# Chapter 5

## Angular Momentum and Spin

I think you and Uhlenbeck have been very lucky to get your spinning electron published and talked about before Pauli heard of it. It appears that more than a year ago Kronig believed in the spinning electron and worked out something; the first person he showed it to was Pauli. Pauli rediculed the whole thing so much that the first person became also the last ...

- Thompson (in a letter to Goudsmit)

The first experiment that is often mentioned in the context of the electron's spin and magnetic moment is the Einstein–de Haas experiment. It was designed to test Ampère's idea that magnetism is caused by "molecular currents". Such circular currents, while generating a magnetic field, would also contribute to the angular momentum of a ferromagnet. Therefore a change in the direction of the magnetization induced by an external field has to lead to a small rotation of the material in order to preserve the total angular momentum.

For a quantitative understanding of the effect we consider a charged particle of mass mand charge q rotating with velocity v on a circle of radius r. Since the particle passes through its orbit  $v/(2\pi r)$  times per second the resulting current  $I = qv/(2\pi r)$ , which encircles an area  $A = r^2 \pi$ , generates a magnetic dipole moment  $\mu = IA/c$ ,

$$I = \frac{qv}{2\pi r} \qquad \Rightarrow \qquad \mu = \frac{IA}{c} = \frac{qv r^2 \pi}{2\pi r c} = \frac{qvr}{2c} = \frac{q}{2mc}L = \gamma L, \qquad \gamma = \frac{q}{2mc}, \tag{5.1}$$

where  $\vec{L} = m\vec{r} \times \vec{v}$  is the angular momentum. Now the essential observation is that the **gyromagnetic ratio**  $\gamma = \mu/L$  is independent of the radius of the motion. For an arbitrary distribution of electrons with mass  $m_e$  and elementary charge e we hence expect

$$\vec{\mu}_e = g \,\mu_B \,\frac{\vec{L}}{\hbar} \qquad \text{with} \qquad \mu_B = \frac{e\hbar}{2m_e c},$$
(5.2)



Figure 5.1: Splitting of a beam of silver atoms in an inhomogeneous magnetic field.

where the **Bohr magneton**  $\mu_B$  is the expected ratio between the magnetic moment  $\vec{\mu}_e$  and the dimensionless value  $\vec{L}/\hbar$  of the angular momentum. The **g-factor** parametrizes deviations from the expected value g = 1, which could arise, for example, if the charge density distribution differs from the mass density distribution. The experimental result of Albert Einstein and Wander Johannes de Haas in 1915 seemed to be in agreement with Lorentz's theory that the rotating particles causing ferromagnetism are electrons.<sup>1</sup>

Classical ideas about angular momenta and magnetic moments of particles were shattered by the results of the experiment of Otto Stern and Walther Gerlach in 1922, who sent a beam of Silver atoms through an inhomogeneous magnetic field and observed a split into two beams as shown in *fig. 5.1*. The magnetic interaction energy of a dipole  $\vec{\mu}$  in a magnetic field  $\vec{B}$  is

$$E = \vec{\mu}\vec{B} = \gamma\vec{L}\vec{B} \tag{5.3}$$

which imposes a force  $\vec{F} = -\vec{\nabla}(\vec{\mu}\vec{B})$  on the dipole. If the beam of particles with magnetic dipoles  $\vec{\mu}$  passes through the central region where  $B_z \gg B_x, B_y$  and  $\frac{\partial B_z}{\partial z} \gg \frac{\partial B_z}{\partial x}, \frac{\partial B_z}{\partial y}$  the force

$$F_z \approx -\gamma L_z \frac{\partial B_z}{\partial z} \tag{5.4}$$

<sup>&</sup>lt;sup>1</sup> The experiment was repeated by Emil Beck in 1919 who found "very precisely half of the expected value" for  $L/\mu$ , which we now know is correct. At that time, however, g was still believed to be equal to 1. As a result Emil Beck only got a job as a high school teacher while de Haas continued his scientific career in Leiden.

points along the z-axis. It is proportional to the gradient of the magnetic field, which hence needs to be inhomogeneous. For an unpolarized beam the classical expectation would be a continuous spreading of deflections. Quantum mechanically, any orbital angular momentum  $L_z$ would be quantized as  $L_z = m\hbar$  with an odd number  $m = -l, 1 - l, \ldots, l - 1, l$  of split beams. But Stern and Gerlach observed, instead, *two* distinct lines as shown in *fig. 5.2*.



Figure 5.2: Stern and Gerlach observed two distinct beams rather than a classical continuum.

In 1924 Wolfgang Pauli postulated two-valued quantum degrees of freedom when he formulated his exclution principle, but he first opposed the idea of rotating electrons. In 1926 Samuel A. Goudsmit and George E. Uhlenbeck used that idea, however, to successfully guess formulas for the hyperfine splitting of spectral lines,<sup>2</sup> which involved the correct spin quantum numbers. Pauli pointet out an apparent discrepancy by a factor of two between theory and experiment, but this issue was resolved by Llewellyn Thomas. Thus Pauli dropped his objections and formalized the quantum mechanical theory of spin in 1927.

The unexpected experimental value g = 2 for the electron's g-factor could only be understood in 1928 when Paul A.M. Dirac found the relativistic generalization of the Schrödinger equation, which we will discuss in chapter 7. Almost 20 years later, Raby et al. discovered a deviation of the magnetic moment from Dirac theory in 1947, and at the same time Lamb et al. reported similar effects in the spectral lines of certain atomic transitions. By the end of that year Julian Schwinger had computed the leading quantum field theoretical correction  $a_e$ to the quantum mechanical value,

$$g/2 \equiv 1 + a_e = 1 + \frac{\alpha}{2\pi} + \mathcal{O}(\alpha^2) = 1 + 0.001161 + \mathcal{O}(\alpha^2)$$
(5.5)

and within a few years Schwinger, Feynman, Dyson, Tomonaga and others developed quantum electrodynamics (QED), the quantum field theory (QFT) of electrons and photons, to a level that allowed the consistent computation of perturbative corrections. Present theoretical calculations of the anomalous magnetic moment  $a_e$  of the electron, which include terms through order  $\alpha^4$ , also need to take into account corrections due to strong and weak nuclear forces. The impressive agreement with the experimental result

$$h_e = \begin{cases} 0.001\,159\,652\,1884\ (43) & \text{experimental} \\ 0.001\,159\,652\,2012\ (27) & \text{theory}\ (\text{QFT}) \end{cases}$$
(5.6)

<sup>&</sup>lt;sup>2</sup> The history as told by Goudsmit can be found in his very recommendable jubilee lecture, whose transcript is available at http://www.lorentz.leidenuniv.nl/history/spin/goudsmit.html.

