

Spin 1/2: The prototypical 2-state quantum system

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1 Introduction

Quantum mechanical spin is a subject often treated only after angular momentum; Liboff introduces it in §11.6. While spin is a kind of angular momentum it is also an intrinsic property of certain particles. Spin cannot be related to anything in classical mechanics so one must accept the fact that it is represented using bras and kets corresponding to no wave function; the bras and kets are the basic elements in this case. The same rules apply to these vectors, and the operators which act on them, as to the more familiar wave-function-derived beasts. You solve spin problems using the same formal, mathematical manipulation of operators, bras and kets.

Once this is accepted spins form a compact 2-dimensional quantum mechanical system; the entire space is spanned by 2 orthogonal states, rather than the infinite set required by e.g. the particle in a box. This means that all operators are simple 2×2 matrices and no superposition of states can involve more than two terms. This vast reduction in complexity makes it far easier to do a wide range of quantum mechanical problems with spins. For this reason I have opted to introduce quantum mechanical spin at this point. Later it will turn out to be easier to solve other problems in quantum mechanics, such as the simple harmonic oscillator, by ignoring the wave functions and simply manipulating bras and kets. By getting used to working this way with spins this mathematical sleight-of-hand will seem less alien later on.

2 The electron in a magnetic field

It turns out that an electron at rest in a magnetic field can be in one of two energy states. I say it is at rest so we don't concern ourselves with its position or momentum. If the electron were moving it would have kinetic energy as well; we will ignore that whenever we talk of spin. (The two energies can be combined and no doubt they will be in later courses.) The electron energy states we are concerned with have no relationship to classical properties so we cannot learn about them from the electron's wave function. We can, however, use our quantum language to describe this system even though there is no wave function. We simply denote each state by its own ket. The states are generally called "spin up" and "spin down" and some books use pair of kets $|+\rangle$ and $|-\rangle$ to denote them; other books, including Liboff, use the less-informative pair $|\alpha\rangle$ and $|\beta\rangle$. I prefer use a different notation which can be changed according to the orientation of the magnetic field. The symbol inside the ket cannot relate to a wave function — there isn't one — so it can be selected to give a clear indication of which state it is.

When the magnetic field is $\mathbf{B} = B\hat{\mathbf{z}}$ I will denote the two energy eigenstates by the kets $|\uparrow\rangle$ and $|\downarrow\rangle$ (the arrows are vertical since $\hat{\mathbf{z}}$ is generally thought of as up.) The Hamiltonian operator is (as always) denoted $\hat{H}$ and these two states are its only two eigenstates:

$$\hat{H}|\uparrow\rangle = E_+|\uparrow\rangle \tag{1}$$

$$\hat{H}|\downarrow\rangle = E_-|\downarrow\rangle \tag{2}$$

where E_+ and E_- are the energies of the two states.

Since $\hat{H}$ is a Hermitian operator (as it always must be) its eigenstates are orthogonal

$$\langle \uparrow | \downarrow \rangle = 0 \quad . \quad (3)$$

This expression looks very strange if you confuse the little arrows inside the bras and kets with vectors — they are only reminders of the electron's spin state. We will naturally take each ket to be normalized so

$$\langle \uparrow | \uparrow \rangle = \langle \downarrow | \downarrow \rangle = 1 \quad . \quad (4)$$

Relations (1)–(4) are all we know about electron spin, and they are all we need to know — everything else will follow from them. This may seem like cheating — for the particle-in-a-box system we worked quite hard to derive a Hamiltonian operator, find its energy eigenvalues, its energy eigenstates, to normalize them and show they were orthogonal. Now it looks like we've skipped all the hard work. We have, but in a way it is not necessary since expressions (1)–(4) are *inevitable* once we have established experimentally that the electron has two energy states rather than 3, or 5, or 17. There must be a Hamiltonian operator. It must have eigenstates defined by expressions (1) and (2). These must be called something, so why not $|\uparrow\rangle$ and $|\downarrow\rangle$ (the names are not inevitable, which is why different books use different names). The Hamiltonian must be Hermitian so its eigenstates must be orthogonal.

The states $|\uparrow\rangle$ and $|\downarrow\rangle$ are the only eigenstates the electron can have so any state can be expanded in terms of them:

$$|\chi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle \quad ,$$

where α and β are constants — each possibly complex. It is a simple exercise in the application of (3) and (4) to show that

$$\langle \chi | \chi \rangle = |\alpha|^2 + |\beta|^2 \quad .$$

In order that $|\chi\rangle$ be normalized we require that $|\alpha|^2 + |\beta|^2 = 1$.

