

Excursions in Computing Science: Week 6. Spin

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I. Prefatory Notes

1. States.

Light has two polarization states: \uparrow and \rightarrow

(This is a little oversimplified, but we clean it up in Note 13.)

Every other state has some amplitude of being in either of these “base” states. (As we saw, amplitudes give rise to probabilities.)

$$\begin{aligned} \nearrow_{\theta} &= \cos \theta \rightarrow + \sin \theta \uparrow \\ \nwarrow_{\theta} &= -\sin \theta \rightarrow + \cos \theta \uparrow \end{aligned}$$

$$\begin{pmatrix} \nearrow \\ \nwarrow \end{pmatrix} = \begin{pmatrix} \mathbf{c} & \mathbf{s} \\ -\mathbf{s} & \mathbf{c} \end{pmatrix} \begin{pmatrix} \rightarrow \\ \uparrow \end{pmatrix}$$

This allows us to view a polarization state, say the one at angle θ , from the perspective of “horizontal” and “vertical”.

2. An electron also has two “polarization” states.

They are abstract, so we won’t draw pictures, but write

“spin up”: $|+\rangle$

“spin down”: $|-\rangle$

“Up” and “down” are relative to some given z-axis in 3D. (The “polarization” might be thought of as the electron spinning about this axis. But it is a quantum-mechanical property, quantized in

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only two directions instead of all possible directions.)

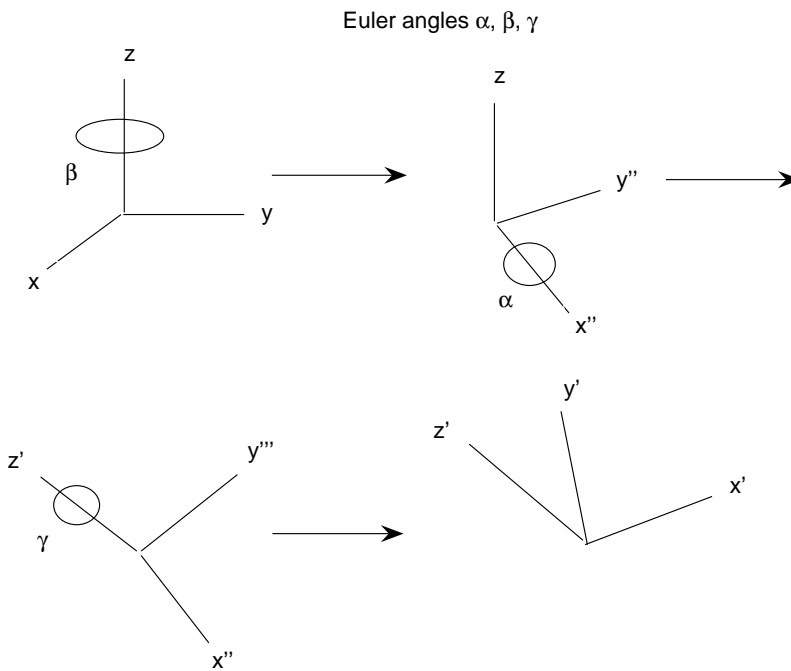
We want to know what happens when we change to the perspective of some other system of axes, x', y', z' .

The transformation matrix must be 2×2 , since there are two states. Any alternative state is some linear combination of the two,

$$a_+ | + \rangle + a_- | - \rangle$$

3. We can get any new axes, x', y', z' , from x, y, z by:

1. rotate through angle β about z ;
2. rotate through angle α about new x'' ;
3. rotate through angle γ about new z' ;



I won't prove this. Or the next step, which is carefully worked through by Feynman [FLS64, Sects.6-3-6-6]. He makes it easy, but it is too long to go through here.