shows the remarkable precision of QFT, which is the theoretical basis of elementary particle physics. Modern precision experiments measure  $a_e$  in Penning traps, which are axially symmetric combinations of a strong homogeneous magnetic field with an electric quadrupole, in which single particles or ions can be trapped, stored and worked with for several weeks.<sup>3</sup>

## 5.1 Quantization of angular momenta

Compelled by the experimental facts discussed above we now investigate general properties of angular momenta in order to find out how to describe particles with spin  $\hbar/2$ . In the previous chapter we found the commutation relations

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \qquad \Rightarrow \qquad [\vec{L}^2, L_i] = 0 \tag{5.7}$$

of the *orbital* angular momentum  $\vec{L} = \vec{X} \times \vec{P}$  with eigenfunctions  $Y_{lm}$  and eigenvalues

$$\vec{L}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}, \qquad L_z Y_{lm} = \hbar m Y_{lm}$$
(5.8)

of  $\vec{L}^2$  and  $L_z$  so that all states with total angular momentum quantum number l come in an odd number 2l + 1 of incarnations with magnetic quantum number  $m = -l, \ldots l$ . We thus want to understand how the electron can have an even number *two* of incarnations, as is implied by the Stern–Gerlach experiment and also by the double occupation of orbitals allowed by the Pauli principle.

If we think of the total angular momentum  $\vec{J} = \vec{L} + \vec{S}$  as the sum of a (by now familiar) orbital part  $\vec{L}$  and an (abstract) spin operator  $\vec{S}$  then it is natural to expect that the total angular momentum  $\vec{J}$  should obey the same kind of commutation relations

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k \qquad \Rightarrow \qquad [\vec{J}^2, J_i] = 0 \tag{5.9}$$

so that, for example, the commutator with  $\frac{1}{i\hbar}J_z$  rotates  $J_x$  into  $J_y$  and  $J_y$  into  $-J_x$ . We will now refrain, however, from a concrete interpretation of  $\vec{J}$  and call any collection of three selfadjoint operators  $J_i = J_i^{\dagger}$  obeying (5.9) an *angular momentum algebra*. Like in the case of the harmonic oscillator we will see that this algebra is sufficient to determine all eigenstates, which

<sup>&</sup>lt;sup>3</sup> The high precision of almost 12 digits can be achieved because  $1 + a_e = \omega_s/\omega_c$  is the ratio of two frequencies, the spin flip frequency  $\omega_s = g\mu_B B_z/\hbar$  and the cyclotron frequency  $\omega_c = \frac{e}{m_e c} B_z$ , and independent of the precise value of  $B_z$ . The cyclotron frequeny corresonds to the energy spacings between the Landau levels of electrons circling in a magnetic field: Landau invented a nice trick for the computation of the associated energy quanta: If we use the gauge  $\vec{A} = B_z X \vec{e_y}$  for a magnetic field  $\vec{B} = B_z \vec{e_z}$  in z-direction then the Hamiltonian becomes  $H = \frac{1}{2m_e} \left(P_x^2 + (P_y - \frac{e}{c}B_z X)^2 + P_z^2\right)$ . The operators  $P_x$  and  $\tilde{X} = X - \frac{c}{eB_z}P_y$ , which determine the dynamics in the xy-plan via the Hamiltonian  $H_{xy} = \frac{1}{2m_e}P_x^2 + \frac{e^2B_z^2}{2m_e c^2}\tilde{X}^2$  of a harmonic oscillator, obviously satisfy a Heisenberg algebra  $[P_x, \tilde{X}] = \frac{\hbar}{i}$ . Recalling the (algebraic) solution of the harmonic oscillator we thus obtain the energy eigenvalues  $E_n = (n + \frac{1}{2})\hbar\omega_c$  of the Landau levels with  $\omega_c = \frac{eB_z}{m_e c} = 2\mu_B B_z/\hbar$  [Landau-Lifschitz].

we denote by  $|j, \mu\rangle$ . The eigenvalues of the maximal commuting set of operators  $J^2$  and  $J_z$  can be parametrized as

$$\vec{J}^{2}|j,\mu\rangle = \hbar^{2}j(j+1)|j,\mu\rangle$$
(5.10)

$$J_z |j,\mu\rangle = \hbar \mu |j,\mu\rangle \tag{5.11}$$

with  $j \ge 0$  because  $\vec{J}^2$  is non-negative. We also impose the normalization  $\langle j', \mu' | j, \mu \rangle = \delta_{jj'} \delta_{\mu\mu'}$ , where orthogonality for different eigenvalues is implied by  $J_i^{\dagger} = J_i$ .

**Ladder Operators.** As usual in quantum mechanics the general strategy is to diagonalize as many operators as possible. In order to diagonalize the action of  $J_z$ , i.e. a rotation in the *xy*-plane, we define the ladder operators

$$J_{\pm} = J_x \pm i J_y, \tag{5.12}$$

where an analogy with the Harmonic oscillator would relate H to  $J_3$  and  $(\mathcal{X}, \mathcal{P})$  to  $(J_x, J_y)$ , which are transformed into one another by the commutator with H and  $J_3$ , respectively. In any case we find

$$[J_z, J_{\pm}] = [J_z, J_x] \pm i[J_z, J_y] = i\hbar J_y \mp i(i\hbar)J_x = \pm\hbar J_{\pm}$$
(5.13)

and

$$[J_+, J_-] = [J_x + iJ_y, J_x - iJ_y] = -i[J_x, J_y] + i[J_y, J_x] = 2\hbar J_z.$$
(5.14)

Since  $[J_z, J_{\pm}] = \pm \hbar J_{\pm}$  the ladder operators  $J_{\pm}$  shift the eigenvalues of  $J_z$  by  $\pm \hbar$ ,

$$J_z \ J_{\pm} |j,\mu\rangle = (J_{\pm}J_z \pm \hbar J_{\pm})|j,\mu\rangle = \hbar(\mu \pm 1) \ J_{\pm}|j,\mu\rangle, \tag{5.15}$$

so that

$$J_{\pm} |j,\mu\rangle = N_{\pm} |j,\mu\pm1\rangle.$$
 (5.16)

