Experiment 2
Multiparticle Systems

1 Introduction

We have already seen that the spin–$\frac{1}{2}$ degree of freedom can be represented by a two-dimensional quantum state

$$|\psi\rangle \;\; = \;\; \alpha\,|+\rangle + \beta\,|-\rangle\,, \tag{1}$$

where α and β are complex numbers such that $|\alpha|^2 + |\beta|^2 = 1$. This lab focuses on how to represent *multiple* spin degrees of freedom. We need at least two particles to discuss quantum entanglement. Furthermore, the humble proton and neutron–each a spin–$\frac{1}{2}$ degree of freedom–are actually each composed of three *quarks*. Each quark is itself a spin–$\frac{1}{2}$ degree of freedom, so it is not immediately clear how protons and neutrons can be spin–$\frac{1}{2}$ particles. The machinery we develop is also capable of describing the color charge degree of freedom in quarks. Collections of two or more particles can also *interact* with each other, and we can examine particular states which minimize energy.

2 Higher spins

Up to this point, we have been concerned with spin–$\frac{1}{2}$ degrees of freedom which are analogous to classical spin vectors of magnitude $\frac{\hbar}{2}$. Angular momentum is quantized in units of $\frac{\hbar}{2}$, so a spin–$\frac{1}{2}$ particle consists of the smallest "lump" of angular momentum allowed by quantum mechanics. However, we could also have systems with any integer multiple of $\frac{\hbar}{2}$. A general spin-s system has total angular momentum $s\hbar$ and has dimension $N = 2s + 1$. For $s = \frac{1}{2}$ ($N = 2$) we recover the structure of spin-$\frac{1}{2}$ discussed previously. For $s > \frac{1}{2}$, the spin operators can be represented by $N \times N$ matrices whose entries are given by

$$\left[\hat{S}^x\right]_{ab} \;\; = \;\; \frac{\hbar}{2}\left(\delta_{a,b+1} + \delta_{a+1,b}\right)\sqrt{(s+1)(a+b-1) - ab}, \tag{2}$$

$$\left[\hat{S}^y\right]_{ab} \;\; = \;\; \frac{i\hbar}{2}\left(\delta_{a,b+1} - \delta_{a+1,b}\right)\sqrt{(s+1)(a+b-1) - ab}, \tag{3}$$

$$\left[\hat{S}^z\right]_{ab} \;\; = \;\; \frac{\hbar}{2}(s+1-a)\delta_{ab}. \tag{4}$$

The functions `spinx(n)`, `spiny(n)`, `spinz(n)` in the template notebook implement these expressions and return $\hat{S}^x$, $\hat{S}^y$, $\hat{S}^z$, respectively, as $N \times N$ matrices (in units where $\hbar \to 1$).

1. Generate $\hat{S}^x$, $\hat{S}^y$ and $\hat{S}^z$ for $s = 2$ and calculate the commutator

$$\left[\hat{S}^x, \hat{S}^y\right] \tag{5}$$

explicitly as a 5×5 matrix. What is the result for general s? You can write it in terms of the spin matrices and the identity.

2. Calculate $\hat{\mathbf{S}}^2 \equiv \left[\hat{S}^x\right]^2 + \left[\hat{S}^y\right]^2 + \left[\hat{S}^z\right]^2$ for several values of s. What is the result for general s?

3. For $s = \frac{3}{2}$, calculate the commutator of $\hat{\mathbf{S}}^2$ with:

   (a) $\hat{S}^x$

   (b) $\hat{S}^y$

   (c) $\hat{S}^z$

   Does the result hold for other values of s?

4. Verify that

$$\left[\hat{S}^x\right]^2 \;=\; \left[\hat{S}^y\right]^2 \;=\; \left[\hat{S}^z\right]^2 \;=\; \frac{1}{4}\hat{I}, \tag{6}$$

   for $s = \frac{1}{2}$. Does this relation hold for $s > \frac{1}{2}$?

3 Two spins: entanglement

Let us consider the case of two spins. In the case where the first spin is described by $|\psi_1\rangle$ and the second spin by $|\psi_2\rangle$, the formalism is to consider the **tensor product** as the full state vector

$$|\psi\rangle \;=\; |\psi_1\rangle \otimes |\psi_2\rangle\,. \tag{7}$$

Later in this document (and within the McIntyre text), you will see the notation $|\psi\rangle = |\psi_1\rangle\,|\psi_2\rangle$ in which the tensor product is implied. Additionally, special cases such as $|\psi_1\rangle = |+\rangle$, $|\psi_2\rangle = |-\rangle$ are sometimes given explicit labels for the particles such as $|\psi\rangle = |+\rangle_1\,|-\rangle_2$. We will assume the ordering of the kets is consistent so that such labels are not needed to specify which particle is in which state.