We may also write a state vector $|\chi\rangle$ as a traditional column vector with the coefficients along the column:

$$|\chi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \quad .$$

In this notation, the top row contains the coefficient of $|\uparrow\rangle$ and the bottom the coefficient of $|\downarrow\rangle$. The basis vectors themselves are therefore unit column vectors in this notation

$$|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad , \quad |\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad .$$

Bras are row vectors formed by transposing the column and taking the complex conjugates of its elements

$$\langle \chi | = [\alpha^*, \beta^*] \quad , \quad \langle \uparrow | = [1, 0] \quad , \quad \langle \downarrow | = [0, 1] \quad .$$

The actual energies of the eigenstates, E_+ and E_- are traditionally taken to have equal magnitude and opposite sign — zero energy therefore represents the energy the electron would have if it did not have spin or if there were no magnetic field. The experimental fact is that

$$E_{\pm} = \pm \mu_b B \quad ,$$

where μ_b is called the Bohr magneton. For the electron its value, found experimentally, is $\mu_b = 9.25 \times 10^{-21}$ ergs/Gauss. In a magnetic field directed in the $+\hat{\mathbf{z}}$ direction, with a magnitude $B = 10^4$ Gauss (equal to one Tesla, a respectable laboratory magnetic field), the state $|\uparrow\rangle$ will have positive energy $E_+ = 9.25 \times 10^{-17}$ ergs or 5.8×10^{-5} electron Volts — a fairly small energy, but a measurable one. The state $|\downarrow\rangle$ has a lower energy: $E_- = -9.25 \times 10^{-17}$ ergs. Making the magnetic field weaker will decrease the energy difference until, at $B = 0$, there is no difference at all: they are degenerate eigenstates.

3 Spin operators

In the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis the Hamiltonian operator is a 2×2 matrix. Since these basis vectors are its eigenstates it will be diagonal:

$$\hat{H} = \begin{bmatrix} E_+ & 0 \\ 0 & E_- \end{bmatrix} = 2\mu_b B \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{bmatrix} . \quad (5)$$

The constants have been factored out to leave the simple operator (matrix) called the *spin* operator

$$\hat{S}_z = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{bmatrix} . \quad (6)$$

The Hamiltonian is therefore $\hat{H} = 2\mu_b B \hat{S}_z$, and the eigenstates of $\hat{S}_z$ are the same as those of $\hat{H}$ namely $|\uparrow\rangle$ and $|\downarrow\rangle$. The eigenvalues of the spin operator are simply $+\frac{1}{2}$ and $-\frac{1}{2}$

$$\hat{S}_z |\uparrow\rangle = +\frac{1}{2} |\uparrow\rangle \quad , \quad \hat{S}_z |\downarrow\rangle = -\frac{1}{2} |\downarrow\rangle . \quad (7)$$

This is why you will hear Physicists refer to the electron as a “spin one-half” particle. This is also why $|\uparrow\rangle$ is called spin “up” and $|\downarrow\rangle$ is called spin “down”. When using this short-hand remember that expression (3) can be read “up is orthogonal to down” — a quantum Physics koan if ever there was one! It seems that the electron has *higher* energy when its spin is parallel to the magnetic field than when its spin is anti-parallel: electrons “want” to line up against the field.¹ Since the spin is a Hermitian operator it must be an observable: we can measure the component of spin along $\hat{\mathbf{z}}$ and we will find it to be either $+\frac{1}{2}$ or $-\frac{1}{2}$ — never any other value.

Certainly there is nothing special about the $\hat{\mathbf{z}}$ direction. It must be possible to measure the component of spin along a different direction, say $\hat{\mathbf{x}}$. That means, according to the first postulate of quantum mechanics, there must be an operator, $\hat{S}_x$, corresponding to such an observation and its eigenvalues will be the possible outcomes of the observation. The amazing fact is that the electron’s spin state is always described by a vector from the same 2-dimensional state-space spanned by $\{|\uparrow\rangle, |\downarrow\rangle\}$. Expressed in this basis $\hat{S}_x$ will be a 2×2 Hermitian matrix, although possibly not diagonal. The same will be true of the operator $\hat{S}_y$ corresponding to a measurement of the electron’s spin along $\hat{\mathbf{y}}$. Expressed in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis the operators are the matrices²

$$\hat{S}_x = \begin{bmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix} \quad , \quad \hat{S}_y = \begin{bmatrix} 0 & -i\frac{1}{2} \\ i\frac{1}{2} & 0 \end{bmatrix} . \quad (8)$$

¹If you remember anything about magnetic dipoles, you might recall that they want to line up *parallel* to the magnetic field. Electrons also do this, but since they have negative electrical charge their magnetic moment points in the direction opposite to their spin axis — Thank you again, Ben Franklin!