Since the eigenstates  $|j,\mu\rangle$  are normalized by assumption, the normalization factors  $N_{\pm}$  can be computed by evaluating the norms

$$||(J_{\pm}|j,\mu\rangle)||^{2} = \langle j,\mu|J_{\mp}J_{\pm}|j,\mu\rangle = |N_{\pm}|^{2}\langle j,\mu\pm1|j,\mu\pm1\rangle = |N_{\pm}|^{2},$$
(5.17)

where we used that  $J_{\pm}^{\dagger} = J_{\mp}$ . The expectation values of  $J_{\mp}J_{\pm}$  are evaluated by relating these operators to  $J^2$  and  $J_z$ . We first compute

$$J_{\pm}J_{\pm} = (J_x \pm iJ_y)(J_x \pm iJ_y) = J_x^2 + J_y^2 \pm i[J_x, J_y] = J_x^2 + J_y^2 \pm \hbar J_z$$
(5.18)

and since  $J^2 = J_x^2 + J_y^2 + J_z^2$  we can express everything in terms of the diagonalized operators

$$J_{\pm}J_{\pm} = J^2 - J_z^2 \mp \hbar J_z \tag{5.19}$$

and obtain

$$|N_{\pm}|^{2} = \hbar^{2} \left( j(j+1) - \mu(\mu \pm 1) \right) = \hbar^{2} \left( j \mp \mu \right) (j \pm \mu + 1)$$
(5.20)

so that we end up with the important formula

$$J_{\pm} |j,\mu\rangle = \hbar \sqrt{(j \mp \mu)(j \pm \mu + 1)} |j,\mu \pm 1\rangle$$
(5.21)

for the ladder operators in the basis  $|j, \mu\rangle$ .

Quantization. The quantization condition for j can now be derived as follows. Since  $J_x^2$  and  $J_y^2$  are positive operators  $J^2 = J_x^2 + J_y^2 + J_z^2 \ge J_z^2$ , so that all eigenvalues of  $J_z^2$  are bounded by the eigenvalue of  $J^2$ ,

$$|\mu| \le \sqrt{j(j+1)}.\tag{5.22}$$

For fixed total angular momentum quantum number j we conclude that  $\mu$  is bounded from below and from above. Since the ladder operators  $J_{\pm}$  do not change j, repeated raising and repeated lowering must both terminate,

$$J_{+} |j, \mu_{max}\rangle = 0, \qquad J_{-} |j, \mu_{min}\rangle = 0.$$
 (5.23)

But this implies

$$J_{-}J_{+} |j, \mu_{max}\rangle = |N_{+}|^{2} |j, \mu_{max}\rangle = 0, \qquad (5.24)$$

$$J_{+}J_{-} |j, \mu_{min}\rangle = |N_{-}|^{2} |j, \mu_{min}\rangle = 0, \qquad (5.25)$$

and hence

$$\mu_{min} = -j, \quad \mu_{max} = j, \qquad \mu_{max} - \mu_{min} = 2j \in \mathbb{N}_0$$
 (5.26)

where 2j must be a non-negative integer because we get from  $|j, \mu_{min}\rangle$  to  $|j, \mu_{max}\rangle$  with  $(J_+)^k$ for  $k = \mu_{max} - \mu_{min} = 2j$ . We thus have shown that quantum mechanical spins are quantized in half-integral units  $j \in \frac{1}{2}\mathbb{N}_0$  with  $\mu$  ranging from -j to j in integral steps. The magnetic quantum number hence can have 2j + 1 different values for fixed total angular momentum. In particular, a doublet like observed in Stern–Gerlach is consistent and implies j = 1/2.

Naively one might expect that the eigenvalue of  $J^2$  is the square of the maximal eigenvalue of  $J_z$ . But this is not possible because of an uncertainty relation, as can be seen from the following chain of inequalities:

$$J^{2} = J_{x}^{2} + J_{y}^{2} + J_{z}^{2} \ge J_{z}^{2} + (\Delta J_{x})^{2} + (\Delta J_{y})^{2} \ge J_{z}^{2} + 2\Delta J_{x} \Delta J_{y}$$
(5.27)

because  $A^2 = (\Delta A)^2 + (\langle \Delta A \rangle)^2 \ge (\Delta A)^2$  and  $(a - b)^2 = a^2 + b^2 - 2ab \ge 0$ . Combining this with the uncertainty relation  $\Delta J_x \Delta J_y \ge \frac{1}{2} |\langle [J_x, J_y] \rangle|$ , where  $[J_x, J_y] = i\hbar J_z$ , we obtain

$$J^{2} \ge J_{z}^{2} + \hbar |J_{z}| = \hbar^{2} (\mu^{2} + |\mu|).$$
(5.28)

This explains our parametrization of the eigenvalue of  $J^2$  as  $\hbar^2 j(j+1)$  and the above derivation of the eigenvalue spectrum shows that the inequality is saturated for  $\mu_{max} = j$  and  $\mu_{min} = -j$ . We conclude that it does not make sense to think of the angular momentum of a particle as pointing into a particular direction: Due to the uncertainty relation between  $J_i$  and  $J_j$  for  $i \neq j$ it is impossible to simultaneously measure different components of the angular moment, just like it is impossible to measure position and momentum of a particle simultaneously. Expectation values  $\langle \psi | \vec{J} | \psi \rangle$ , on the other hand, are usual vectors that do point into a particular direction.

### 5.2 Electron spin and the Pauli equation

According to general arguments of rotational invariance and angular momentum conservation we expect that the total angular momentum  $\vec{J} = \vec{L} + \vec{S}$  is the sum of an intrinsic and an orbital part, which can be measured independently and hence ought to commute,

$$\vec{J} = \vec{L} + \vec{S}, \qquad [L_i, S_j] = 0.$$
 (5.29)

Moreover, each of these angular momentum vectors obeys the same kind of algebra

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k, \qquad [L_i, L_j] = i\hbar\varepsilon_{ijk}L_k, \qquad [S_i, S_j] = i\hbar\varepsilon_{ijk}S_k. \tag{5.30}$$

and transforms as a vector under a rotation of the complete system (i.e. of the position *and* of the spin of a particle)

$$[J_i, L_j] = i\hbar\varepsilon_{ijk}L_k, \qquad [J_i, S_j] = i\hbar\varepsilon_{ijk}S_k, \qquad [J_i, J_j] = i\hbar\varepsilon_{ijk}J_k.$$
(5.31)

More generally, we can decompose the total angular momentum into a sum of (commuting) contributions of independent subsystems  $\vec{J} = \sum_i \vec{L}_{(i)} + \sum_i \vec{S}_{(i)}$  for systems composed of several spinning particles with respective orbital angular momenta  $\vec{L}_{(i)} = \vec{X}_{(i)} \times \vec{P}_{(i)}$  and spins  $\vec{S}_{(i)}$ .

