Quantum Magnetism Prof. J. Knolle 13/10/23 PROBLEM SHEET 1 Winter Term 2023/24

Submission deadline for the homework questions: 20/10/2023 (hand in via moodle).

Please prepare the remaining questions for the tutorials in the following week and be ready to present the questions marked with a star (*).

Exercise 1.1*: Classical Dipoles

- (a) For a classical magnetic dipole, define its magnetic moment $\vec{\mu}$ in terms of its angular momentum and a constant.
- (b) Discuss how these may be interpreted if the source of the moment is a current loop.
- (c) What is the energy of this dipole configuration when an external field **B** is applied?
 - Discuss the effect of this magnetic interaction on the orientation and position of the dipole.
- (d) By once again considering the source of the dipole as being an infinitesimal element of a current carrying wire, argue that the force this part of the dipole $\vec{\mu}$ experiences in the field B is

$$d\mathbf{F} = I \, d\mathbf{r} \times \mathbf{B}. \tag{1}$$

Therefore, by integrating over the loop of wire, derive the expression for the torque $\vec{\tau}$ that the dipole experiences.

(e) By equating the torque to the rate of change of angular momentum, and using part (a), show that the magnetic moment precesses with a frequency of $\omega_L = \gamma B$.

Exercise 1.2: Angular Momentum & Spin (Homework Question)

(a) Argue semiclassically that the magnetic moment of an electron in the ground state of a hydrogen atom is given by $\mu = -\mu_B = -e\hbar/2m_e$, where μ_B is the Bohr magneton.

To do this, consider the orbit as a single-electron current with radius r_e .

What are the gyromagnetic ratio and Lamor frequency for this singleelectron system?

(b) This question will discuss the group structure of angular momentum in a quantum mechanical context.

In 2D the group of rotations on the plane is Spin(2) = SO(2), with elements that are the rotation matrices. Write a quantum mechanical operator $U_L(\theta)$ which acts on the coordinates in this way

$$U_L(\theta) \begin{pmatrix} x \\ y \end{pmatrix} U_L^{\dagger}(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{2}$$

(i) Now argue that one may write this generator of rotations in terms of the Hermitian angular momentum operator

$$U_L(\theta) = \exp(iL\theta/\hbar),$$
 (3)

by showing that for infinitesimal θ , (2) gives the correct commutation relation for L.

(ii) Use the fact that the coordinates are unchanged by a 2π rotation to show that L has quantised eigenvalues.

We may define the spin operator S as being a new operator which generates the same group as L but without modifying the coordinate eigenstates. Does S have quantised eigenvalues in 2D?

(c) In 3D the rotation group is SO(3), generated by rotations in three directions. The operators which generate the quantum spin group are S_i satisfying

$$[S_i, S_j] = i\hbar \epsilon_{ijk} S_k \tag{4}$$

(i) Show that the Pauli matrices $S_i = (\hbar/2)\sigma_i$ satisfy this commutation relation (4).

This is the spin-1/2 representation of the Spin(3) = SU(2) algebra (or the 2 × 2 traceless Hermitian matrices).

Show that the general such matrix can be written as $\vec{\sigma} \cdot \mathbf{d}$, where $\mathbf{d} = (d_x, d_y, d_z)$ and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$.

Furthermore show that the eigenvalues of such a matrix are $\pm |\mathbf{d}|$.

(ii) Now we will investigate spin-s reps of SU(2).

What does the non-commuting nature of the spin operators S_i mean for the possibility of simultaneous measurement of the components?

Therefore argue why we must label states by $|s, s_z\rangle$ where s is the total spin eigenvalue and s_z the S_z eigenvalue.

(iii) Show that we may define raising and lowering operators

$$S_{\pm} = S_x \pm iS_y \tag{5}$$

and, through finding the commutation relations with S_z and S^2 , show that these operators move between s_z states in a space of constant-s states.

- (iv) Write S^2 in terms of S_{\pm} and S_z . Given that there exists a highest weight state $|s,s\rangle$ which is annihilated by S_+ , show that $S^2 |s,s\rangle = \hbar^2 s(s+1) |s,s\rangle$, and generalise to all s_z .
- (v) By considering $\langle s, s_z | S_{\pm} S_{\pm} | s, s_z \rangle$, show that

$$S_{\pm}|s,s_z\rangle = \sqrt{(s \mp s_z)(s \pm s_z + 1)}|s,s_z \pm 1\rangle.$$
 (6)

Show that there exists a lowest weight (s_z) representation, and therefore find the degeneracy of a spin-s state.

- (vi) What are the operators S_{\pm} , S^2 in the spin-1/2 Pauli basis?
- (d) (i) The Dirac equation of electrons can be approximated in the non-relativistic setting to give

$$\left[\left[\frac{1}{2m_e} (p + eA)^2 - e\phi \right] \mathbf{1} + \frac{e}{m_e} \mathbf{S} \cdot \mathbf{B} \right] |\psi\rangle = E |\psi\rangle.$$
 (7)

Where $|\psi\rangle$ is a 2-component spinor. What does this equation predict as the magnetic moment g?

Discuss why the kinetic term has this form.

- (ii) Argue why (7) implies that the total spin $s = \frac{\hbar}{2}$ for the electron. Using the fact that rotations around the z-axis are generated by $U_S(\theta) = \exp(i\sigma_z\theta/2)$, show that $U_S(2\pi)|\psi\rangle = -|\psi\rangle$, and discuss its interpretation.
- (iii) With $\mathbf{B} = B\mathbf{z}$, calculate evolution of spin eigenstates under the time-dependent Schrödinger equation to show the electrons undergo Lamor precession (take the electron to not be moving).

