Chapter 2
Spin States and Spin Polarization

Quantum mechanics deals with statistical statements about the result of measurements on an ensemble of states (particles, beams, targets). In other words: by giving an expectation value of operators it provides probabilitites (better: probability amplitudes) for the result of a measurement on an ensemble. Here two limiting cases can be distinguished. One is the case that our knowledge about the system is complete e.g. when all members of an ensemble are in the same spin state. This state will then be characterized completely by a state vector (ket). A special case is the spin state of a *single* particle which is always completely (spin-)polarized.

Example In the classic Stern–Gerlach experiment [1] (see Chap. 8.1) an inhomogeneous magnetic field (the "polarizer") spatially separates silver atoms according to two projections $m_S = +1/2$ and $m_S = -1/2$ of a spin S $= 1/2$ system.[1] By cutting out one of these partial beams by a stopper the remaining ensemble will be completely spin-polarized, see Fig. 8.1. The general state vector of such a system (as well as of each single particle in the beam) is

$$|\Psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle \tag{2.1}$$

with $|\uparrow\rangle$ and $|\downarrow\rangle$ denoting the basis states which characterize such a system completely, i.e. the UP or DOWN spin projections with respect to one direction, e.g. that of the magnetic field. a and b are the probability amplitudes for the two basis states with the normalization $|a|^2 + |b|^2 = 1$. Like for every two-state system the dimension of this system is N = 2 (=2S + 1) and therefore the description of this system is complete if $|\uparrow\rangle$ and $|\downarrow\rangle$ are orthogonal. The choice of the quantization axis is in principle arbitrary. It is, however, obvious that—though e.g. the occupation of the substates under the rotation transformation of this axis is not changed—the phase relation between $|\uparrow\rangle$ and $|\downarrow\rangle$ and therefore the description will be changed. $|\Psi\rangle$ is a

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[1] At the time of this completely unexpected discovery neither the notion of a spin S nor of its 2S + 1 projections was possible. Whenever we discuss spin in general the symbols S and m_S are used. The symbols J and m_J are used for the electron spin of atoms (and sometimes for nuclear spin states), and I, m_I are reserved for the nuclear spins.

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coherent superposition of the basis states. Denoting as usual the polar and azimuthal angles of the "spin" by β and ϕ

$$\frac{a}{b} = \frac{\cos\frac{\beta}{2}}{e^{i\phi}\sin\frac{\beta}{2}} \tag{2.2}$$

The solution of this equation shows that one has a state in which the spins of all particles point into a well-defined direction (β, ϕ). In the Stern–Gerlach case we can check the direction dependence of a and b with a second Stern–Gerlach magnet (the "analyzer") which is rotatable around the beam axis: the intensities behave as $\sin^2(\beta/2)$ or $\cos^2(\beta/2)$, respectively. This double Stern–Gerlach experiment has been used to introduce a number of basic features of quantum mechanics such as the anti-commutation and commutation relations for the spin and other properties of the spin operators, the projection-operator formalism etc., see e.g. [2, 3, 4, 5].

In classical optics this is quite analogous to the behaviour of light polarization only that the angle $\beta/2$ has to be replaced by β when rotating polarization filters. (The factor 1/2 characterizes the spin as an entirely non-classical phenomenon).

A state for which we have complete knowledge about all particles of the ensemble is a *pure state*.

The other limiting case is that where the magnetic field of the Stern–Gerlach system is turned off. Then for symmetry reasons the spins of all particles of the ensemble will point in all spatial directions with equal probability (completely unpolarized ensemble). It is clear that this system cannot be described solely by one state vector and also that for such a system we do not know in which direction the spin of each individual particle is pointing. It is clearly a state of non-maximal information (even, as we shall see, it is a state of minimal information). A Stern–Gerlach analyzer would not detect any dependence on direction. There is also no fixed phase relation between basis states. As in classical (statistical) physics the adequate description of the state is that of an incoherent weighted superposition of pure states. In contrast to the case of the pure states it should not matter with reference to which direction the pure UP/DOWN basis states have been defined.