We now focus on the spin degree of freedom and consider the case  $s = \frac{1}{2}$  that is relevant for electrons, protons and neutrons. The basis in which  $S^2$  and  $S_z$  are diagonal consists of two states  $|\frac{1}{2}, \pm \frac{1}{2}\rangle$  which span the Hilbert space  $\mathcal{H} = \mathbb{C}^2$ . We can hence identify  $|\frac{1}{2}, \pm \frac{1}{2}\rangle$  with the natural basis vectors  $e_1 = {1 \choose 0}$  and  $e_2 = {0 \choose 1}$ . In order to save some writing it is useful to introduce the abbreviations  $|\pm\rangle = |\frac{1}{2}, \pm \frac{1}{2}\rangle$  and

$$\left|\frac{1}{2}, +\frac{1}{2}\right\rangle = \left|+\right\rangle = \left|\uparrow\right\rangle \equiv \begin{pmatrix}1\\0\end{pmatrix}, \qquad \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \left|-\right\rangle = \left|\downarrow\right\rangle \equiv \begin{pmatrix}0\\1\end{pmatrix}. \tag{5.32}$$

According to (5.21) the action of the spin operators is

 $S_z|\uparrow\rangle = +\frac{\hbar}{2}|\uparrow\rangle, \qquad S_+|\uparrow\rangle = 0, \qquad \qquad S_-|\uparrow\rangle = \hbar|\downarrow\rangle$  (5.33)

$$S_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle, \qquad S_+|\downarrow\rangle = \hbar|\uparrow\rangle, \qquad S_-|\downarrow\rangle = 0$$
(5.34)

which corresponds to the matrices

$$S_{z} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad S_{+} = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad S_{-} = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{5.35}$$

in the natural basis. Solving  $S_{\pm} = S_x \pm iS_y$  for  $S_x = \frac{1}{2}(S_+ + S_-)$  and  $S_y = \frac{1}{2i}(S_+ - S_-)$  we find

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix}, \qquad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i\\ i & 0 \end{pmatrix}, \qquad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix}.$$
(5.36)

We hence can write the spin operator as

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma} \tag{5.37}$$

where  $\vec{\sigma}$  are the **Pauli–matrices** 

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.38}$$

The  $\sigma$ -matrices obey the following equivalent sets of identities,

$$(\sigma_i)^2 = 1, \qquad \sigma_i \sigma_j = -\sigma_j \sigma_i = i \varepsilon_{ijk} \sigma_k \quad \text{for} \quad i \neq j,$$

$$(5.39)$$

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}, \qquad [\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k, \tag{5.40}$$

$$\sigma_i \sigma_j = \delta_{ij} \mathbb{1} + i \varepsilon_{ijk} \sigma_k.$$
(5.41)

They are traceless,

$$\operatorname{tr} \sigma_i = 0, \qquad \operatorname{tr} \sigma_i \sigma_j = 2\delta_{ij}, \tag{5.42}$$

and it is easily checked for Hermitan  $2 \times 2$  matrices  $A = A^{\dagger}$  that

$$A = \frac{1}{2} \left( \mathbb{1} \operatorname{tr} A + \vec{\sigma} \operatorname{tr} (A\vec{\sigma}) \right), \qquad (5.43)$$

where  $\vec{\sigma} \operatorname{tr} A \vec{\sigma} \equiv \sum_{i=1}^{3} \sigma_i \operatorname{tr} A \sigma_i$  is a linear combination of the three matrices  $\sigma_i$  with coefficients  $\operatorname{tr}(A\sigma_i)$ . The Pauli matrices hence form a basis for the 3-dimensional linear space of all traceless Hermitian  $2 \times 2$  matrices.

The complete state of an electron is now specified by the position and spin degrees of freedom  $|\vec{x} \in \mathbb{R}^3, s = \frac{1}{2}, \mu = \pm \frac{1}{2}\rangle$ . Once we agree that electrons have spin  $s = \frac{1}{2}$  we can omit this redundant information. In the  $S_z$  basis we find

$$|\psi\rangle = \sum_{\substack{\mu=\pm\\x\in\mathbb{R}^3}} |x,\mu\rangle\langle x,\mu|\psi\rangle = \psi_+(x) |\frac{1}{2},\frac{1}{2}\rangle + \psi_-(x) |\frac{1}{2},-\frac{1}{2}\rangle = \psi_+(x)|\uparrow\rangle + \psi_-(x)|\downarrow\rangle = \begin{pmatrix}\psi_+(x)\\\psi_-(x)\end{pmatrix},$$
(5.44)

i.e. the spinning electron is described by two wave functions  $\psi_{\pm}(x)$ .<sup>4</sup>

<sup>&</sup>lt;sup>4</sup> More familiarly, a vector field  $\vec{v}(x)$ , i.e. a wave function with spin 1, is described by *three* component functions  $v_i(x)$ .

#### 5.2.1 Magnetic fields: Pauli equation and spin-orbit coupling

Due to the experimental value g = 2 the total magnetic moment of the electron is

$$\vec{\mu}_{total} = \frac{e}{2m_e c} \left( \vec{L} + 2\vec{S} \right) = \frac{e}{2m_e c} \left( \vec{L} + \hbar \vec{\sigma} \right)$$
(5.45)

and the corresponding interaction energy with a magnetic field is

$$H_{int} = \vec{\mu}_{total}\vec{B} = \mu_B \left(\frac{1}{\hbar}\vec{L} + \vec{\sigma}\right)\vec{B} = \frac{\mu_B}{\hbar} \left(\vec{L} + 2\vec{S}\right)\vec{B},\tag{5.46}$$

where  $\mu_B = \frac{e\hbar}{2m_e c}$  is the Bohr magneton. The complete Hamiltonian thus becomes

$$H_{Pauli} = \frac{\vec{P}^{\,2}}{2m} + V(\vec{x}) + \frac{\mu_B}{\hbar} \left(\vec{L} + 2\vec{S}\right) \vec{B}.$$
(5.47)

The corresponding Schrödinger equation is called **Pauli equation** (without spin-orbit coupling)

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\vec{\hbar}^2}{2m}\Delta + V(\vec{x}) + \frac{\mu_B}{\hbar}\left(\vec{L} + 2\vec{S}\right)\vec{B}\right)\psi,\tag{5.48}$$

which is a system of differential equations for the two components  $\psi_{\pm}(x)$  of the wave function **spinor**  $\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$  that are coupled by the magnetic interaction term  $\vec{S}\vec{B}$ .

