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# Moderne Theoretische Physik I

## Grundlagen der Quantenmechanik

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Exercise Sheet 10

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The problems whose solutions you need to upload are designated with stars.

### ★ Problem 1 ★ Fun with orbital angular momentum

The orbital angular momentum operator is given by  $\hat{\mathbf{L}} = (\hat{L}_x, \hat{L}_y, \hat{L}_z) = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$ . In spherical coordinates

$$x = r \sin \theta \cos \phi, \quad y = r \sin \theta \sin \phi, \quad z = r \cos \theta \quad \text{with } r = \sqrt{x^2 + y^2 + z^2} \quad (1)$$

and the gradient is given by

$$\nabla_{r,\theta,\phi} = \hat{\mathbf{e}}_r \frac{\partial}{\partial r} + \hat{\mathbf{e}}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\mathbf{e}}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \quad (2)$$

with

$$\hat{\mathbf{e}}_r = \sin \theta \cos \phi \hat{\mathbf{e}}_x + \sin \theta \sin \phi \hat{\mathbf{e}}_y + \cos \theta \hat{\mathbf{e}}_z, \quad (3)$$

$$\hat{\mathbf{e}}_\theta = \cos \theta \cos \phi \hat{\mathbf{e}}_x + \cos \theta \sin \phi \hat{\mathbf{e}}_y - \sin \theta \hat{\mathbf{e}}_z, \quad (4)$$

$$\hat{\mathbf{e}}_\phi = -\sin \phi \hat{\mathbf{e}}_x + \cos \phi \hat{\mathbf{e}}_y \quad (5)$$

1. Show that the angular momentum operator in spherical coordinates has the following form:

$$\hat{L}_x = \frac{\hbar}{i} \left( -\sin \phi \frac{\partial}{\partial \theta} - \frac{\cos \phi}{\tan \theta} \frac{\partial}{\partial \phi} \right), \quad \hat{L}_y = \frac{\hbar}{i} \left( \cos \phi \frac{\partial}{\partial \theta} - \frac{\sin \phi}{\tan \theta} \frac{\partial}{\partial \phi} \right), \quad \hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \quad (6)$$

2. Suppose a particle described by the following wave function

$$\psi(\mathbf{r}) = (x + y + 2z)N e^{-r^2/\alpha^2} \quad (7)$$

where  $N$  and  $\alpha$  both are real numbers and  $N$  is a normalization constant.

By applying

$$\hat{\mathbf{L}}^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} \right) \quad (8)$$

to the state  $\psi(\mathbf{r})$ , show that  $\psi(\mathbf{r})$  is an eigenstate of the  $\hat{\mathbf{L}}^2$ . i.e.

$$\hat{\mathbf{L}}^2 \psi(\mathbf{r}) = l(l+1) \hbar^2 \psi(\mathbf{r}) \quad (9)$$

and determine the value of  $l$ .

3. Now express the wave function Eq. (7) by a superposition of suitable spherical harmonics. Which values can be measured for the  $z$ -component  $\hat{L}_z$  of the orbital angular momentum? With what probability are these measured?

## Solution 1

1. We now show that the angular momentum operator in spherical coordinates has the form:

$$\hat{L}_x = \frac{\hbar}{i} \left( -\sin \phi \frac{\partial}{\partial \theta} - \frac{\cos \phi}{\tan \theta} \frac{\partial}{\partial \phi} \right), \quad \hat{L}_y = \frac{\hbar}{i} \left( \cos \phi \frac{\partial}{\partial \theta} - \frac{\sin \phi}{\tan \theta} \frac{\partial}{\partial \phi} \right), \quad \hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \quad (10)$$

Using Eq. (2) and the fact that

$$\hat{e}_r \times \hat{e}_\theta = \hat{e}_\phi, \quad \hat{e}_\theta \times \hat{e}_\phi = \hat{e}_r, \quad \hat{e}_\phi \times \hat{e}_r = \hat{e}_\theta, \quad (11)$$

the angular momentum operator is now given by

$$\begin{aligned} \frac{i}{\hbar} \hat{\mathbf{L}} &= \hat{\mathbf{r}} \times \hat{\mathbf{p}} = \hat{\mathbf{r}} \times \nabla = r \hat{e}_r \times \left( \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right) \\ &= \hat{e}_\phi \frac{\partial}{\partial \theta} - \hat{e}_\theta \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \\ &= \left( -\sin \phi - \frac{\cos \phi}{\tan \theta} \frac{\partial}{\partial \phi} \right) \hat{e}_x + \left( \cos \phi \frac{\partial}{\partial \theta} - \frac{\sin \phi}{\tan \theta} \frac{\partial}{\partial \phi} \right) \hat{e}_y + \frac{\partial}{\partial \phi} \hat{e}_z \end{aligned} \quad (12)$$

