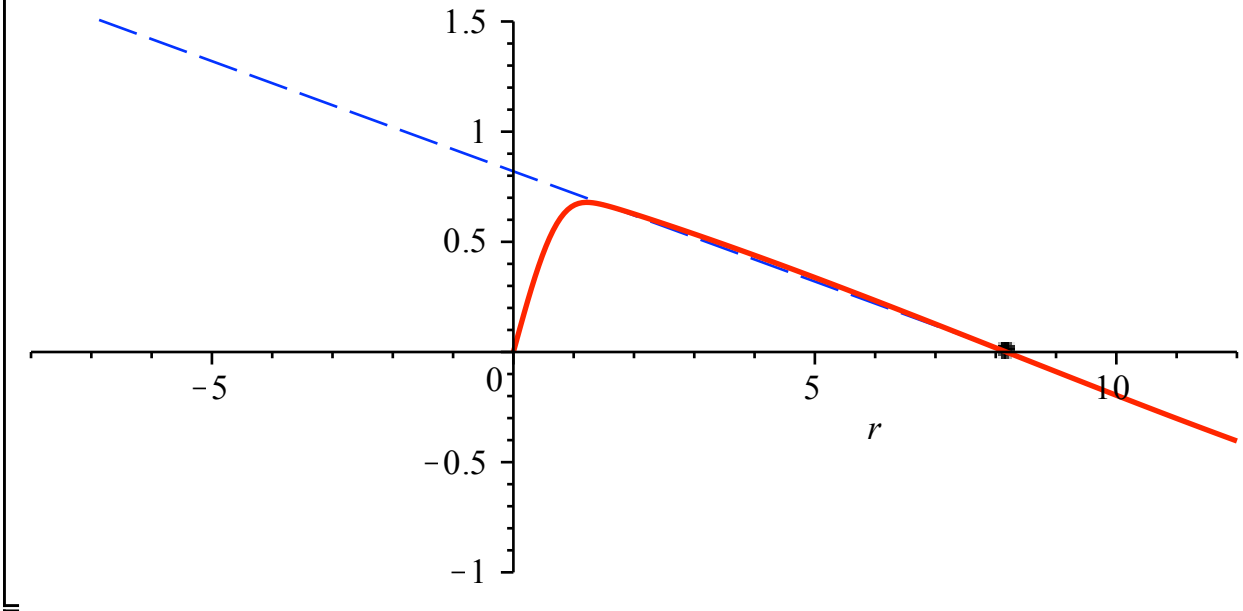
The precise value of the slope of the blue line will depend on how far out you go, and (as I check below) at some point the linear approximation outside will start to break down, so we already see this can only make
sense for a "truncated" domain.
Now increase the well depth:

```
> V := V2 :
> sol := dsolve( [subs(E = 0.01, SE), u(0) = 0, D(u)(0) = 1], u(r), numeric) :
> display(plot(0.1 (r + 7.2), r = −8 ..8, color = blue, linestyle = dash), point( [−7.2, 0], symbol
      = solidcircle, symbolsize = 15), odeplot(sol, [r, u(r)], 0 ..5, thickness = 2), view = [−8 ..5, 0
      ..1.5])
```



We see one of the key points, that *a* moves out to the left and can be much bigger in absolute value than R.
At some point *a* "crosses from negative to positive infinity", i.e. goes over to large values on the positive x-axis,
i.e. the blue dashed line "flips over" through horizontal, as we see in the deepest of our three wells:

```
> V := V3 :
> sol := dsolve( [subs(E = 0.01, SE), u(0) = 0, D(u)(0) = 1], u(r), numeric) : plotkeep := plot(
      -0.1 (r - 8.2), r = -8..8, color = blue, linestyle = dash), point( [8.2, 0], symbol
      = solidcircle, symbolsize = 15), odeplot(sol, [r, u(r)], 0..12, thickness = 2), view = [-8
      ..12, -1..1.5] :
> display(plotkeep)
```