The transformation matrix is, in terms of these Euler angles,

$$\begin{aligned}
 R(\alpha, \beta, \gamma) &= \begin{pmatrix} c_\alpha(c_{\beta+\gamma} + is_{\beta+\gamma}) & is_\alpha(c_{\beta-\gamma} - is_{\beta-\gamma}) \\ is_\alpha(c_{\beta-\gamma} + is_{\beta-\gamma}) & c_\alpha(c_{\beta+\gamma} - is_{\beta+\gamma}) \end{pmatrix} \\
 &= c_\alpha c_{\beta+\gamma} I + ic_\alpha s_{\beta+\gamma} \sigma_z + is_\alpha c_{\beta-\gamma} \sigma_x + is_\alpha s_{\beta-\gamma} \sigma_y
 \end{aligned}$$

where $c_\alpha = \cos \frac{\alpha}{2}$, $s_\alpha = \sin \frac{\alpha}{2}$, $c_{\beta \pm \gamma} = \cos \frac{\beta \pm \gamma}{2}$, $s_{\beta \pm \gamma} = \sin \frac{\beta \pm \gamma}{2}$
 and $I = \begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$, $\sigma_x = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$, $\sigma_y = \begin{pmatrix} & -i \\ i & \end{pmatrix}$.

4. Note the *half* angles. These normally appear when we do rotations in 3D (see Week 7c). They mean, in some circumstances, that we must rotate through 4π (720°) to get back where we started. This can actually happen. [Demonstration here.] Here, the rotated object is *tethered*—part of a system.

In quantum mechanics, with 2-number matrix entries, it can just happen, never mind any tethers—and it does with electrons.

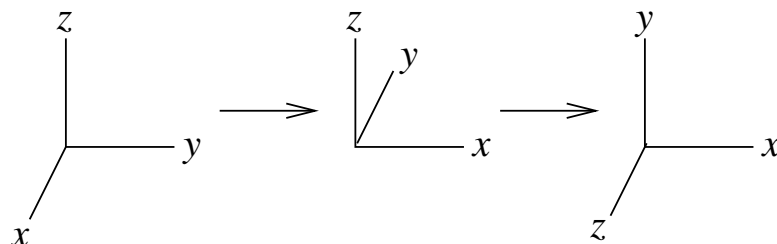
Because of this 720° rotation to get back to square 1, we say electrons have “spin $\frac{1}{2}$ ”.

5. Note the “Pauli matrices” $I, \sigma_z, \sigma_y, \sigma_x$. They have interesting properties.

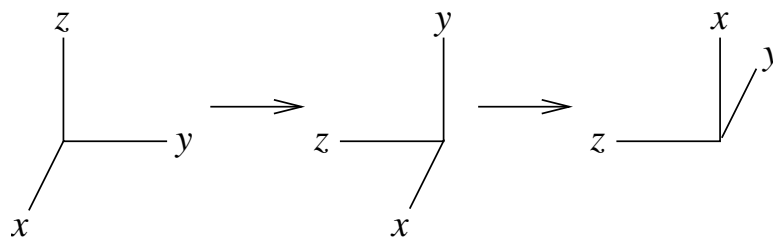
$$\begin{aligned} \sigma_z \sigma_z &= \sigma_x \sigma_x = \sigma_y \sigma_y = I \\ \sigma_x \sigma_y &= i \sigma_z & \sigma_y \sigma_z &= i \sigma_x \\ \sigma_z \sigma_x &= i \sigma_y & \sigma_j \sigma_k &= -\sigma_k \sigma_j \end{aligned}$$

The latter is the “anticommutative” property, $\sigma_j \sigma_k + \sigma_k \sigma_j = 0$ for any $j, k \in \{x, y, z\}$. (Compare this with ordinary numbers, a, b , which commute: $ab - ba = 0$.)

Rotations in 3D are not commutative: e.g. $x \rightarrow y$ then $y \rightarrow z$ gives the cycle $x \rightarrow y \rightarrow z \rightarrow x$



while $y \rightarrow z$ then $x \rightarrow y$ gives another cycle, $z \rightarrow -y \rightarrow x \rightarrow z$.