**Spin–Orbit coupling.** When an electron moves with a velocity  $\vec{v}$  in the electric field produced by a nucleus it observes, in its own frame of reference, a modified magnetic field according to the transformation rule

$$\vec{B}' = \vec{B} - \frac{1}{c} \left( \vec{v} \times \vec{E} \right), \tag{5.49}$$

where  $\vec{B}$  is the magnetic field in the rest frame (of the nucleus). We can therefore try to take into account relativistic corrections to the Pauli equation by considering the interaction of this field with the magnetic moment  $\vec{\mu}_e = \frac{e}{m_e c} \vec{S}$  of the electron.

If we ignore the weak magnetic field of the nucleus<sup>5</sup>  $\vec{B} \approx 0$  then its electric field

$$\vec{E} = \frac{1}{e} \frac{dV}{dr} \frac{\vec{x}}{r} \tag{5.50}$$

induces a velocity-dependent magnetic field

$$\vec{B}' = -\frac{1}{ecr} \frac{dV}{dr} \underbrace{(\vec{v} \times \vec{x})}_{=-\frac{1}{m_e} \vec{L}} = \frac{1}{ecr} \frac{dV}{dr} \left(\frac{1}{m_e} \vec{L}\right).$$
(5.51)

The corresponding interaction energy  $\Delta E = \vec{\mu}_e \vec{B}'$  suggests the spin-orbit correction

$$\vec{\mu}_e = \frac{e}{m_e c} \vec{S} \qquad \Rightarrow \qquad \Delta E_{\text{naiv}} = \frac{1}{m_e^2 c^2 r} \frac{dV}{dr} \left(\vec{L}\vec{S}\right).$$
 (5.52)

<sup>&</sup>lt;sup>5</sup> Note that the magnetic moment  $\mu = g \frac{q}{2mc}$  is proportional to the inverse mass.

The correct **spin-orbit interaction** energy differs from this by a factor  $\frac{1}{2}$  and will be derived from the fully relativistic Dirac equation in chapter 7,

$$H_{SO} = \frac{1}{2m_e^2 c^2 r} \frac{dV}{dr} \left(\vec{L}\vec{S}\right) = \frac{1}{2m_e^2 c^2} \vec{L}\vec{S} \frac{Ze^2}{r^3}$$
(5.53)

where Z is the atomic number of the nucleus.

### 5.3 Addition of Angular Momenta

The spin-orbit interaction is an instance of the more general phenomenon that angular momenta  $\vec{J}_1$  and  $\vec{J}_2$  coming from different degrees of freedom interact so that only the total angular momentum  $\vec{J} = \vec{J}_1 + \vec{J}_2$  is conserved. In order to be able to take advantage of this conservation it is therefore necessary to reorganize the Hilbert space spanned by the  $N = (2j_1 + 1)(2j_2 + 1)$  states  $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$  into a new basis  $|j, m, \ldots\rangle$  in which

$$\vec{J}^2 = \vec{J}_1^2 + \vec{J}_2^2 + 2\vec{J}_1\vec{J}_2$$
 and  $J_z = J_{1z} + J_{2z}$  (5.54)

are diagonal. In order to simplify the notation we use, in the present section, the indices 1 and 2 exclusively to label the angular momenta  $\vec{J_1}$  and  $\vec{J_2}$ , and we use x, y, z to label the different components. Since

$$[\vec{J}_1 \vec{J}_2, J_{1z}] = [J_{1x}, J_{1z}]J_{2x} + [J_{1y}, J_{1z}]J_{2y} = -i\hbar J_{1y}J_{2x} + i\hbar J_{1x}J_{2y}$$
(5.55)

the commutator

$$[J^2, J_{1z}] = 2i\hbar(J_{1x}J_{2y} - J_{1y}J_{2x}) = -[J^2, J_{2z}]$$
(5.56)

is non-zero so that we can not diagonalize  $J_{1z}$  or  $J_{2z}$  simultaneously with  $J^2$  and  $J_z$ . But  $\vec{J}_1^2$ and  $\vec{J}_2^2$  both commute with  $J^2$  and  $J_z$  and we can continue to use their eigenvalues to label the states in the new basis by  $|j, m, j_1, j_2\rangle$  with

$$J^{2} |j, m, j_{1}, j_{2}\rangle = \hbar^{2} j(j+1) |j, m, j_{1}, j_{2}\rangle, \qquad (5.57)$$

$$J_z |j, m, j_1, j_2\rangle = \hbar m \qquad |j, m, j_1, j_2\rangle, \qquad (5.58)$$

$$J_1^2 |j, m, j_1, j_2\rangle = \hbar^2 j_1(j_1 + 1) |j, m, j_1, j_2\rangle, \qquad (5.59)$$

$$J_2^2 |j, m, j_1, j_2\rangle = \hbar^2 j_2(j_2 + 1) |j, m, j_1, j_2\rangle.$$
(5.60)

During the course of our analysis we will show that j and m completely characterize the new basis so that no further independent commuting operators exist. For fixed j the angular momentum algebra implies that all magnetic quantum numbers with  $-j \leq m \leq j$  are present and all of them can be obtained from a single one by repeated application of the ladder operators  $J_{\pm}$ . Such a **multiplet** of 2j + 1 states is called an **irreducible representation**  $R_j$  of the

$m = m_1 + m_2$	number of states	$m_{\blacktriangle}$	
$j_1 + j_2$	1	imar	$ \qquad \qquad  j_1,j_1\rangle\otimes j_2,j_2\rangle $
$j_1 + j_2 - 1$	2	5111000	$\checkmark J_{-}( j_1,j_1\rangle \otimes  j_2,j_2\rangle)$
$j_1 + j_2 - 2$	3		
$j_1 - j_2 + 1$	$2j_2$		
$j_1 - j_2$	$2j_2 + 1$	$+ j_{min}$	
$j_1 - j_2 - 1$	$2j_2 + 1$		
		<b>+</b> 0	
$-j_1 + j_2 + 1$	$2j_2 + 1$		
$-j_1 + j_2$	$2j_2 + 1$	$-j_{min}$	
$-j_1 + j_2 - 1$	$2j_2$		
$-j_1 - j_2 + 2$	3		
$-j_1 - j_2 + 1$	2		
$-j_1 - j_2$	1	$-j_{max}$	j

Table 5.1: Reorganization of the Hilbert space of states  $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$ .

angular momentum algebra and the change of basis that we are about to construct is called a decomposition of the tensor product  $R_{j_1} \otimes R_{j_2}$  into a direct sum of irreducible representations  $R_j$ . The result of our analysis will be that  $|j_1 - j_2| \leq j \leq j_1 + j_2$ .