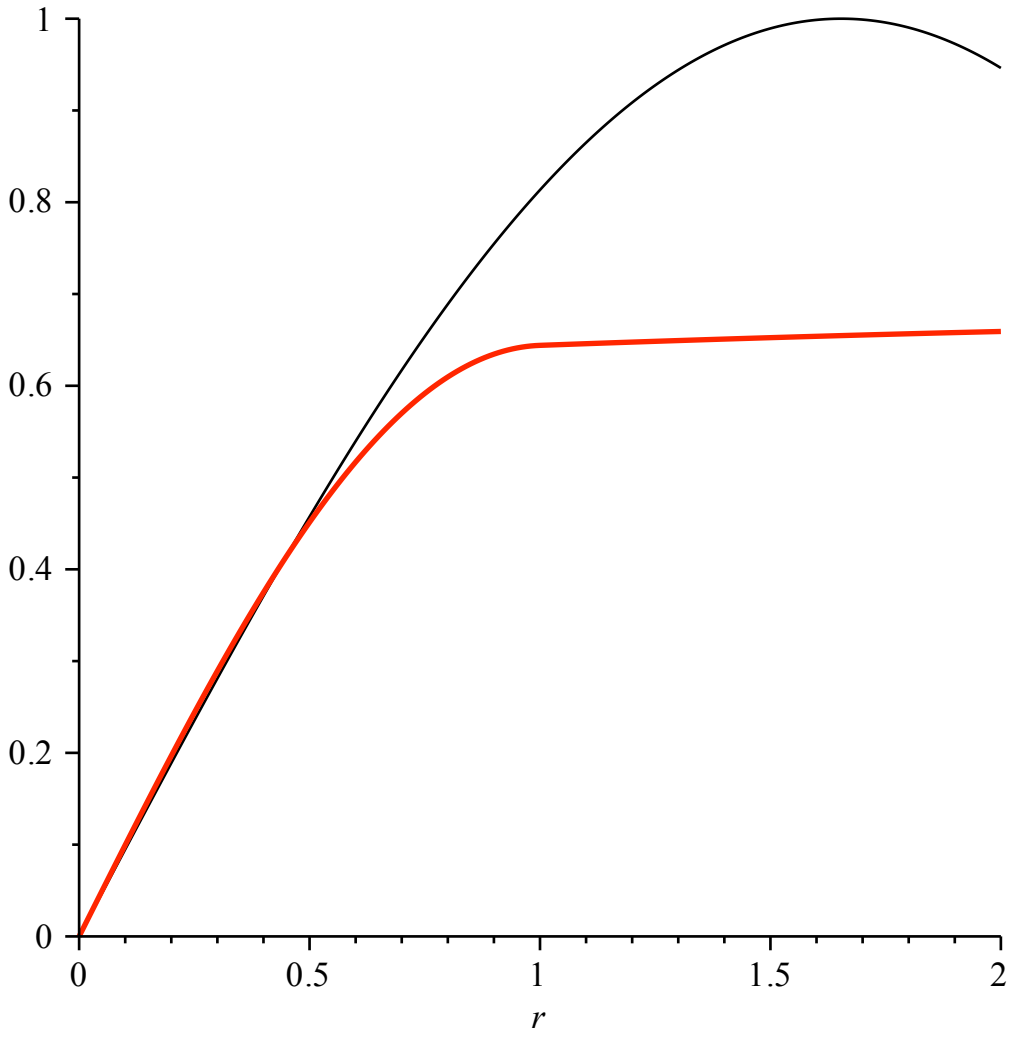


When we match inside/outside at R ~ 1, for the interior solution we would try to use a sine function as approximation, but because the potential is smooth, we expect it to be a bad approximation right around R = 1:

> $matchingsine := \sin(0.95\,r)$;

$$matchingsine := \sin(0.95\,r) \quad \textbf{(2)}$$

> $display(plot(\text{matchingsine}, r = 0..2, \text{color} = \text{black}), odeplot(sol, [r, u(r)], 0..2, thickness = 2))$