6. Special cases.

1. rotate by ϕ around z -axis

$$\begin{aligned} \alpha &= 0, \beta = \phi, \gamma = 0 \\ R_z(\phi) &= c_\phi I + i s_\phi \sigma_z = \begin{pmatrix} \cos(\phi/2) + i \sin(\phi/2) & \\ & \cos(\phi/2) - i \sin(\phi/2) \end{pmatrix} \end{aligned}$$

2. rotate by ϕ around x -axis

$$\begin{aligned} \alpha &= \phi, \beta = 0, \gamma = 0 \\ R_x(\phi) &= c_\phi I + i s_\phi \sigma_x = \begin{pmatrix} \cos(\phi/2) & i \sin(\phi/2) \\ i \sin(\phi/2) & \cos(\phi/2) \end{pmatrix} \end{aligned}$$

3. rotate by ϕ around y -axis

$$\alpha = \phi, \beta = \pi/2, \gamma = -\pi/2$$

$$R_y(\phi) = c_\phi I + i s_\phi \sigma_y = \begin{pmatrix} \cos(\phi/2) & \sin(\phi/2) \\ -\sin(\phi/2) & \cos(\phi/2) \end{pmatrix}$$

7. The matrix

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} = \begin{pmatrix} \cos(\alpha/2)e^{i(\beta+\gamma)/2} & i \sin(\alpha/2)e^{-i(\beta-\gamma)/2} \\ i \sin(\alpha/2)e^{i(\beta-\gamma)/2} & \cos(\alpha/2)e^{-i(\beta+\gamma)/2} \end{pmatrix}$$

(why is this the same matrix as $R(\alpha, \beta, \gamma)$?)

means that an electron which is spin up, $|+\rangle$, in x, y, z

has amplitude a of being spin up, $|+\prime\rangle$, in x', y', z'

and amplitude b of being spin down, $|-\prime\rangle$, in x', y', z'

and that an electron which is spin down, $|-\rangle$, in x, y, z

has amplitude c of being spin up, $|+\prime\rangle$, in x', y', z'

and amplitude d of being spin down, $|-\prime\rangle$, in x', y', z' , i.e.,

$$\begin{aligned} |+\prime\rangle &= a |+\rangle + c |-\rangle \\ |-\prime\rangle &= b |+\rangle + d |-\rangle \end{aligned}$$

Dirac wrote this (he called them “<bra|ket>s”)

$$\begin{aligned} a &= \langle +\prime | + \rangle \\ b &= \langle -\prime | + \rangle \\ c &= \langle +\prime | - \rangle \\ d &= \langle -\prime | - \rangle \end{aligned}$$

8. In quantum computing, an electron, or any spin- $\frac{1}{2}$ particle, with two states, could serve as a bit: a “q-bit”.

So what do 2 q-bits look like?

For that matter, how do 2 electrons transform?

Here’s a new kind of matrix product, the “tensor product”, \otimes .

$$\begin{aligned} \begin{pmatrix} |+\prime\rangle \\ |-\prime\rangle \end{pmatrix} & \begin{pmatrix} |+\rangle & |-\rangle \\ \left(\begin{array}{cc} a & c \\ b & d \end{array} \right) \end{pmatrix} \otimes \begin{pmatrix} |+\prime\rangle \\ |-\prime\rangle \end{pmatrix} & \begin{pmatrix} |+\rangle & |-\rangle \\ \left(\begin{array}{cc} a & c \\ b & d \end{array} \right) \end{pmatrix} = \\ \begin{pmatrix} |+\prime+\prime\rangle \\ |+\prime-\prime\rangle \\ |-\prime+\prime\rangle \\ |-\prime-\prime\rangle \end{pmatrix} & \begin{pmatrix} |++\rangle & |+-\rangle & |--\rangle & |---\rangle \\ \left(\begin{array}{cc|cc} aa & ac & ca & cc \\ ab & ad & cb & cd \\ \hline ba & bc & da & dc \\ bb & bd & db & dd \end{array} \right) \end{pmatrix} \end{aligned}$$

This has 4 states.