2.1 Measurement Process, Pure and Mixed States, Polarization

From the foregoing discussion the recipe of how to describe a general non-pure state (mixed state, mixed ensemble or "mixture") results: one has to state with which probability p_i (not probability amplitude, but statistical weight!) a number of pure states contribute to the mixture. In detail:

- $p_i \geq 0$ and $\sum_i p_i = 1$
- Choose a "basis" of pure states described by state vectors $\Psi^{(i)}$ which do not necessarily have to be orthogonal!
  Example: one could combine one pure state completely polarized in $+x$ direction

with a contribution of $P_1 = 20\%$ with another one completely polarized in the $-z$ direction with a contribution of $P_2 = 80\%$

- The number of these states needs not be equal to the dimension N of the state space (spin space) but can be larger! E.g. one could imagine a partially polarized ensemble of spin 1/2 particles produced from three pure states in the following way: $P_1 = 30\%$ of the particles fully polarized in the $+z$ direction, $P_2 = 40\%$ fully polarized in the $+x$ and $P_3 = 30\%$ fully polarized in the $-y$ direction.
- In the limit an infinite number of subsystems each completely polarized in arbitrary directions can be imagined. If their statistical weights would all be equal the measured spin polarization would be zero.
  Example: Modern Stern–Gerlach magnets as they are used in atomic-beam sources for polarized particle beams are multipole magnets, see Sect. 8.3.3 (quadrupoles and sextupoles). In such magnets all field directions around the z axis appear with equal weight because of rotational symmetry. This means that even though the magnet focuses and therefore selects all atoms in one spin substate and therefore produces partial beams completely polarized with respect to one field direction the polarization in the magnet interior will be zero. This results from the *incoherent* superposition of the *pure, i.e. fully polarized* subsystems with equal weights. Only after guiding the atoms (adiabatically!) into a field region with a dominant field direction will there be a net polarization.

2.2 Expectation Value and Average of Observables in Measurements

Carrying out a number of measurements of an observable **A** on a (generally) mixed ensemble results in an expectation value which is the statistical ensemble average of the quantum-mechanical expectation values $\langle\Psi^{(i)}|A|\Psi^{(i)}\rangle$ with respect to the pure states $|\Psi^{(i)}\rangle$ present (or considered) in the ensemble. These should be expandable in an eigenstate basis $|u_n\rangle$ (i.e. $A|u_n\rangle = a_n|u_n\rangle$) with $\langle u_n|u_m\rangle = \delta u_{nm}$:

$$\langle \mathbf{A}\rangle = \sum_i p_i\langle\Psi^{(i)}|A|\Psi^{(i)}\rangle = \sum_i\sum_n p_i|\langle u_n|\Psi^{(i)}\rangle|^2 a_n \tag{2.3}$$

with

$$|\Psi^{(i)}\rangle = \sum_n \langle u_n|\Psi^{(i)}\rangle\langle|u_n\rangle = \sum_n c_n^{(i)}|u_n\rangle \tag{2.4}$$

Probabilities appear here twice: once as $|\langle u_n|\Psi^{(i)}\rangle|^2$, which is the probability to find the state $|\Psi^{(i)}\rangle$ in an eigenstate $|u_n\rangle$ of A (with eigenvalue a_n) in the measurement, but also as the probability p_i of finding the ensemble in a quantum mechanical state characterized by $|\Psi^{(i)}\rangle$. By choosing an even more general basis (see e.g. [5]) $|b\rangle$ one can represent the ensemble average more generally as

$$
\begin{aligned}
\langle \boldsymbol{A} \rangle &= \sum_i p_i \sum_n \sum_m \langle \Psi^{(i)} | b_n \rangle \langle b_n | A | b_m \rangle \langle b_m | \Psi^{(i)} \rangle \\
&= \sum_n \sum_m \left(\sum_i p_i \langle b_m | \Psi^{(i)} \rangle \langle \Psi^{(i)} | b_n \rangle \right) \langle b_n | \mathbf{A} | b_m \rangle
\end{aligned}
\tag{2.5}
$$

The number of terms in the n, m sums is N each while i depends on the composition of the statistical ensemble. In this representation the properties of the ensemble and of the obervable **A** factorize.

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