For fixed  $j_1$  and  $j_2$  there are  $2j_1 + 1$  different values of  $m_1$  and  $2j_2 + 1$  different values of  $m_2$ . Since  $J_z = J_{1z} + J_{2z}$  the eigenvalues in the old basis  $|j_1j_2m_1m_2\rangle = |j_1m_1\rangle \otimes |j_2m_2\rangle$  and in the new basis  $|jj_1j_2m\rangle$  are related by  $m = m_1 + m_2$ , but since  $[J^2, J_{1z}] \neq 0$  a specific vector  $|j_1j_2m_1m_2\rangle$  may contribute to states with different total angular momentum j. In order to find the possible values of j and the linear combinations of the eigenstates of  $J_{1z}$  and  $J_{2z}$  that are eigenstates of  $J^2$  we organize the Hilbert space according to the total magnetic quantum number m, as shown in table 5.1. For fixed m we draw as many boxes in the respective row as there are independent combinations  $m_1 + m_2 = m$  with  $|m_1| \leq j_1$  and  $|m_2| \leq j_2$ . The numbers of boxes in one row are listed for the case  $j_1 \geq j_2$  (otherwise exchange  $J_1$  and  $J_2$ ).

The next step is to understand the horizontal position of the boxes along the *j*-axis between  $j_{min} = |j_1 - j_2|$  and  $j_{max} = j_1 + j_2$ . For the maximal value  $j_1 + j_2$  of *m* there is only one box, which corresponds to the state  $|j_1m_1\rangle \otimes |j_2m_2\rangle$ . This box must belong to a spin multiplet  $R_j$  with angular momentum  $j = j_1 + j_2$  because  $j \ge m = j_1 + j_2$  and for a larger value of *j* a state with a larger value of *m* would have to exist. Hence  $j_{max} = m_{1max} + m_{2max}$  and  $|j_{max}, m_{max}\rangle = |j_1, j_2, m_{1max}, m_{2max}\rangle$ . Having identified the state  $|j, m\rangle$  with  $j = m = j_1 + j_2$  we can obtain all other states of  $R_{j_{max}}$  by repeated application of the lowering operator  $J_- = J_{1-} + J_{2-}$  with

$$(J_{-})^{k}|j_{1}+j_{2},j_{1}+j_{2}\rangle = (J_{1-}+J_{2-})^{k}|j_{1},j_{2},j_{1},j_{2}\rangle = \sum_{l=0}^{k} {\binom{k}{l}}(J_{1-})^{l}|j_{1}j_{1}\rangle \otimes (J_{2-})^{k-l}|j_{2}j_{2}\rangle.$$
(5.61)

Iterating the formula (5.21) we find  $J_{-}^{k}|j,j\rangle = \hbar^{k} k! \sqrt{\binom{2j}{k}} |j,j-k\rangle$ . With  $m = j_{1} + j_{2} - k$ ,  $m_{1} = j_{1} - l$  and  $m_{2} = j_{2} - k + l = m - m_{1}$  we hence obtain

$$\sqrt{\binom{2j_1+2j_2}{j_1+j_2-m}} |j_1+j_2,m\rangle = \sum_{m_1+m_2=m} \sqrt{\binom{2j_1}{j_1-m_1}} |j_1,m_1\rangle \otimes \sqrt{\binom{2j_2}{j_2-m_2}} |j_2,m_2\rangle.$$
(5.62)

If we now remove the  $2j_1 + 2j_2 + 1$  states of the form (5.62), i.e. the last column in table 5.1, then the important observation is that we are left with a single box of maximal m, which now is  $m_{max} = j' = j_1 + j_2 - 1$ . Repeating the above argument we hence conclude that there is a unique angular momentum multiplet  $R_{j'}$ . The state with the largest magnetic quantum number  $|j', j'\rangle$  is determined by orthogonality to the state  $|j_1 + j_2, j_1 + j_2 - 1\rangle$  in (5.62), which has the same magnetic quantum number m = j' but a different total angular momentum. Iteration of this procedure until all states are exhausted shows that there is a unique multiplet with total angular momentum j with

$$|j_1 - j_2| \le j \le j_1 + j_2. \tag{5.63}$$

As a check we count the number of states in the new basis. Assuming  $j_1 \ge j_2$  the number of columns in table 5.1 is  $2j_2 + 1$  and

$$\sum_{j=j_1-j_2}^{j_1+j_2} (2j+1) = (2j_2+1) \frac{(2j_1+2j_2+1)+(2j_1-2j_2+1)}{2} = (2j_1+1)(2j_2+1)$$
(5.64)

in accord with the dimension of the tensor product. Having determined the range of eigenvalues of  $J^2$  and having established their non-degeneracy we now turn to the discussion of the unitary change of basis.

#### 5.3.1 Clebsch-Gordan coefficients

The matrix elements  $\langle j_1 j_2 m_1 m_2 | j m j_1 j_2 \rangle$  of the unitary change of basis

$$|jmj_{1}j_{2}\rangle = \sum_{m_{1}+m_{2}=m} |j_{1}j_{2}m_{1}m_{2}\rangle \langle j_{1}j_{2}m_{1}m_{2}|jmj_{1}j_{2}\rangle$$
(5.65)

are called Clebsch–Gordan (CG) coefficients, for which a number of notations is used,

$$\langle j_1 j_2 m_1 m_2 | j m j_1 j_2 \rangle \equiv \langle j_1 j_2 m_1 m_2 | j m \rangle \equiv C_{m_1 m_2 m}^{j_1 j_2 j} \equiv C_{m_1 m_2}^j.$$
 (5.66)

For the shorthand notation  $C_{m_1m_2}^j$  the values  $j_1, j_2$  must be known from the context; also the order of the quantum numbers and the index position may vary. Note that the elements of the CG matrix can be chosen to be real, so that the CG matrix becomes orthogonal.