Exercise 1.3: Paramagnetism (Homework Question)

(a) Let us calculate the paramagnetic behaviour of non-interacting classical spins at a finite temperature.

(i) Apply a magnetic field B along the z-direction, and parameterise the spins with polar angle θ .

Writing the partition function of a single spin at temperature T as a sum over θ states, show that

$$Z = \int_0^{\pi} \exp(\mu B \cos \theta / k_B T) \sin \theta \, d\theta \,, \tag{8}$$

up to a constant coefficient.

(ii) Therefore show that the magnetisation is

$$M = n \langle \mu_z \rangle = n\mu \left[\coth \left(\frac{\mu B}{k_B T} \right) - \frac{k_B T}{\mu B} \right], \tag{9}$$

where n is the number density of spins.

Sketch this function and discuss its behaviour in low and high field B.

- (iii) For low field, show that the susceptibility obeys Curie's law.
- (b) Now we would like to investigate the paramagnetic response of a spin-1/2 system (with g=2) in a magnetic field.

Show the energies of the states are $\pm \mu_B B$.

Hence show $Z = 2 \cosh(\mu_B B/k_B T)$ and by calculating $F = -nk_B T \log Z$, show

$$M = -\left(\frac{\partial F}{\partial B}\right)_T = M_s \tanh\left(\frac{\mu B}{k_B T}\right),\tag{10}$$

and find the saturation magnetisation M_s .

(c) Show that for a quantum system with spin-J, the partition function is

$$Z = \sum_{m_J = -J}^{J} \exp(m_J g_J \mu_B B / k_B T). \tag{11}$$

Therefore find the magnetisation is given in terms of the Brillouin function, and confirm the results from (a) and (b) are recovered in the appropriate limits.

Exercise 1.4: Coupled Spins (Homework Question)

(a) Consider coupling two spin-1/2 particles a,b with a Heisenberg exchange term

$$H = J\mathbf{S}_a \cdot \mathbf{S}_b. \tag{12}$$

The total spin is given by $\mathbf{S}_{\text{tot}} = \mathbf{S}_a + \mathbf{S}_b$.

- (i) Write down all states in the combined Hilbert space, in the simple tensor product basis.
 - Are these states eigenvalues of $\mathbf{S}_{\text{tot}}^2$ and $\mathbf{S}_{\text{tot},z}$?
- (ii) Find a linear combination of these states which are eigenvalues of $\mathbf{S}_a \cdot \mathbf{S}_b$. Show that these are the singlet (S=0) and triplet (S=1) states, and write down the energies.
- (iii) What is a perturbation which could be added to H that could split the triplet state?
- (b) Generally, when taking tensor products of spin states by decomposing the spins under the eigenvalues of the combined spin operator, the product of a spin-S with spin-1/2 space, may be decomposed as follows

$$\mathcal{H}_S \otimes \mathcal{H}_{1/2} = \mathcal{H}_{S-1/2} \oplus \mathcal{H}_{S+1/2}. \tag{13}$$

Use this to show

$$\mathcal{H}_{1/2} \otimes \mathcal{H}_{1/2} \otimes \mathcal{H}_{1/2} = \mathcal{H}_{3/2} \oplus \mathcal{H}_{1/2} \oplus \mathcal{H}_{1/2}. \tag{14}$$

Confirm that the dimensions of the product space is the same as the sum of dimensions of the three spaces we decompose into.

(c) Define the chiral spin operator

$$\chi = \mathbf{S}_1 \cdot (\mathbf{S}_2 \times \mathbf{S}_3),\tag{15}$$

which commutes with the total spin operator **S**. We may therefore categorise states as $|S, M_S; \chi\rangle$.

- (i) Show $\left|\frac{3}{2}, \frac{3}{2}; 0\right\rangle = \left|\uparrow\uparrow\uparrow\uparrow\right\rangle$, and find an expression for all $\left|\frac{3}{2}, M; 0\right\rangle$ in terms of this, using the lowering operator S_{-} .
- (ii) Argue that $\chi \left| \frac{3}{2}, M; 0 \right\rangle = 0$ by thinking about the symmetry of the eigenstate under exchanging pairs of spins.
- (iii) Show that

$$\chi = \frac{i}{2} \left[-S_{-,1}S_{+,2}S_{z,3} + S_{+,1}S_{-,2}S_{z,3} + S_{-,1}S_{z,2}S_{+,3} - S_{+,1}S_{z,2}S_{-,3} - S_{z,1}S_{-,2}S_{+,3} + S_{z,1}S_{+,2}S_{-,3} \right]$$
(16)

(iv) Now there are two spaces of spin-1/2 subspaces in the three-particle product space. We will distinguish these by their chiral eigenvalue. Show that the following state is an eigenstate of χ and evaluate its eigenvalue

$$\left|\frac{1}{2}, \frac{1}{2}; + \right\rangle = \frac{1}{\sqrt{3}} \left[|\uparrow\uparrow\downarrow\rangle + \exp(2\pi i/3) |\uparrow\downarrow\uparrow\rangle + \exp(-2\pi i/3) |\downarrow\uparrow\uparrow\rangle \right]. \tag{17}$$

- (v) Find an orthogonal state with $S = \frac{1}{2}$ and $M_S = \frac{1}{2}$ which has the negative eigenvalue $\left|\frac{1}{2}, \frac{1}{2}; -\right\rangle$.
 - How are the states $\left|\frac{1}{2}, -\frac{1}{2}; +\right\rangle$ related to these previous states?