9. But if we’re doing physics, not qbits, we must consider nature’s preference for pure symmetry and pure antisymmetry (in exchange of the two spin- $\frac{1}{2}$ particles):

not $|+-\rangle$ and $| -+\rangle$ but

$|\text{symm}\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + | -+\rangle)$ and

$$|\text{asym}\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - | -+\rangle)$$

This gives an interesting matrix.

$$\begin{array}{l} |++\rangle \\ |'+'\rangle \\ |\text{symm}'\rangle \\ |-'-\rangle \\ |\text{asym}'\rangle \end{array} \begin{array}{l} |++\rangle \\ |\text{symm}\rangle \\ |--\rangle \\ |\text{asym}\rangle \end{array} \begin{pmatrix} a^2 & ac\sqrt{2} & c^2 & & \\ ab\sqrt{2} & ad+bc & cd\sqrt{2} & & \\ b^2 & bd\sqrt{2} & d^2 & & \\ & & & ad-bc & \\ & & & & \end{pmatrix}$$

Note that the first three are symmetric in the exchange of particles and the fourth is antisymmetric in the exchange of particles. Note also that

$$ad - bc = \det \begin{pmatrix} a & c \\ b & d \end{pmatrix} = 1$$

so the antisymmetric state transforms to itself, $|\text{asym}'\rangle = |\text{asym}\rangle$, and thus this state is just a number, not a vector.

The antisymmetric state describes spin 0: $0 = \frac{1}{2} - \frac{1}{2}$.

The symmetric state describes spin 1: $1 = \frac{1}{2} + \frac{1}{2}$.

(See [FLS64, p.12-16].)

10. Let's compare spin-1 to polarized light. We must work out the elements of the symmetric, 3×3 part of the matrix:

$$\begin{aligned} a^2 &= \left(\cos \frac{\alpha}{2} e^{i\frac{\beta+\gamma}{2}}\right)^2 \\ &= \cos^2 \frac{\alpha}{2} e^{i(\beta+\gamma)} \\ &= \frac{1}{2}(1 + \cos \alpha) e^{i(\beta+\gamma)} \end{aligned}$$

and so on:

$$\frac{1}{2} \begin{pmatrix} (1 + \cos \alpha) e^{i(\beta+\gamma)} & i\sqrt{2} \sin \alpha e^{i\gamma} & (\cos \alpha - 1) e^{-i(\beta-\gamma)} \\ i\sqrt{2} \sin \alpha e^{i\beta} & \cos \alpha & i\sqrt{2} \sin \alpha e^{-i\beta} \\ (\cos \alpha - 1) e^{i(\beta-\gamma)} & i\sqrt{2} \sin \alpha e^{-i\gamma} & (1 + \cos \alpha) e^{-i(\beta+\gamma)} \end{pmatrix}$$

Note: there are no more half-angles.

Remember this is the matrix that transforms the description (amplitudes) of a quantum-mechanical entity of spin-1 when we change the coordinate system from x, y, z by the Euler angles α, β, γ to x', y', z' .

If we take the special case $\alpha = 0 = \gamma$, the z -axis is fixed ($z' = z$), and β describes a rotation of the x, y coordinates into new x', y' coordinates. This would be an appropriate thing to do if the entity is travelling in the z direction.

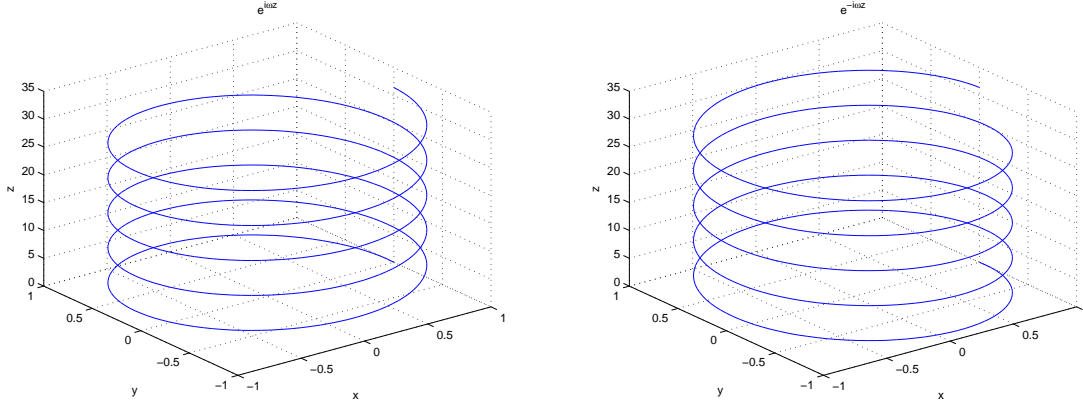
$$\begin{pmatrix} e^{i\beta} & & \\ & 1 & \\ & & e^{-i\beta} \end{pmatrix} \begin{pmatrix} |++\rangle \\ |\text{symm}\rangle \\ |--\rangle \end{pmatrix} = \begin{pmatrix} e^{i\beta} |++\rangle \\ |\text{symm}\rangle \\ e^{-i\beta} |--\rangle \end{pmatrix}$$