The tensor product operation on kets, $\otimes$, can be represented by the **Kronecker product** when the states are represented by column vectors. While the discussion generalizes, we will specialize to the case $s = \frac{1}{2}$. The Kronecker product of two vectors is

$$\begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} \;\equiv\; \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix}. \tag{8}$$

That is, a two-spin system should have dimension $(2s)^2 = 4$ corresponding to $|+\rangle\,|+\rangle$, $|+\rangle\,|-\rangle$, $|-\rangle\,|+\rangle$ and $|-\rangle\,|-\rangle$. For n spins, the dimension grows frighteningly quickly as 2^n. The tensor-product construction provides *one* way of assembling multiparticle states, but it does not capture all such states (as we'll see in a moment!).

With larger states, we will need larger matrices to serve as operators. Individually, each spin can be "acted on" by the ordinary spin–$\frac{1}{2}$ matrices, but we need a way of representing this single-spin operation as

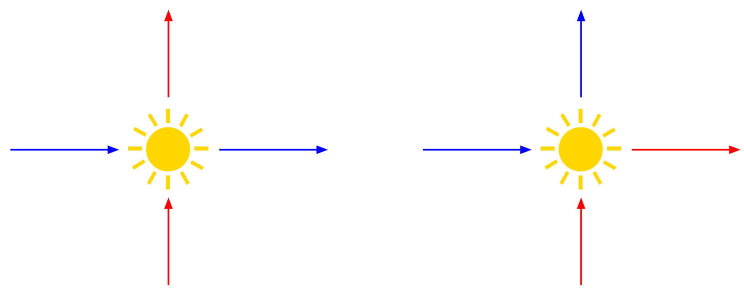

Fig. 1: Classically, it is possible to determine the paths taken by incident particles in a scattering event: the two possibilities depicted are distinguishable. Quantum mechanically, identical particles *cannot* be distinguished and the amplitudes corresponding to the two possibilities *both* contribute to the process.

an action on the full, two-spin state vector. Again, the Kronecker product provides the answer. Applied to matrices,

$$\begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \otimes \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} \equiv \begin{pmatrix} a_1 a_2 & a_1 b_2 & b_1 a_2 & b_1 b_2 \\ a_1 c_2 & a_2 d_2 & b_1 c_2 & b_1 d_2 \\ c_1 a_2 & c_1 b_2 & d_1 a_2 & d_1 b_2 \\ c_1 c_2 & c_1 d_2 & d_1 c_2 & d_1 d_2 \end{pmatrix}. \tag{9}$$

Explicit calculations become cumbersome quickly, so we will make use of `kron()`, which is built into NUMPY. As it pertains to our needs, we use the Kronecker product to define the spin operators acting on individual particles. For example,

$$\hat{S}^x_1 = \hat{S}^x \otimes \hat{I}, \tag{10}$$

represents the ordinary operator $\hat{S}^x$ acting on the first spin with no action (indicated by the identity operator) acting on the second spin. Such an operator has the correct dimension to act on the state vector. When such calculations can be done analytically, it the tensor product property can be used to simplify calculations,

$$\left[\hat{S}^x \otimes \hat{I}\right] \left[|\psi_1\rangle \otimes |\psi_2\rangle\right] = \left[\hat{S}^x |\psi_1\rangle\right] \otimes \left[|\psi_2\rangle\right]. \tag{11}$$

We can also define the *total* spin components,

$$\hat{S}^x = \hat{S}^x_1 + \hat{S}^x_2 = \hat{S}^x \otimes \hat{I} + \hat{I} \otimes \hat{S}^x. \tag{12}$$

Note that Eq. (12) is *not* a simple product of two single-site operators. Its eigenstates therefore might not be simple products of single spin states.

An important concept which arises in quantum mechanics is that of **indistinguishability**. Classically, we can always (hypothetically) "label" the particles in our system. But because all electrons are exactly identical, quantum mechanics takes advantage of this ambiguity and allows for "interference" between classical possibilities.