In chapter 6 we will need to know the CG coefficients for the total angular momentum  $\vec{J} = \vec{L} + \vec{S}$  of a spin $-\frac{1}{2}$  particle. From (5.62) we can read off the CG coefficients

$$\langle j_1 j_2 m_1 m_2 | jm \rangle = \sqrt{\binom{2j_1}{j_1 - m_1} \binom{2j_2}{j_2 - m_2} / \binom{2j}{j - m}} \quad \text{for} \quad j = j_1 + j_2.$$
 (5.67)

Specializing to the case  $j_1 = l$  and  $j_2 = \frac{1}{2}$ , so that  $m_s = \pm \frac{1}{2}$  and  $m_l = m_j \mp \frac{1}{2}$ , we observe that  $\binom{2s}{s\pm m_s} = 1$  and

$$\binom{2l}{l-m_l} / \binom{2j}{j-m_j} = \frac{(2l)!}{(l-m_l)!(l+m_l)!} \frac{(j-m_j)!(j+m_j)!}{(2l+1)!},$$
(5.68)

which yields the first line of the orthogonal matrix

$$\begin{array}{c|cccc}
C_{m_l,m_s}^j & m_s = \frac{1}{2} & m_s = -\frac{1}{2} \\
j = l + \frac{1}{2} & \sqrt{\frac{l + m_j + 1/2}{2l + 1}} & \sqrt{\frac{l - m_j + 1/2}{2l + 1}} \\
j = l - \frac{1}{2} & -\sqrt{\frac{l - m_j + 1/2}{2l + 1}} & \sqrt{\frac{l + m_j + 1/2}{2l + 1}} \\
\end{array}$$
(5.69)

The second line follows from unitarity with signs chosen such that the determinant is positive.<sup>6</sup>

Explicit formulas for general CG coefficients have been derived by Racah and by Wigner (see [Grau] appendix A6 or [Messiah] volume 2). The coupling of three (or more) angular momenta can be analyzed by iteration. It is easy to see that now there are degeneracies, i.e. the resulting states are no longer uniquely described by  $|j,m\rangle$  with  $m = m_1 + m_2 + m_3$ . The 8 states of the coupling of three spins  $j_1 = j_2 = j_3 = \frac{1}{2}$ , for example, organize themselves into a unique spin 3/2 "quartet" and two non-unique spin 1/2 "doublet" representations. The resulting basis depends on the order of the iteration  $\vec{J} = \vec{J}_{12} + \vec{J}_3 = \vec{J}_1 + \vec{J}_{23}$  with  $\vec{J}_{12} = \vec{J}_1 + \vec{J}_2$  and  $\vec{J}_{23} = \vec{J}_2 + \vec{J}_3$ . The recoupling coefficients, which are matrix elements of the corresponding unitary change of basis, can be expressed in terms of the Racah W-coefficients or in terms of the Wigher 6-j symbol, which essentially differ by sign conventions.<sup>7</sup> These quantities are used in atomic physics.

 $^{6}$  Recursion relations that can be used to compute all CG coefficients follow from

$$\langle j_1, j_2, m_1, m_2 | J_{\pm} | j, m \rangle = \langle j_1, j_2, m_1, m_2 | (J_{1\pm} + J_{2\pm}) | j, m \rangle$$
(5.70)

where  $J_{i\pm}$  can be evaluated on the bra-vector and  $J_{\pm}$  on the ket,

$$\sqrt{(j \mp m)(j \pm m + 1)}\langle j_1, j_2, m_1, m_2 | j, m \pm 1 \rangle = \sqrt{(j_1 \pm m_1)(j_1 \mp m_1 + 1)}\langle j_1, j_2, m_1 \mp 1, m_2 | j, m \rangle 
+ \sqrt{(j_2 \pm m_2)(j_2 \mp m_2 + 1)}\langle j_1, j_2, m_1, m_2 \mp 1 | j, m \rangle.$$
(5.71)

Possible values of  $m_1$  and  $m_2$  for fixed  $j_1$ ,  $j_2$  and j are shown in the following graphics, where the corner X



can be used as the starting point of the recursion because the linear equations (5.71) relate corners of the triangles  $\sum_{m_2-1}^{m_1,m_2} \max_{m_1,m_2} \sum_{m_1+1}$  (the overall normalization has to be determined from unitarity). <sup>7</sup> The Wigner 6*j*-symbols and the Racah W-coefficients, which describe the recoupling of 3 spins, are related

#### 5.3.2 Singlet, triplet and EPR correlations

Another interesting case is the addition of two spin-1/2 operators

$$\vec{S} = \vec{S}_1 + \vec{S}_2 \tag{5.74}$$

The four states in the tensor product basis are  $|\pm\rangle \otimes |\pm\rangle$ , or  $|\uparrow\uparrow\rangle$ ,  $|\uparrow\downarrow\rangle$ ,  $|\downarrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$ . The total spin can have the values 0 and 1, and the respective multiplets, or representations, are called singlet and triplet, respectively.<sup>8</sup> The **triplet** consists of the states

$$|1, 1\rangle = |\uparrow\uparrow\rangle, \tag{5.75}$$

$$|1, 0\rangle = \frac{1}{\sqrt{2}\hbar}S_{-}|\uparrow\uparrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right), \qquad (5.76)$$

$$|1,-1\rangle = \frac{1}{\sqrt{2}\hbar} S_{-}|1,0\rangle = |\downarrow\downarrow\rangle.$$
(5.77)

The singlet state is the superposition of the  $S_z = 0$  states  $|\uparrow\downarrow\rangle$  and  $|\downarrow\uparrow\rangle$  orthogonal to  $|1,0\rangle$ ,

$$|0, 0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right). \tag{5.78}$$

An important application for a system with two spins is the hyperfine structure of the ground state of the hydrogen atom, which is due to the magnetic coupling between the spins of the proton and of the electron. The energy difference between the ground state singlet and the triplet excitation corresponds to a signal with 1420.4 MHz, the famous 21 cm hydrogen line, which is used extensively in radio astronomy. Due to the weakness of the magnetic interaction the lifetime of the triplet state is about 10<sup>7</sup> years.

In order to derive a formula for the projectors to singlet and triplet states we note that  $\vec{S}^2 = \vec{S_1}^2 + \vec{S_2}^2 + 2\vec{S_1}\vec{S_2}$  with

$$\vec{S}^2|1,m\rangle = 2\hbar^2|1,m\rangle, \qquad \vec{S}^2|0,0\rangle = 0 \quad \text{and} \quad \vec{S}_1^2 = \vec{S}_2^2 = \frac{3}{4}\hbar^2 \mathbb{1}.$$
 (5.79)

The operator  $\vec{S}_1 \vec{S}_2 = \frac{1}{2} \vec{S}^2 - \frac{3}{4} \hbar^2 \mathbb{1}$  therefore has eigenvalue  $-\frac{3}{4} \hbar^2$  on the singlet and  $\frac{1}{4} \hbar^2$  on triplet states. With the tensor product notation  $\vec{S}_1 = \vec{S} \otimes \mathbb{1}$  and  $\vec{S}_2 = \mathbb{1} \otimes \vec{S}$ , i.e.

$$\vec{S}_1 \, \vec{S}_2 \equiv \vec{S} \otimes \vec{S} = \frac{\hbar^2}{4} \vec{\sigma} \otimes \vec{\sigma} \tag{5.80}$$

by

$$\begin{cases} j_1 \ j_2 \ J_{12} \\ j_3 \ J \ J_{23} \end{cases} = (-1)^{j_1 + j_2 + j_3 + J} W(j_1 j_2 J j_3; J_{12} J_{23}).$$
(5.72)

The Wigner 3j-symbols and the Racah V-coefficients are related to the Clebsch Gordan coefficients by

$$\begin{cases} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{cases} = (-1)^{j-j_1+j_2} V(j_1 j_2 j; m_1 m_2 m) = \frac{(-1)^{m+j_1-j_2}}{\sqrt{2j+1}} \langle j_1 j_2 m_1 m_2 | jm \rangle.$$
 (5.73)

Wigner's sign choices have the advantage of higher symmetry; see [Messiah] vol. II and, for example, http://mathworld.wolfram.com/Wigner6j-Symbol.html and http://en.wikipedia.org/wiki/Racah\_W-coefficient.

