Theoretical Physics II B – Quantum Mechanics

Lecture 17

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Solutions to previous control questions

16.1 As a first step, rewrite the wave function $\psi(\theta,\,\phi)$ through spherical harmonics:

$$\psi(\theta,\,\phi) = N\left[\sqrt{4\pi}\,Y_{10} - \sqrt{\frac{2\pi}{3}}(Y_{11} - Y_{1-1}) - i\sqrt{\frac{2\pi}{3}}(Y_{11} + Y_{1-1})\right]$$

(a) The normalisation can be obtained by realising that the spherical harmonics are normalised. Therefore

$$1 = \int\limits_0^{4\pi} \mathrm{d}\Omega|\psi|^2 = |N|^2\left[4\pi + 4\frac{2\pi}{3}\right] = |N|^2\frac{20\pi}{3}$$

leading to $N = \sqrt{3/(20\pi)}$.

(b) The expectation value of $\underline{\mathcal{L}}^2$ is given by

$$\left\langle \psi \left| \hat{\underline{L}}^2 \right| \psi \right\rangle = \hbar^2 l(l+1) = 2\hbar^2 \,,$$

because the state ψ is a pure spin-$l = 1$ state - the admixture of different values of m does not change this.

(c) Similarly,

$$\mathcal{P}_{l=1,m=0} = |\langle 10|\psi\rangle|^2 = \frac{3\hbar}{20\pi}\,[4\pi] = \frac{3\hbar}{5}\,.$$

16.2 (a) Orient the ring such that the z-axis goes through its centre and that the ring lies in the x-y-plane. Then the remaining degree of freedom is the angle ϕ around the z-axis, which yields the position of the particle on the ring: $x = r\cos\phi$ and $y = r\sin\phi$

The classical Lagrange-function thus reads (with $\dot{\phi} = \partial\phi/\partial t$):

$$L(\dot{\phi},\, \phi,\, t) = \frac{mr^2}{2}\dot{\phi}^2 = \frac{I}{2}\dot{\phi}^2\,,$$

and the generalised momentum therefore is given by $p_\phi = \frac{\partial L}{\partial\dot{\phi}} = I\dot{\phi}$.

This results in the classical Hamilton function for this system to read

$$H(\phi,\, p_\phi,\, t) = \dot{\phi}p_\phi - L = \frac{p_\phi^2}{2I} = \frac{L_z^2}{2I}\,,$$

where the generalised momentum related to the angle ϕ has been identified with the orbital angular momentum L_z.

The Hamilton operator emerges from the classical function by making all dynamical quantities operators:

$$\hat{H} = \frac{\hat{L}_z^2}{2I}\,.$$

(b) Since the Hamiltonian, being equal to the square of $\hat{L}_z$, it commutes with $\hat{L}_z$. Thus, naively, one would expect the energy eigenkets to be the $|lm\rangle$. However, the extra condition, $\hat{\underline{L}}^2 = \hat{L}_z^2$, implies that the angular momenta around the x and y-axes, $\hat{L}_x$ and $\hat{L}_y$, have been measured to be equal to 0. This is in obvious contradiction with the uncertainty principle, manifest by the observation that the eigenvalues of $\hat{L}_z^2 = m^2\hbar^2$ and of $\hat{\underline{L}}^2 = l(l+1)\hbar^2$ cannot be satisfied at the same time with integer values for l and m. Therefore, the $|lm\rangle$ cannot be the eigenkets of the Hamiltonian.
Instead, we can label the eigenkets with as $|m\rangle$ only. The corresponding energy eigenvalues then are given by $E_m = \frac{m^2\hbar^2}{2I}$ and the energy eigenfunctions read $\psi_m(\phi) = e^{im\phi}$, where m denotes any integer, implying a two-fold degeneracy for non-zero energies: $E_m = E_{-m}$.
The correctness of the energy eigenfunctions can be checked by realising that, with $\psi(\phi) = e^{im\phi}$,

$$E\psi_m(\phi) = \frac{\hat{L}_z^2}{2I}\psi(\phi) = \frac{1}{2I}\frac{-(i\hbar\partial)^2}{\partial\phi^2}\psi(\phi) = \frac{\hbar^2 m^2}{2I}\psi(\phi)\,.$$

(c) In lecture 9 we have seen that the time evolution of the expectation value of an observable with no explicit time-dependence is governed by its commutator with the Hamiltonian. Thus

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathcal{L}_z\rangle_{\text{any state}} = \left\langle\left[\hat{H},\,\hat{L}_z\right]\right\rangle_{\text{any state}} = 0\,,$$

and therefore the angular momentum around the z-axis is a constant of motion.