One consequence of this indistinguishability is that proper two-particle states involving indistinguishable (identical) particles should be possess a certain symmetry with respect to the *exchange* of particles. Let us define the operator $\hat{\Pi}$ as the particle-exchange operator. Its action is to exchange the roles of the spins. That is,

$$\begin{aligned}
\hat{\Pi}\,|+\rangle\,|+\rangle &= |+\rangle\,|+\rangle\,, \\
\hat{\Pi}\,|+\rangle\,|-\rangle &= |-\rangle\,|+\rangle\,, \\
\hat{\Pi}\,|-\rangle\,|+\rangle &= |+\rangle\,|-\rangle\,, \\
\hat{\Pi}\,|-\rangle\,|-\rangle &= |-\rangle\,|-\rangle\,.
\end{aligned} \tag{13}$$

The states $|+\rangle\,|+\rangle$ and $|-\rangle\,|-\rangle$ are invariant under $\hat{\Pi}$, while the mixed states are not. It should be clear upon reflection that $\hat{\Pi}^2 = \hat{I}$, and this requires the eigenvalues of this operator to be ± 1. The eigenstates of $\hat{\Pi}$ are the proper states for two-particle systems. Though the -1 might seem troubling, it is just a phase $e^{\pm i\pi} = -1$ which has no affect on the observables.

1. Consider the basis states $|+\rangle\,|+\rangle$, $|+\rangle\,|-\rangle$, $|-\rangle\,|+\rangle$, $|-\rangle\,|-\rangle$. By hand, calculate these using the single-spin representations

$$|+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{14}$$

   Define representations of $|\pm\rangle$ in your JUPYTER notebook and use `kron()` to verify the tensor products. One way to enter the arrays is

```
u1 = array([1.0,0.0])
u1.shape = (2,1)

u2 = array([0.0,1.0])
u2.shape = (2,1)
```

   The Kronecker product can be called as `kron(u1,u2)`. Does order matter? That is, does `kron(u2,u1)` give the same result?

2. Each of the $|\pm\rangle\,|\pm\rangle$ basis states involves each spin being in a well-defined state of $\hat{S}^z$. If a measurement of $\hat{S}^z = \hat{S}^z_1 + \hat{S}^z_2$ were performed, what would be the value for each of the basis states? You can infer this from the states (adding up the components since they're parallel) or verify numerically. The operator $\hat{S}^z$ follows from

$$\hat{S}^z \;\to\; \texttt{kron(sz,so)+kron(so,sz)}, \tag{15}$$

   where `so = eye(2)` is the identity matrix. The expectation value can be a bit clunky, but one way to write it is

$$\langle\psi|\,\hat{O}\,|\psi\rangle \;\to\; \texttt{asscalar(dot(conj(psi.transpose()),O*psi))}, \tag{16}$$

   where the state vector is `psi` and the matrix representation of the operator is `O`.

3. This question involves the operator $\hat{\Pi}$ whose action is defined by Eq. (13).

   (a) Construct a matrix representation of $\hat{\Pi}$ in the basis $|+\rangle\,|+\rangle$, $|+\rangle\,|-\rangle$, $|-\rangle\,|+\rangle$, $|-\rangle\,|-\rangle$. You can define a matrix of zeros and fill in the nonzero entries (of which there are only a few) using, for example,

```
Pi = matrix(zeros((4,4)))
Pi[0,0] = 1.0
...
```

(b) Show explicitly that $\hat{\Pi}^2 = \hat{I}$.

(c) Obtain the eigenvalues and eigenvectors of $\hat{\Pi}$ corresponding to the "proper" two-particle states which respect the indistinguishability of the spins and group these states by eigenvalue. Use `eigh()`, and observe that the eigenvectors are normalized.

(d) Write the eigenstates of $\hat{\Pi}$ in terms of the basis kets.

4. In the standard basis, construct the operator $\hat{\mathbf{S}}^2$ by using the *total* spin components (e.g., Eq. (12)). Though the basis states are eigenstates of $\hat{S}^z$, they are not necessarily eigenstates of the total (squared) spin operator. Group the eigenvectors by eigenvalue and comment on the following.

   (a) What does the eigenvalue of $\hat{\mathbf{S}}^2$ signify?

   (b) How do the eigenvectors of $\hat{\mathbf{S}}^2$ compare to those of $\hat{\Pi}$?

   (c) The state $\frac{1}{\sqrt{2}}(|+\rangle|-\rangle - |-\rangle|+\rangle)$ is called the **singlet**. Physically, how does it differ from the state $\frac{1}{\sqrt{2}}(|+\rangle|-\rangle + |-\rangle|+\rangle)$?

5. Calculate the expectation values $\langle \hat{S}^z_1 \rangle$, $\langle \hat{S}^z_2 \rangle$ and $\langle \hat{S}^z \otimes \hat{S}^z \rangle$ for the states

   (a) $|+\rangle|+\rangle$

   (b) $\frac{1}{\sqrt{2}}(|+\rangle|-\rangle - |-\rangle|+\rangle)$

   (c) $\frac{1}{\sqrt{2}}(|+\rangle|-\rangle + |-\rangle|+\rangle)$

   (d) $|-\rangle|-\rangle$

6. What does it mean to say states (c) and (d) are *entangled*?