2. First we write the given wave function in spherical coordinates

$$\begin{aligned} \psi(r, \theta, \phi) &= (r \sin \theta \cos \phi + r \sin \theta \sin \phi + 2r \cos \theta) N e^{-r^2/\alpha^2} \\ &= (\sin \theta \cos \phi + \sin \theta \sin \phi + 2 \cos \theta) f(r) \end{aligned} \quad (13)$$

where the  $f(r) = r N e^{-r^2/\alpha^2}$

Now we apply  $\hat{\mathbf{L}}^2$  to the wave function

$$\hat{\mathbf{L}}^2 \psi(r, \theta, \phi) = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} \right) (\sin \theta \cos \phi + \sin \theta \sin \phi + 2 \cos \theta) f(r) \quad (14)$$

$$\frac{\partial^2}{\partial \theta^2} (\sin \theta \cos \phi + \sin \theta \sin \phi + 2 \cos \theta) = -(\sin \theta \cos \phi + \sin \theta \sin \phi + 2 \cos \theta), \quad (15)$$

$$\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} (\sin \theta \cos \phi + \sin \theta \sin \phi + 2 \cos \theta) = -\frac{1}{\sin \theta} (\cos \phi + \sin \phi), \quad (16)$$

$$\frac{1}{\tan \theta} \frac{\partial}{\partial \theta} (\sin \theta \cos \phi + \sin \theta \sin \phi + 2 \cos \theta) = \frac{\cos^2 \theta}{\sin \theta} (\cos \phi + \sin \phi) - 2 \cos \theta \quad (17)$$

As a result,

$$\hat{\mathbf{L}}^2 \psi(r, \theta, \phi) = 2\hbar^2 (\sin \theta \cos \phi + \sin \theta \sin \phi + 2 \cos \theta) f(r) = 2\hbar \psi(r, \theta, \phi) \quad (18)$$

Thus  $\psi(r, \theta, \phi)$  is an eigenfunction with the eigenvalue  $2\hbar = l(l+1)\hbar$ , from which  $l = 1$  can be read directly.

3. The spherical harmonics are complete and orthogonal. The coefficients could therefore be found by projecting onto these states. However, since we already know that  $l = 1$ , the state can only be expressed by a superposition of the functions  $Y_{l=1}^m(\theta, \phi)$ . We therefore only need the three spherical harmonics

$$Y_1^0(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta, \quad Y_1^1(\theta, \phi) = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}, \quad Y_1^{-1}(\theta, \phi) = \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi} \quad (19)$$

and find the coefficients by comparing with Eq. (13).

$$\begin{aligned} \psi(r, \theta, \phi) &= \left( -\sqrt{\frac{2\pi}{3}} (Y_1^1(\theta, \phi) - Y_1^{-1}(\theta, \phi)) + i\sqrt{\frac{2\pi}{3}} (Y_1^1(\theta, \phi) + Y_1^{-1}(\theta, \phi)) + 2\sqrt{\frac{4\pi}{3}} Y_1^0(\theta, \phi) \right) f(r) \\ &= (c_1 Y_1^1(\theta, \phi) + c_0 Y_1^0(\theta, \phi) + c_{-1} Y_1^{-1}(\theta, \phi)) f(r) \end{aligned} \quad (20)$$

where

$$c_1 = -\sqrt{\frac{2\pi}{3}}(1-i), \quad c_0 = 4\sqrt{\frac{\pi}{3}}, \quad c_{-1} = \sqrt{\frac{3\pi}{3}}(1+i). \quad (21)$$