This leads us into a discussion of the outside solution
. Sakurai is saying is that there is a "bound state wavefunction"
exp(-kappa r) that is valid *outside* R and for *negative* E.
The confusing point is that *E is positive,* so what does this mean? But small positive E is "close to being negative",
in the sense that for small k^2, sine and constant and exponential
are all close to each other in some limited region in r.
If you accept this, we know the exponent kappa in the
bound state exponential from Sakurai's discussion, it's approximately kappa = 1/a (for R << a):

> $\kappa := \frac{1}{8.2}$

$$\kappa := 0.1219512195 \quad \textbf{(3)}$$

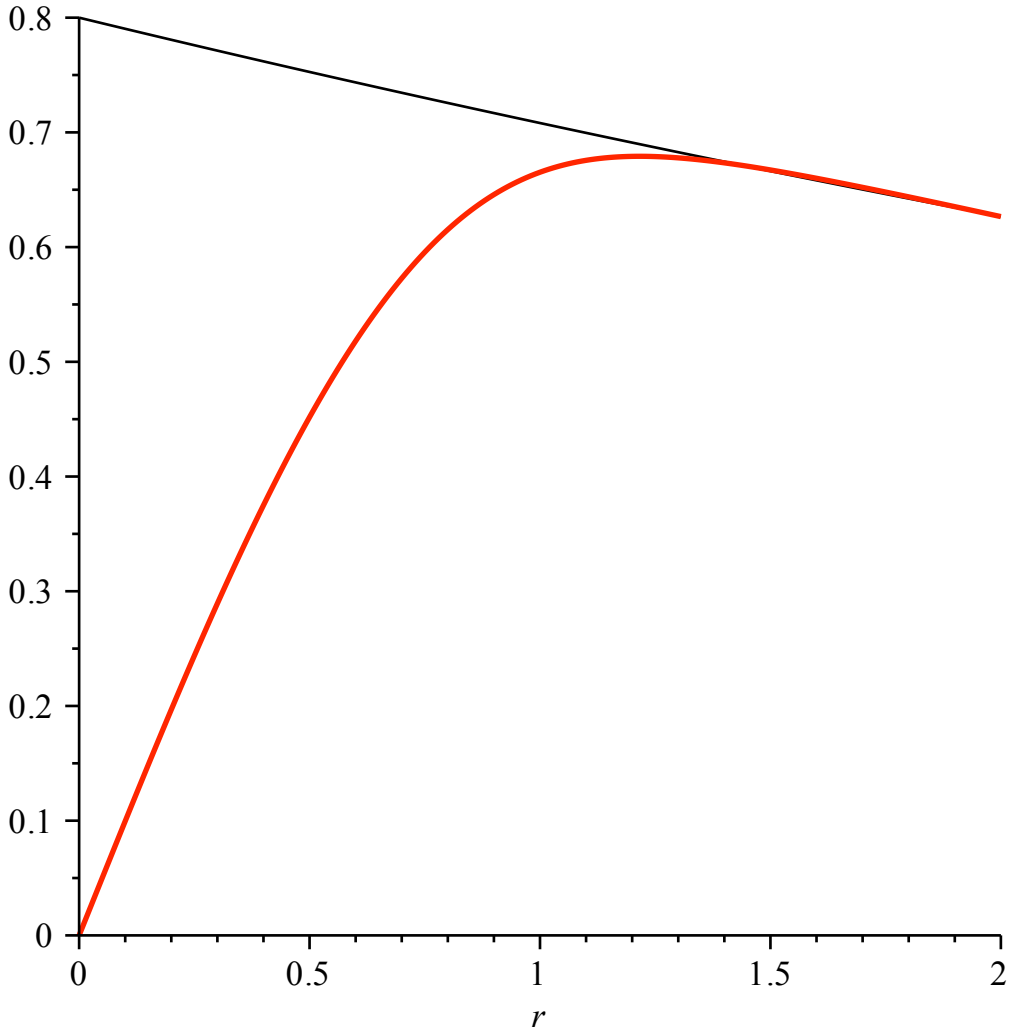
The normalization is not given by that discussion, we have to fix it ourselves:

> $boundstate := 0.8\,e^{-\kappa r}$

$$boundstate := 0.8\,e^{-0.1219512195\,r} \quad \textbf{(4)}$$

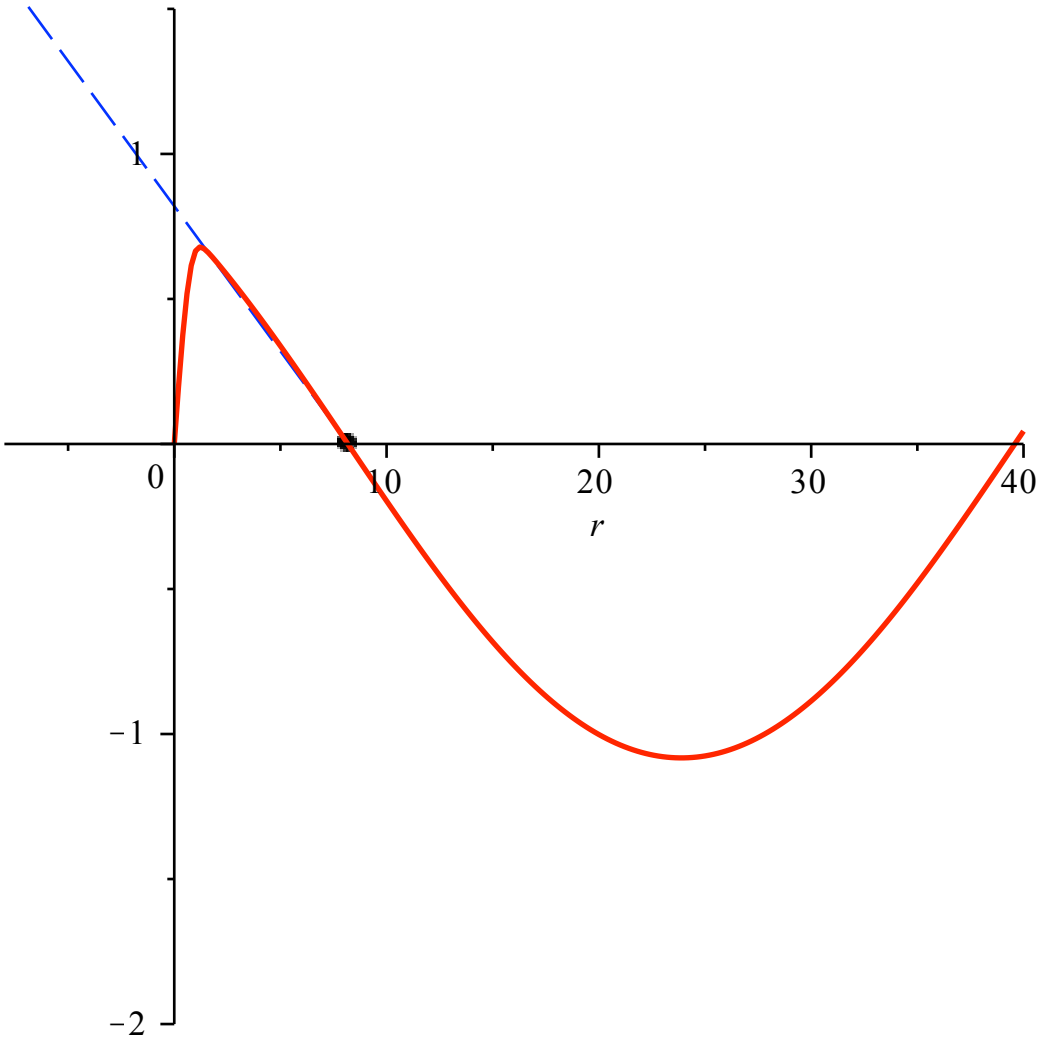
This gets it right outside :

```
> display(plot(boundstate, r = 0 ..2, color = black), odeplot(sol, [r, u(r)], 0 ..2, thickness = 2))
```



We can think of this as "loosely bound" since kappa (corresponding to the bound state energy) is fairly small.
Of course, all this is based on *cutting everything off* at some point and effectively *matching* to E=0, since otherwise the
linear approximation outside always fails at some large radius :