This is just a phase change of $+\beta$ if the entity is “spinning” “upwards”, and of $-\beta$ if the entity is “spinning” “downwards”.

11. If the entity is light (a *photon*), we can interpret $|++\rangle$ as right circular polarization. To get away from thinking about the two spin- $\frac{1}{2}$ components we started with and to think instead of the

single spin-1 photon, we'll replace $|++\rangle$ by $|+1\rangle$, or just $|R\rangle$ (for *Right* circular polarization). Similarly, we interpret $|--\rangle$ as left circular polarization and rename it $| -1\rangle$, or $|L\rangle$ (*Left* circular polarization).

We might think of the photon as a helical motion in the z direction, spinning right-handedly ($|R\rangle = \frac{1}{\sqrt{2}}e^{i\omega z} = \frac{1}{\sqrt{2}}(\cos \omega z + i \sin \omega z)$) or left-handedly ($|L\rangle = \frac{1}{\sqrt{2}}e^{-i\omega z} = \frac{1}{\sqrt{2}}(\cos \omega z - i \sin \omega z)$):



How do we get x -polarized light, $|x\rangle$, and y -polarized light, $|y\rangle$?

Try

$$|x\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle) = \cos \omega z$$

$$|y\rangle = \frac{-i}{\sqrt{2}}(|R\rangle - |L\rangle) = \sin \omega z$$

Conversely,

$$\begin{pmatrix} |R\rangle \\ |L\rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \end{pmatrix}$$

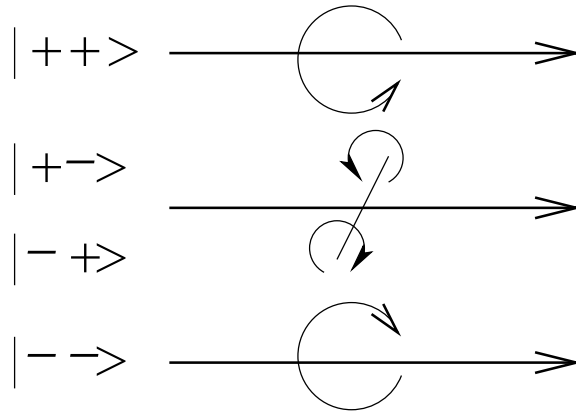
12. How do $|x\rangle$ and $|y\rangle$ transform under rotation of the x, y axes?

$$\begin{aligned} \begin{pmatrix} |x'\rangle \\ |y'\rangle \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \begin{pmatrix} |R'\rangle \\ |L'\rangle \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \begin{pmatrix} e^{i\beta} & \\ & e^{-i\beta} \end{pmatrix} \begin{pmatrix} |R\rangle \\ |L\rangle \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \begin{pmatrix} e^{i\beta} & \\ & e^{-i\beta} \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \end{pmatrix} \\ &= \begin{pmatrix} \cos \beta & -\sin \beta \\ \sin \beta & \cos \beta \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \end{pmatrix} \end{aligned}$$

This is just a rotation in two dimensions—the very same transformation we gave for polarized light in Week 2.

13. But we've left out $|\text{symm}\rangle$. What happened to it?

It turns out that, since photons travel at lightspeed, they cannot “spin” about any axis not in the direction of their motion. Here's a picture which claims to show that $|+-\rangle, |-+\rangle$ and, of course, $|\text{symm}\rangle$ would have part of their circular arrows actually going faster than light. (Think of these photons as *tumbling*, while $|++\rangle$ and $|--\rangle$ have right- and left-handed *screwing* motion.)



lightspeed!

(This is not a very precise argument, and we'll find considerations in Week 9 which appear to contradict it, but it will have to do for this course.)