<sup>8</sup>The German names for  $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$  are Singulett, Dublett, Triplett, Quartett, ..., respectively.

we thus obtain the **projector**  $P_0$  onto the singlet state

$$P_0 = |0,0\rangle\langle 0,0| = \frac{1}{4}\mathbb{1} - \frac{1}{\hbar^2}\vec{S}_1\vec{S}_2 = \frac{1}{4}\left(\mathbb{1} - \vec{\sigma}\otimes\vec{\sigma}\right)$$
(5.81)

and the projector  $P_1$  onto triplet states

$$P_1 = \sum_{m=-1}^{1} |1, m\rangle \langle 1, m| = \frac{3}{4} \mathbb{1} + \frac{1}{\hbar^2} \vec{S}_1 \vec{S}_2 = \frac{1}{4} \left( 3\mathbb{1} + \vec{\sigma} \otimes \vec{\sigma} \right),$$
(5.82)

which we now apply to the computation of probabilities.

**Correlations in the EPR experiment.** We want to compute the conditional probability  $P(\vec{\alpha}|\vec{\beta})$  for the measurement of spin up in the direction of a unit vector  $\vec{\alpha}$  for one particle if we measure spin up in the direction of a unit vector  $\vec{\beta}$  for the other decay product of a quantum mechanical system composed of two spin  $\frac{1}{2}$  particles that has been prepared in the singlet state  $|0,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ , i.e. in Bohm's version of the EPR experiment.

The conditional probability  $P(\vec{\alpha}|\vec{\beta}) = P(\vec{\alpha} \wedge \vec{\beta})/P(\vec{\beta})$  is the probability that we measure spin up in direction  $\vec{\alpha}$  for the first particle and spin up in direction  $\vec{\beta}$  for the second particle divided by the probability for the latter. It is easily seen that  $\Pi_{\pm} = \frac{1}{2}(\mathbb{1} \pm \sigma_z)$  is the projector  $|\pm\rangle\langle\pm|$  onto the  $S_z$  eigenstate  $|\pm\rangle$ . More generally, the spin operator  $\vec{\alpha}\vec{S}$  for a spin measurement in the direction  $\vec{\alpha}$  has eigenvalues  $\pm \frac{\hbar}{2}$ , so that  $\vec{\alpha}\vec{\sigma}$  has eigenvalues  $\pm 1$ . Therefore the projectors  $\Pi_{\pm\vec{\alpha}}$  onto the eigenspaces of spin up and spin down in the direction of the unit vector  $\vec{\alpha}$  are

$$\Pi_{\pm\vec{\alpha}} = \frac{1}{2} (\mathbb{1} \pm \vec{\alpha}\vec{\sigma}) \tag{5.83}$$

and the probability for spin up in direction  $\vec{\beta}$  for the second particle in the singlet state is

$$P(\vec{\beta}) = \operatorname{tr}(P_0 \Pi_{\vec{\beta}}^{(2)}) = \operatorname{tr}\left(\frac{1}{4}(\mathbb{1} \otimes \mathbb{1} - \sigma_i \otimes \sigma_i) \circ (\mathbb{1} \otimes \Pi_{\vec{\beta}})\right)$$
$$= \frac{1}{4}\operatorname{tr}\left(\mathbb{1} \otimes \Pi_{\vec{\beta}} - \sigma_i \otimes \sigma_i \Pi_{\vec{\beta}}\right) = \frac{1}{4}\left(\operatorname{tr} \mathbb{1} \cdot \operatorname{tr} \Pi_{\vec{\beta}} - \operatorname{tr} \sigma_i \cdot \operatorname{tr}(\sigma_i \Pi_{\vec{\beta}})\right)$$
(5.84)

where we used the factorization  $\operatorname{tr}(\mathcal{O}_1 \otimes \mathcal{O}_2) = \operatorname{tr} \mathcal{O}_1 \cdot \operatorname{tr} \mathcal{O}_2$  of traces of product operators shown in (3.68). In the two-dimensional one-particle spin spaces the traces are

$$\operatorname{tr} \mathbb{1} = 2, \quad \operatorname{tr} \sigma_i = 0, \quad \operatorname{tr} \Pi_{\vec{\beta}} = \frac{1}{2} \operatorname{tr} \mathbb{1} = 1, \quad \operatorname{tr}(\sigma_i \Pi_{\vec{\beta}}) = \frac{1}{2} \operatorname{tr}(\sigma_i + \sigma_i \sigma_j \beta_j) = \beta_i \quad (5.85)$$

and we find  $P(\vec{\beta}) = 1/2$ , as we had to expect because of rotational symmetry. For the conditional probability we thus obtain

$$P(\alpha|\beta) = P(\alpha \wedge \beta) / P(\beta) = 2P(\alpha \wedge \beta) = 2\operatorname{tr} P_0 \Pi_{\vec{\alpha}}^{(1)} \Pi_{\vec{\beta}}^{(2)}$$
(5.86)

$$= 2 \operatorname{tr} \left( \frac{1}{4} \left( \mathbb{1} \otimes \mathbb{1} - \sigma_i \otimes \sigma_i \right) \circ \left( \Pi_{\vec{\alpha}} \otimes \Pi_{\vec{\beta}} \right) \right)$$
(5.87)

$$= \frac{1}{2} \left( \operatorname{tr}(\Pi_{\vec{\alpha}}) \operatorname{tr}(\Pi_{\vec{\beta}}) - \operatorname{tr}(\sigma_i \Pi_{\vec{\alpha}}) \operatorname{tr}(\sigma_i \Pi_{\vec{\beta}}) \right) = \frac{1}{2} \left( 1 - \vec{\alpha} \vec{\beta} \right) = \frac{1}{2} \left( 1 - \cos(\vec{\alpha}, \vec{\beta}) \right), \quad (5.88)$$

which is the result we used in the discussion of EPR in chapter 3.