In a measurement of  $\hat{L}_z$ , the values  $\hbar m$  with  $m = -1, 0, 1$  can be found. We have not normalized the wave function, i.e.  $f(r)$  is only known up to a constant factor  $N$ . However, when calculating the measurement probabilities of the various angular momentum values,  $f(r)$  is eliminated

$$P(m = -1) = \frac{|c_{-1}|^2}{|c_{-1}|^2 + |c_0|^2 + |c_1|^2} = \frac{1}{6} \quad (22)$$

$$P(m = 0) = \frac{|c_0|^2}{|c_{-1}|^2 + |c_0|^2 + |c_1|^2} = \frac{2}{3} \quad (23)$$

$$P(m = 1) = \frac{|c_1|^2}{|c_{-1}|^2 + |c_0|^2 + |c_1|^2} = \frac{1}{6} \quad (24)$$

### ★ Problem 2 ★ Particles in a magnetic field - Landau levels

Consider a particle of charge  $q$  in a homogeneous magnetic field  $\mathbf{B} = B\hat{e}_z$ . A clever choice of the vector potential  $\mathbf{A}$  in this case is given by the Landau gauge with  $\mathbf{A} = -By\hat{e}_x$ . Assuming the particle is restricted to the  $x - y$  plane (as in a two-dimensional electron gas), the Hamiltonian is

$$\hat{H} = \frac{1}{2m} \left( \hat{\mathbf{p}} - \frac{q}{c} \mathbf{A} \right)^2 = \frac{1}{2m} \left( \left( \hat{p}_x + \frac{q}{c} B y \right)^2 + \hat{p}_y^2 \right) \quad (25)$$

1. Show  $[\hat{H}, \hat{p}_x] = 0$ , and use the knowledge of the eigenfunctions of  $\hat{p}_x$  to make a separation of variable approach for the wave function  $\psi(x, y)$ .
2. Show that the Schrödinger equation can be brought to the form of a one-dimensional harmonic oscillator and find the characteristic frequency  $\omega_c$  of the eigenenergies  $E_n = \hbar\omega_c(n + \frac{1}{2})$  where  $n \geq 0$ .
3. Now specify the corresponding eigenfunctions  $\psi_{n,p_x}(x, y)$ . Use the magnetic length scale  $l_B = \sqrt{\frac{\hbar c}{qB}}$  in expressing the  $\psi_{n,p_x}(x, y)$ .

Apparently the eigenfunctions depend on the quantum number  $p_x$ , but the energies do not. Thus the Landau energy levels are strongly degenerate. This degeneracy plays an important role for physical applications (e.g., de Haas-van Alphen effect). We now want to determine these degeneracies for a sample with an area  $A = L_x L_y$ .

- 4 Determine the quantization of  $\hat{p}_x$ , assuming periodic boundary conditions  $\psi(x + L_x, y) = \psi(x, y)$ . Also find the distance between adjacent values of  $p_{x,n_x}$ . i.e.  $\Delta p_x = p_{x,n_x+1} - p_{x,n_x}$ .  
(Hint: To do this, perform a discrete Fourier transformation  $\phi(x) = \frac{1}{\sqrt{L_x}} \sum_{p_x} e^{-ip_x x/\hbar} \phi_{p_x}$ .)
- 5 A restriction on the permitted values of  $p_x$  can be found by the condition that the position of the potential minimum  $y_0 = \frac{cp_x}{qB}$  must lie within the dimensions of the sample, i.e.  $0 < y_0 < L_y$ . From this, determine the  $I_{p_x}$  which is length of the interval of permitted  $p_x$  values, and the number  $N = \frac{I_{p_x}}{\Delta p_x}$  (= degree of degeneracy of each Landau level).

### Solution 2

1. We can easily show that  $[\hat{H}, \hat{p}_x] = 0$  from the fact that  $[\hat{y}, \hat{p}_x] = 0$ . So we can make an Ansatz:  $\psi(x, y) = e^{ip_x x/\hbar} \chi(y)$ .