So, while a spin-1 particle generally has a 3-dimensional (3×3) transformation, photons, travelling at lightspeed, are only two dimensional. This was the simplification in Note 1 for this week.

Photons move at lightspeed because they have no mass. (Week 3 shows that no particle with mass can attain lightspeed. A massless particle has little choice but to go at lightspeed—see Week 7a.)

14. Fermions and Bosons.

We said in Week 5 that fermion amplitudes change phase by π when two are exchanged (antisymmetry), while boson amplitudes are unchanged when swapped (symmetry).

This week we have just seen that there are similar phase changes when spin- $\frac{1}{2}$ and spin-1 particles, respectively, are rotated through 2π : spin- $\frac{1}{2}$ particles change phase by π , which is the same as saying they change sign, while spin-1 particles change phase by $2\pi \equiv 0$, which is to say they don't.

We can associate fermions with spin $\frac{1}{2}$ (and generally spin $\frac{n}{2}$ for odd n), and bosons with spin $\frac{n}{2}$ for even n .

The connection between exchanging two identical particles, on one hand, and rotating them through 2π , on the other, is made in Week 7a and Week 9.

Fermions and bosons are fundamental to the physical universe. Fermions are the basis of all matter because they fundamentally avoid each other as we shall see in Week 7a and so provide solidity. Bosons are the basis of all forces. Bosons don't avoid each other and so may be combined to produced effects we can actually feel in the every-day, non-quantum world.

Why don't we encounter particles of spin $\frac{1}{3}$, which would require rotation through 6π to restore their phase, or spin $\frac{1}{4}$, and so on? Week 8 will look at rotations in three dimensions and show that half-angles arise even in ordinary, non-quantum, geometry, but not third-angles or so forth. Week 8c part III gets to the math that shows that spins may be integral or half-integral and nothing else.

15. Summary

(These notes show the trees. Try to see the woods!)

- – Each possibility is a dimension.
- Any state may be a linear combination of other orthogonal states, taken as “base” states.
- Spin $\frac{1}{2}$ has 2 base states. Half angles in the transformation mean that it cannot return to its original state in only one full rotation, but needs two full rotations to do so.

- Spin 1 has 3 base states and no half angles: a normal full rotation suffices to restore it, just as in the familiar world.
- Pauli matrices and anticommutativity: describe electrons (spin- $\frac{1}{2}$, fermions).
- Tensor product: spin- $\frac{1}{2} + \text{spin-}\frac{1}{2} = \text{spin-}1$. Bosons.
- Photons are a special case of spin 1: they travel at lightspeed and are two-dimensional, not three.

II. The Excursions

You've seen lots of ideas. Now *do* something with them!

1. Discuss Feynman's demonstration [FLS64, pages 6-3ff] that the transformation of spin- $\frac{1}{2}$ to rotated coordinates requires the 2×2 2-number matrix given in the lecture.
2. Look up Feynman's discussion of spin 1 [FLS64, p.12-16].
3. Show the reduction of the spin rotation matrix, $R(\alpha, \beta, \gamma)$, to the linear combination of I and the three Pauli matrices.
4. Show that the Pauli matrices have the properties given.
5. Derive the three special cases of $R(\alpha, \beta, \gamma)$ and show that their product, $R_z(\gamma)R_x(\alpha)R_z(\beta)$, is $R(\alpha, \beta, \gamma)$.
6. Is the \times operator (tensor product) on matrices commutative?
7. Why is there a $\sqrt{2}$ in the symmetric combination of $|+-\rangle$ and $| -+\rangle$, $(|+-\rangle + | -+\rangle)/\sqrt{2}$, and in the antisymmetric combination, $(|+-\rangle - | -+\rangle)/\sqrt{2}$?
8. a) Show that the tensor product of $\begin{pmatrix} a & c \\ b & d \end{pmatrix}$ with itself becomes the matrix given (Note 9) when the symmetric and antisymmetric combinations of $|+-\rangle$ and $| -+\rangle$ are taken.
b) Show that the matrix

$$Q = \begin{pmatrix} 1 & & & \\ & 1/\sqrt{2} & 1/\sqrt{2} & \\ & 1/\sqrt{2} & -1/\sqrt{2} & \\ & & & 1 \end{pmatrix}$$

transforms the matrix of Note 8 to that of Note 9.