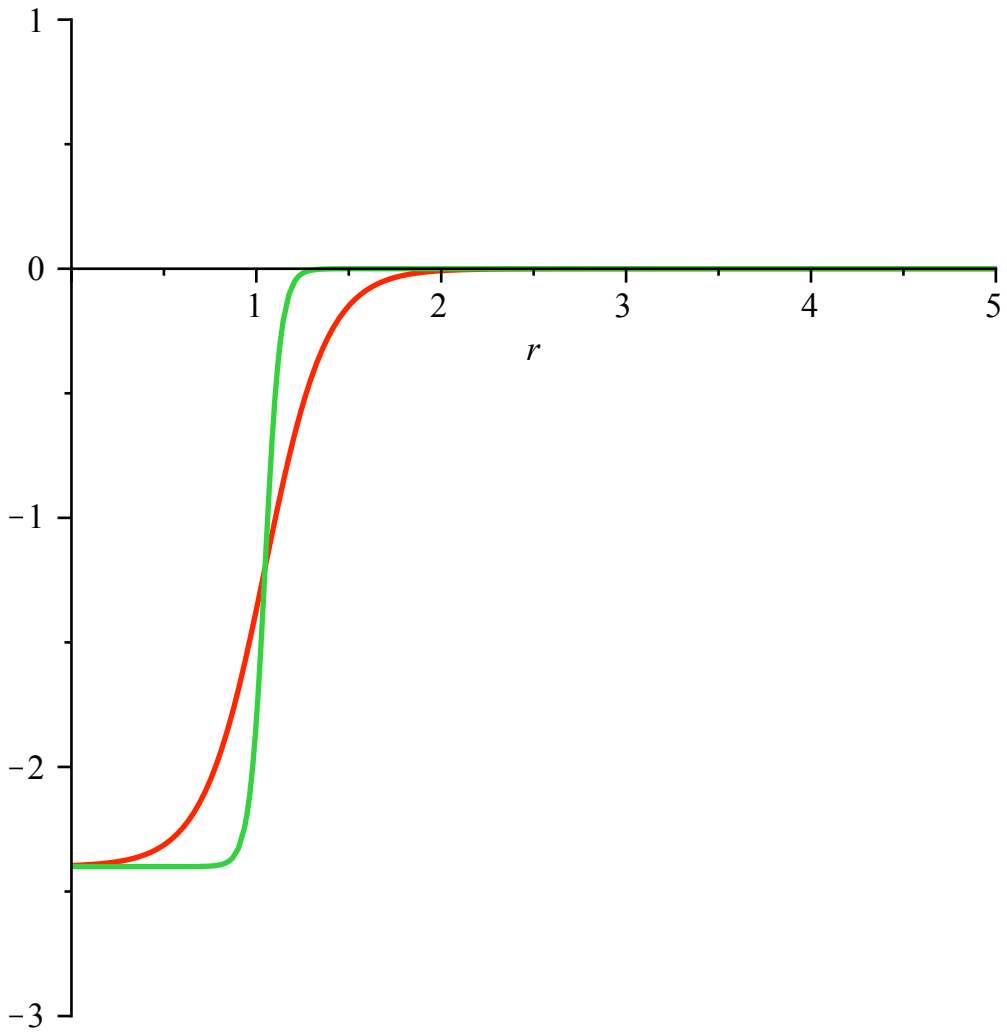
```
> display(plot(-0.1 (r - 8.2), r = -8 ..8, color = blue, linestyle = dash), point([8.2, 0], symbol
      = solidcircle, symbolsize = 15), odeplot(sol, [r, u(r)], 0 ..40, thickness = 2), view = [-8
      ..40, -2 ..1.5])
```