²These are given in Liboff through equation (11.81) and (11.82). His version of $\hat{S}_z$ etc. includes a factor of $\hbar$, and the Pauli spin matrices $\hat{\sigma}_z$ have 1’s in place of the $\frac{1}{2}$ ’s.

What then are the eigenstates of $\hat{S}_x$? An eigenstate $|\chi\rangle$ must satisfy the eigen-equation

$$\hat{S}_x|\chi\rangle = \lambda|\chi\rangle \quad ,$$

where λ is the eigenvalue — which we must also solve for. Substituting the expansion

$$|\chi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \quad ,$$

into the eigen-equation and using the matrix from (8) gives

$$\begin{bmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \lambda \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \quad .$$

The trick to solving eigen-equations is to subtract the right hand vector from both sides of the equation to get

$$\begin{bmatrix} -\lambda & \frac{1}{2} \\ \frac{1}{2} & -\lambda \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = 0 = (\hat{S}_x - \lambda\hat{I})|\chi\rangle \quad (9)$$

where $\hat{I}$ is the identity operator (identity matrix). In order for the product of a vector, $|\chi\rangle$, and a matrix, $(\hat{S}_x - \lambda\hat{I})$, to yield the zero-vector one of two situation must occur. Either the vector itself is zero $|\chi\rangle = 0$ (not very satisfying), or the matrix is a *singular* matrix. Basically a singular matrix is one whose rows are not all linearly independent. You might have come across one when trying to solve N equations to find N unknowns. If one of your N equations is defective (it is a repeat or is a linear combination of the other equations) you will not succeed — your problem is singular. The way to detect a singular matrix is to take its *determinant*. If the determinant of a matrix is exactly zero then the matrix is singular.

The prescription for solving eigen-equation (9), without giving up by setting $|\chi\rangle = 0$, is to find a value of λ which makes the determinant vanish

$$\det \begin{bmatrix} -\lambda & \frac{1}{2} \\ \frac{1}{2} & -\lambda \end{bmatrix} = \det(\hat{S}_x - \lambda\hat{I}) = 0 \quad . \quad (10)$$

This is called the *characteristic* equation, it is a polynomial equation for λ whose multiple solutions are the different eigenvalues. The present case is (thankfully) 2×2 so the determinant is easily computed to give a quadratic characteristic equation

$$\lambda^2 - \left(\frac{1}{2}\right)^2 = 0 \quad .$$

The two eigenvalues which solve this equation are $\lambda_1 = \frac{1}{2}$ and $\lambda_2 = -\frac{1}{2}$.

It seems that the possible values of spin along $\hat{\mathbf{x}}$ are the same as those along $\hat{\mathbf{z}}$. This is logical since there is nothing special about $\hat{\mathbf{z}}$. Repeating the steps above for $\hat{S}_y$ will confirm that its eigenvalues are also $+\frac{1}{2}$ and $-\frac{1}{2}$. The electron has spin one-half no matter which way you look at it.

To find the eigenvector corresponding to a particular eigenvalue, λ_j , one returns to (9). The top row of this equation yields one relation between the two coefficients, α and β

$$\beta = 2\lambda_j\alpha \quad . \quad (11)$$

Will the bottom row provide the second equation from which we can solve for both coefficients? The answer will always be “No”. The second row is basically the same as the first — it yields relation (11) over again. This is natural since we chose λ_j in order to make the matrix singular — its rows are not independent. The eigen-equation determines the directions of all eigen-vectors, but never their magnitude. In this case we find

$$|\chi_j\rangle = \alpha (|\uparrow\rangle + 2\lambda_j|\downarrow\rangle)$$

where $j = 1, 2$ for the two eigenvalues and their corresponding eigenvectors. The unknown coefficient α is now fixed by normalization:

$$\langle\chi_j|\chi_j\rangle = |\alpha|^2(1 + 4\lambda_j^2) = 1 \quad .$$

Since $\lambda_j^2 = 1/4$ for both $j = 1$ and $j = 2$ we see that $\alpha = 1/\sqrt{2}$ (its sign or complex phase being arbitrary).