9. Derive the special cases of the symmetric/antisymmetric matrix in note 9: (1) $\beta = \pi/2, \gamma = -\pi/2$ and (2) $\alpha = 0, \gamma = 0$, given in [FLS64] equations (5.38) and (5.39) respectively. (Why does $\cos^2(\alpha/2) = (1 + \cos(\alpha))/2$?)
10. Show that rotating an electron through 2π about either x or z axes changes the sign of its amplitude. How does the electron resemble a dog on a leash? (Look up Ethan D. Bolker's *The Spinor Spanner* [Bol73].)
11. Combine two spin-1 systems (3 components each) into a spin-2 system (5 components) and others. Show that angles are doubled for the spin-2 system, so a complete revolution is accomplished by rotating through π . What are the other components?
12. Look up Paul Adrien Maurice Dirac, 1902–1984. Which minus sign, ignored by everybody else, did he take seriously?

13. Look up Wolfgang Pauli, 1900–1958. Why did he come up with the exclusion principle? Legendarily, what usually happened when he entered a laboratory?
14. The electrons surrounding atomic nuclei are governed by their states of angular momentum, which is related to spin. We’ve seen that a quantum system with integral spin, s , has $2s + 1$ states (3 for spin 1, 5 for spin 2, etc.). This carries over into the “orbital” angular momenta of electrons, only these angular momenta have upper limits depending on how close the electron is to the atomic nucleus: for “shell” n , the angular momentum, $l = 0, \dots, n - 1$. Each of these values of l in turn has $2l + 1$ states, and in addition to this, each electron can be in a spin up or spin down state (the electron spin, $s = \frac{1}{2}$, so $2s + 1$ gives 2 states). n goes from 1 to about 7 for all the chemical elements. (See Week 8c part III for a more complete treatment.)

With this much information, you can predict the electron configurations of the first 18 elements of the periodic table. Look up “atomic structure” or “atomic spectra” or “atomic physics”, or the periodic table of the elements to check your results. (One book is Gerhard Hertzberg’s *Atomic Spectra and Atomic Structure* [Her44]. This book is not in the style of this course and in reading it you’ll develop the ability to skim what you don’t at first understand, write out a synopsis as you go, and keep revisiting the parts that you think you might begin to understand later. The book proceeds historically, in part, and gives a good lesson in theories being developed, making some progress, and then being replaced by better theories. Quantum mechanics cut its teeth in the 1900s to 1930s on the complex problems of explaining chemistry.)

The elements after 18 begin to show the effects of interference between the “orbital” angular momenta and the electron spins—they are all angular momenta, after all, and obey vector addition rules, but are subject to precession when they interact, which changes their energies—and between the electrons in the outer shell and the electrons closer to the nucleus. The spin of the nucleus itself also has some effect on the energies of the electrons (as shown by the spectra of the light radiated when electrons jump from one level to another) but not on atomic structure. So you’ll find that your predictions begin to go wrong after element 18.

Can you go on from here to explain why chemical reactions combine atoms in the quantities that they do? (To get relative masses, you will also need to know atomic weights, due to the numbers of protons and neutrons in the nuclei, which is the subject of nuclear physics.)

All the foregoing is essential to understand chemistry, but is not necessarily a good way to *do* chemistry or chemical engineering.

15. Relate the 2-number description of polarized light in Note 12 to the relativistic description of magnetism referred to in the Excursions for Week 3.
16. Any part of the lecture that needs working through.

References

- [Bol73] Ethan D. Bolker. The spinor spanner. *The American Mathematical Monthly*, 80(9):977–84, Nov. 1973.
- [FLS64] R. P. Feynman, R. B. Leighton, and M. Sands. *The Feynman Lectures on Physics, Volume III*. Addison-Wesley, 1964.
- [Her44] Gerhard Hertzberg. *Atomic Spectra and Atomic Structure*. Dover Publications, New York, 1944. Prentice-Hall Inc., 1937; translated by J. W. T. Spinks.