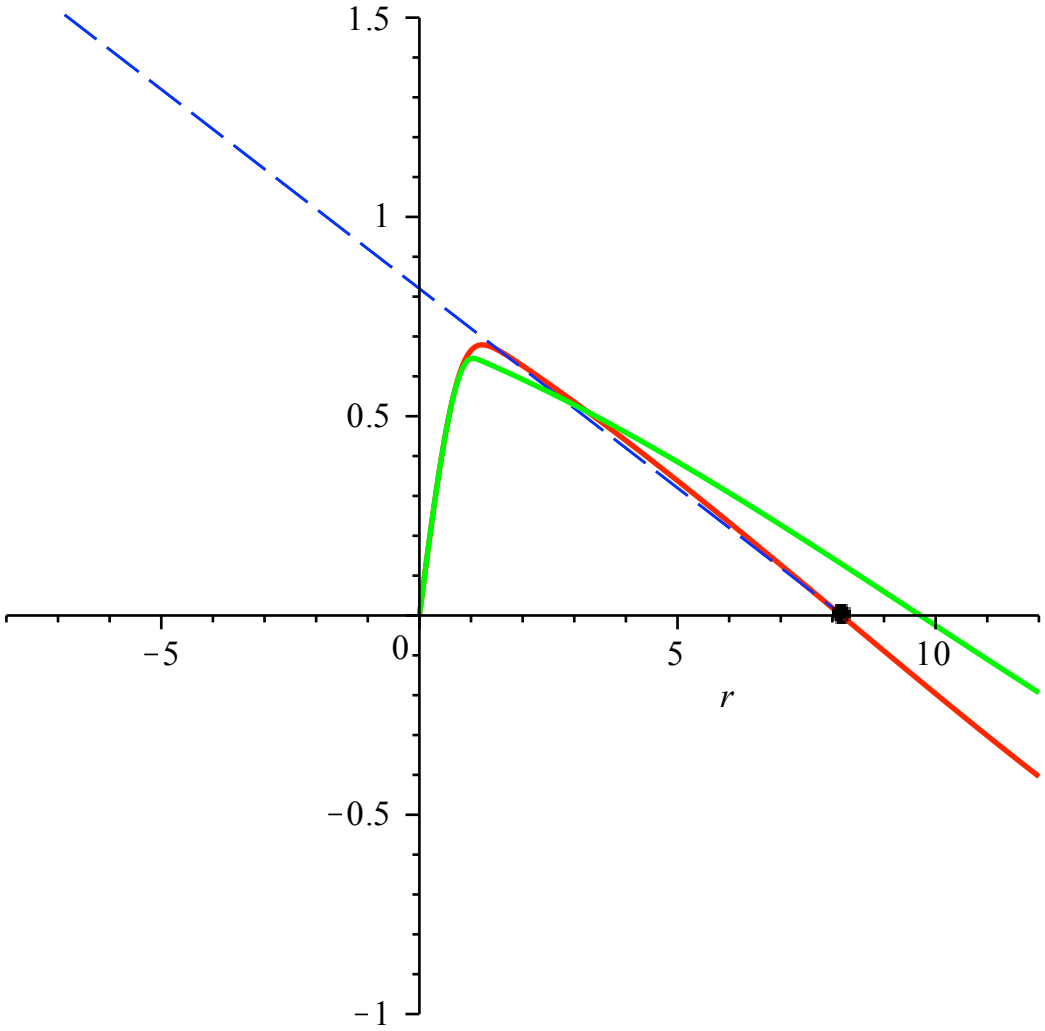
This exhibits the original idea of approximating the outside wavefunction as a constant: it is actually a sine function, so if constant is a decent approximation over some range, then so is exponentially decaying (until it crosses zero, that is).

Finally, let us make the potential steeper, more like the step function of the piecewise constant well:

```
> V4 := 1.2 ( tanh(12 r − 4 π) − 1) :
> plot([V3, V4], r = 0 ..6, view = [0 ..5, −3 ..1], thickness = 2)
```




```
> V := V4 :
> sol := dsolve( [subs (E = 0.01, SE), u(0) = 0, D(u)(0) = 1 ], u(r), numeric) :
> display(plotkeep, plot( -0.1 (r − 8.2), r = -8 ..8, color = blue, linestyle = dash ), point( [8.2, 0 ],
      symbol = solidcircle, symbolsize = 15 ), odeplot(sol, [r, u(r) ], 0 ..12, thickness = 2, color
      = green ), view = [ -8 ..12, -1 ..1.5 ])
```