2. Inserting the ansatz into Schrödinger equation, we immediately get

$$\left[ \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\left(\frac{qB}{mc}\right)^2 \left(y + \frac{cp_x}{qB}\right)^2 \right] \chi(y) = E\chi(y) \quad (26)$$

Let us now introduce the characteristic frequency  $\omega_c = \frac{qB}{mc}$ , and the displacement  $y_0 = \frac{cp_x}{qB}$  and also a variable shift by  $\tilde{y} = y + y_0$ ,  $\hat{p}_y = \hat{p}_{\tilde{y}}$ . Then we get

$$\left[ \frac{\hat{p}_{\tilde{y}}^2}{2m} + \frac{1}{2}m\omega_c^2 \tilde{y}^2 \right] \chi(\tilde{y} - y_0) = E\chi(\tilde{y} - y_0) \quad (27)$$

Here we have a harmonic oscillator with the energies  $E_n = \hbar\omega_c(n + \frac{1}{2})$ , and the eigenfunctions of the harmonic oscillator

$$\chi(\tilde{y} - y_0) = \tilde{\chi}(\tilde{y}) = \left(\frac{m\omega_c}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega_c}{\hbar}} \tilde{y}\right) e^{-\frac{1}{2}\frac{m\omega_c}{\hbar} \tilde{y}^2} \quad (28)$$

3. It is  $\chi(y) = \tilde{\chi}(y + y_0)$ . With the magnetic length scale  $l_B = \sqrt{\frac{\hbar}{m\omega_c}} = \sqrt{\frac{\hbar c}{qB}}$ , we can write the eigenfunctions as follows

$$\begin{aligned} \psi_{n,p_x}(x, y) &= e^{ip_x x/\hbar} \chi(y) = e^{ip_x x/\hbar} \tilde{\chi}(y + y_0) \\ &= e^{ip_x x/\hbar} \frac{1}{\pi^{1/4} \sqrt{l_B} \sqrt{2^n n!}} H_n\left(\frac{y + y_0}{l_B}\right) e^{-\frac{(y+y_0)^2}{2l_B^2}}. \end{aligned} \quad (29)$$

4. To determine the quantization under periodic boundary conditions we perform the Fourier transformation

$$\psi(x, y) = \frac{1}{\sqrt{L_x}} \sum_{p_x} e^{-ip_x x/\hbar} \psi_{p_x}(y) = \psi(x + L_x, y) = \frac{1}{\sqrt{L_x}} \sum_{p_x} e^{-ip_x(x+L_x)/\hbar} \psi_{p_x}(y) \quad (30)$$

$$\Rightarrow p_x L_x = 2\pi\hbar n_x \quad (n_x = 0, \pm 1, \pm 2, \dots) \quad (31)$$

$$\therefore p_x = \frac{2\pi\hbar}{L_x} n_x. \quad (32)$$

Therefore  $\Delta p_x = p_{x, n_x+1} - p_{x, n_x} = \frac{2\pi\hbar}{L_x}$ .

5. Now we require that the position of the potential minimum  $y_0$  lies within the sample i.e.  $0 < y_0 < L_y$  and thus obtain the restriction for  $p_x$ ,  $0 < p_x < \frac{qBL_y}{c}$ . Then the length of the interval of the allowed  $p_x$  is  $I_{p_x} = \frac{qBL_y}{c}$ . As a result, the number of degenerated states is given by

$$N = \frac{I_{p_x}}{\Delta p_x} = \frac{qBA}{2\pi\hbar c} \quad (33)$$

### Problem 3 Detection of directional quantization in the magnetic field and spin precession

In a groundbreaking experiment done by Stern and Gerlach, they were able to demonstrate the directional quantization of the angular momentum. They used a setup with a strongly inhomogeneous magnetic field and observed that a silver atom beam is split into two beams. This setup, also called Stern-Gerlach apparatus shown in Fig. 1, can also be used to investigate spin precession in more detail.

Here we shall consider two Stern-Gerlach apparatuses arranged one behind the other. The first has an inhomogeneous magnetic field along the  $z$ -direction which splits the electron beam into  $|\uparrow\rangle$  and  $|\downarrow\rangle$  states. The second apparatus has an inhomogeneous magnetic field along the  $x$ -direction which also splits the electron beam, this time into spins along  $\pm\hat{x}$ . A homogeneous magnetic field  $B_y$  is applied between the apparatuses in the  $y$ -direction and leads to a precession of the spin during the flight time  $T$  between the two Stern-Gerlach apparatuses. Two points are now observed on a detector screen behind the second apparatus.