With this final piece in place we can exhibit the positive and negative eigenkets of the $\hat{S}_x$ operator, which I call $|\rightarrow\rangle$ and $|\leftarrow\rangle$ respectively,

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\rangle \quad , \quad |\leftarrow\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle \quad (12)$$

Multiplying each of these by the matrix from (8) verify that these are eigenkets

$$\hat{S}_x|\rightarrow\rangle = +\frac{1}{2}|\rightarrow\rangle \quad , \quad \hat{S}_x|\leftarrow\rangle = -\frac{1}{2}|\leftarrow\rangle \quad ,$$

verifies that each is an eigenket and reminds us of its eigenvalue. It is also easy to check that $\langle\rightarrow|\leftarrow\rangle = 0$.

Following the same procedure for the operator $\hat{S}_y$, the second matrix in eq. (8), gives explicit versions of its eigenkets, whose names are my own, and will never be used again (I promise)

$$|\otimes\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{i}{\sqrt{2}}|\downarrow\rangle \quad , \quad |\odot\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle - \frac{i}{\sqrt{2}}|\downarrow\rangle \quad . \quad (13)$$

Once again, a simple multiplication of these by the matrix in (8) serves to check my claim of eigenket-ness and also reveals their respective eigenvalues. It is worth using these expression to verify explicitly that $\langle\otimes|\odot\rangle = 0$ and $\langle\otimes|\otimes\rangle = 1$ since this will test your ability to manipulate factors of i .

Expression (12) contains some fairly remarkable information about spins. First of all, the spin-up state, $|\uparrow\rangle$ and the spin-right state, $|\rightarrow\rangle$ are *not* orthogonal

$$\langle\uparrow|\rightarrow\rangle = \frac{1}{\sqrt{2}}\langle\uparrow|\uparrow\rangle + \frac{1}{\sqrt{2}}\langle\uparrow|\downarrow\rangle = \frac{1}{\sqrt{2}} \quad .$$

This may be somewhat at odds with your intuition — you would think spins in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$ direction would be orthogonal... but then you would *not* expect that spins along the $+\hat{\mathbf{z}}$ and $-\hat{\mathbf{z}}$ directions to be orthogonal to one another and they are.

An electron whose spin is exactly along $\hat{\mathbf{x}}$ is in a mixed state with respect to $\hat{\mathbf{z}}$: it is “half-up and half-down”. The expectation value of such a measurement can be found

$$\langle S_z \rangle = \langle\rightarrow|\hat{S}_z|\rightarrow\rangle = 0 \quad .$$

(You should work out this product to be sure you understand it.) This much is consistent with your classical intuition. But be careful to remember what the expectation value tells us. If you were to measure the component along $\hat{\mathbf{z}}$ you would find it up (in the $|\uparrow\rangle$ state) with a probability

$$P(\uparrow) = |\langle \uparrow | \rightarrow \rangle|^2 = \frac{1}{2} .$$

The probability of finding it in the $|\downarrow\rangle$ state is also one-half — hence the “half up and half down” statement. The expectation value combines these two possible outcomes

$$\langle S_z \rangle = (+\frac{1}{2})P(\uparrow) + (-\frac{1}{2})P(\downarrow) = 0 .$$

Our classical intuition would lead us to think that if the spin is along $\hat{\mathbf{x}}$ then the component along $\hat{\mathbf{z}}$ would be exactly zero — when we measured it we would measure zero. Our quantum experience has told us that a measurement of zero is not an option since zero is not an eigenvalue of $\hat{S}_z$. Our classical intuition must eventually prevail, according to Bohr’s correspondence principle, but only through the expectation value. If you average enough measurements you will find a value of zero (or very, very close). Quantum mechanics, however, applies to the individual measurements, and none of these are zero — ever.

I conclude this section with a quantum parable which helps to illustrate the various postulates. You prepare an electron to be in the spin-up state, $|\uparrow\rangle$. You then measure its z -spin again for good measure. What do you find? Answer: you are guaranteed to find its spin *up* ($P(\uparrow) = 1$). Next you measure its x -spin and find it in the $+\hat{\mathbf{x}}$ direction. You now repeat the z -spin measurement of this same electron. What will you find? Answer: this time the spin has a 50% chance of being *down*. By making an x -spin measurement you have affected the particle; your subsequent z measurement clearly shows this.