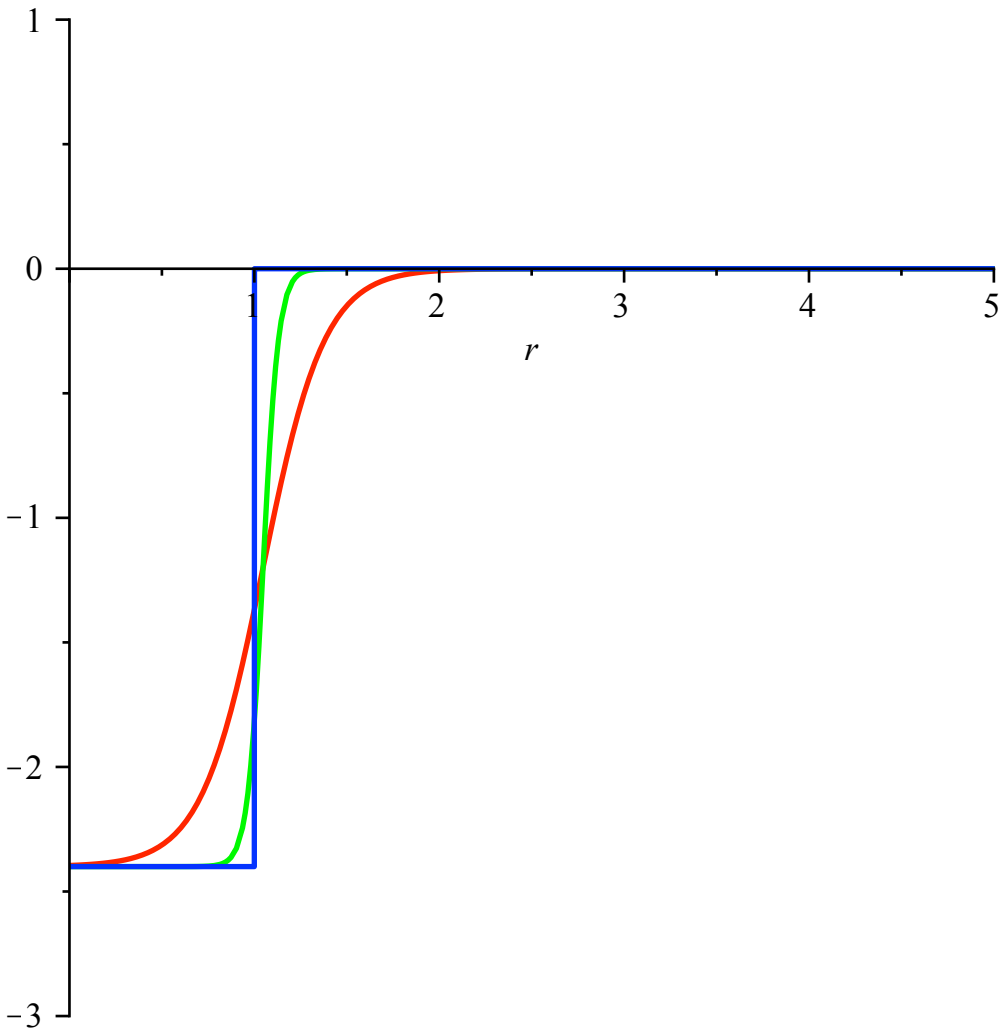


As expected, there is no qualitative change. But if V(r) is truly a step function, though, something changes:

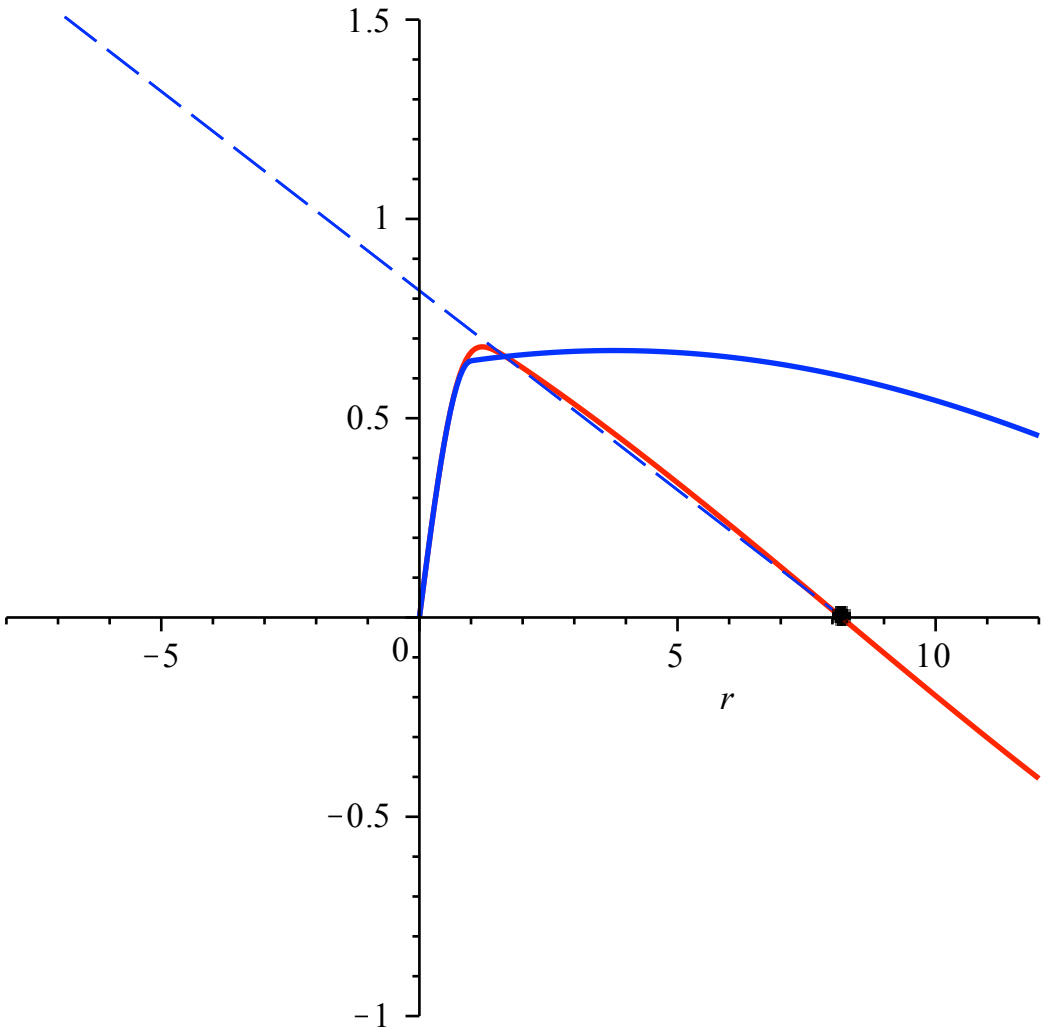
```
> V5 := piecewise(r < 1, -2.4);
```

$$V5 := \begin{cases} -2.4 & r < 1 \\ 0 & otherwise \end{cases} \quad \textbf{(5)}$$

```
> plot([V3, V4, V5], r = 0..6, view = [0..5, -3..1], thickness = 2, color = [red, green, blue])
```




```
> V := V5 :
> sol := dsolve( [subs (E = 0.01, SE), u(0) = 0, D(u)(0) = 1 ], u(r), numeric) :
> display(plotkeep, plot( -0.1 (r − 8.2), r = -8 ..8, color = blue, linestyle = dash ), point( [8.2, 0 ],
      symbol = solidcircle, symbolsize = 15 ), odeplot(sol, [r, u(r) ], 0 ..12, thickness = 2, color
      = blue ), view = [ -8 ..12, -1 ..1.5 ])
```



Now there cannot be smooth matching to something that slopes down, in the "outside linear" approximation:
Indeed at best it can *bend* down to hit the x-axis, as it's starting to do here, but then it is not approximately linear.
So in a sense, this whole discussion rests upon the potential not really being a step function.

>