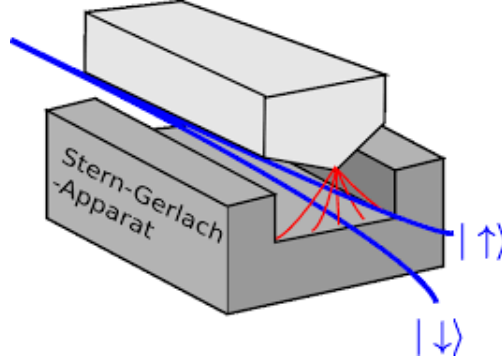
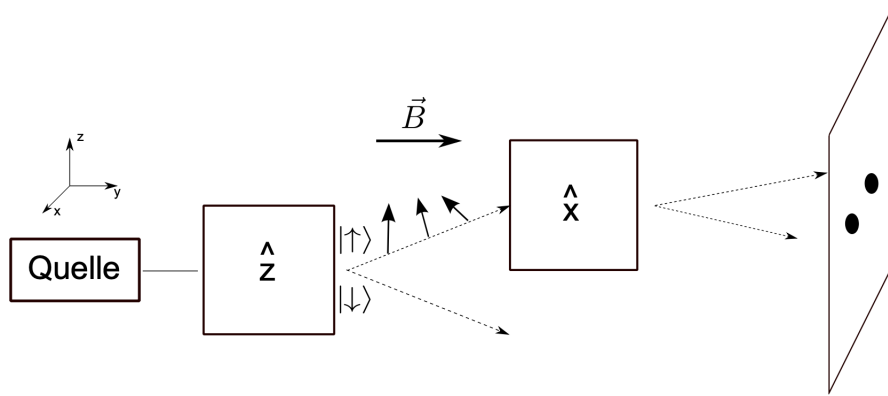


Figure 1: Stern-Gerlach apparatus

1. Sketch the experimental setup including the beam path.
2. The intensities of the two observed points depend on the magnetic field  $B_y$  and the time of flight  $T$ . Calculate this dependence for the two possible prepared initial states ( $|\uparrow\rangle$  and  $|\downarrow\rangle$ ).

### Solution 3

1. Sketch



2. According to the first Stern-Gerlach apparatus, the state of the particles is either  $|\uparrow\rangle$  (for the upper beam, for example) and  $|\downarrow\rangle$  (for the lower beam).

During the flight time from one device to the other, the states evolve due to the external magnetic field applied in the  $y$ -direction

$$|\psi_{\uparrow}(t)\rangle = \frac{e^{-i\omega t/2}}{2}(|\uparrow\rangle + i|\downarrow\rangle) + \frac{e^{i\omega t/2}}{2}(|\uparrow\rangle - i|\downarrow\rangle) = \cos \frac{\omega t}{2}|\uparrow\rangle - \sin \frac{\omega t}{2}|\downarrow\rangle, \quad (34)$$

$$|\psi_{\downarrow}(t)\rangle = \cos \frac{\omega t}{2}|\downarrow\rangle + \sin \frac{\omega t}{2}|\uparrow\rangle, \quad (35)$$

$$(36)$$

with  $\omega = \frac{\mu_B B}{\hbar}$ . The second Stern-Gerlach apparatus splits the states again into the states

$$|\uparrow\rangle_x = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle), \quad (37)$$

$$|\downarrow\rangle_x = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle). \quad (38)$$

Accordingly, the conditional probabilities to measure these after the flight time  $T$  are given by

$$P(\uparrow_x, \uparrow) = \left| \frac{1}{\sqrt{2}} (\langle \uparrow | + \langle \downarrow |) \left( \cos \frac{\omega T}{2} | \uparrow \rangle - \sin \frac{\omega T}{2} | \downarrow \rangle \right) \right|^2 = \frac{1}{2}(1 - \sin \omega T), \quad (39)$$

$$P(\downarrow_x, \uparrow) = \frac{1}{2}(1 + \sin \omega T), \quad (40)$$

$$P(\uparrow_x, \downarrow) = \frac{1}{2}(1 + \sin \omega T), \quad (41)$$

$$P(\downarrow_x, \downarrow) = \frac{1}{2}(1 - \sin \omega T). \quad (42)$$

The intensities of the points on the detector screen are directly proportional to these probabilities.