(d) Time evolution operator:

$$\hat{U}(t,\,t_0) = \exp\left[-\frac{i\hat{H}(t-t_0)}{\hbar}\right] = \exp\left[-\frac{i\hat{L}_z^2(t-t_0)}{2\hbar I}\right]\,.$$

From lecture 10 we know that, in the Heisenberg picture,

$$\hat{L}_z(t) = \hat{U}^\dagger(t,\,t_0)\hat{L}_z(t_0)\hat{U}(t,\,t_0) = \hat{L}_z(t_0)x$$

because $\hat{L}_z$ commutes with $\hat{L}_z^2$ and thus also with its exponential.

Total angular momentum

- Up to now we discussed two instances of angular momentum: spin angular momentum, $\hat{S}$, an *internal degree of freedom*, and orbital angular momentum, $\hat{L}$, an *external degree of freedom*.
- The question arises, what happens if we have a system where combinations of external and internal degrees of freedom matter.

Simple example: State ket of a particle with spin

- Up to now studied systems either with no spin or with spin, but with all other quantum-mechanical degrees of freedom ignored.
- Example: spin-$\frac{1}{2}$ particle in position space.
  Base kets are direct products of position with spin base kets.
- These kets live in a Hilbert space that is a product space of position and spin space. Infinitely dimensional operators living in the space by the $|\underline{x}\rangle$ commute with the two dimensional operators spanned by the $|\pm\rangle$.
- The base kets can also be used, of course, to construct wave functions related to a state ket $|\psi\rangle$, which take a vector (or better: spinor) form:

(Spinors because they have a slightly different transformation behaviour under rotations . . . .)

$$|\underline{x}\,;\,\pm\rangle = |\underline{x}\rangle \otimes |\pm\rangle \quad \text{and} \quad \langle \underline{x}\,;\,\pm|\psi\rangle = \left(\begin{array}{c} \psi_+(\underline{x}) \\ \psi_-(\underline{x}) \end{array} \right) .$$

- In this case the rotation operator still has the form $\exp(-i\underline{\hat{J}} \cdot \underline{\phi}/\hbar)$, but the angular momentum operator $\underline{\hat{J}}$ now reads

$$\underline{\hat{J}} = \underline{\hat{L}} + \underline{\hat{S}}\,,$$

where the first term, the orbital angular momentum $\underline{\hat{L}}$, acts on the spatial components of the state ket only, while the second term, the spin operator $\underline{\hat{S}}$, acts on the spin degrees of freedom. It therefore is maybe more sensible to rewrite this, for the time being as

$$\underline{\hat{J}} = \underline{\hat{L}} \otimes \hat{\mathbf{1}}_{\pm} + \hat{\mathbf{1}}_{\underline{x}} \otimes \underline{\hat{S}}\,,$$

where the identity operators in position and spin space are denoted as $\hat{\mathbf{1}}_{\underline{x}}$ and $\hat{\mathbf{1}}_{\pm}$, respectively.

- Assume now that the system exhibits discrete energy levels. Then it may be sensible to replace the original position eigenket $|\underline{x}\rangle$ with $|nlm\rangle$, where n labels the energy levels E_n and l and m denote the quantum numbers of the orbital angular momentum operators $\hat{\underline{L}}^2$ and $\hat{L}_z$ with $l(l+1)\hbar^2$ and $m\hbar$, respectively. The eigenkets $|\pm\rangle$ of the spin-operators in this case would be $\frac{3}{4}\hbar^2$ for $\hat{\underline{S}}^2$ and $\pm\frac{1}{2}\hbar$ for $\hat{S}_z$.
- In this case, our base kets would read $|nlm_l sm_s\rangle$.
- Instead, as will be seen in the next example, we could also use the eigenvalues of the *total angular momentum operators* $\hat{\underline{J}}^2 = (\hat{\underline{L}} + \hat{\underline{S}})^2$ and $\hat{J}_z = \hat{L}_z + \hat{S}_z$ and either $\hat{L}_z$ and $\hat{S}_z$ or $\hat{\underline{L}}^2$ and $\hat{\underline{S}}^2$.

Simple example: Two spin-$\frac{1}{2}$ particles

- Consider a system of, say, two electrons with their relative orbital angular momentum being suppressed. Usually, the spin is written as

$$\hat{S}_{(1+2)} = \hat{S}_1 + \hat{S}_2$$

with $\hat{S}_{i\{x,y,z\}} = \frac{\hbar}{2}\hat{\sigma}_{x,y,z}$ for each of the two particles $i = 1, 2$.

- The expression above is understood as each of the two spin operators $\hat{S}_i$ acting on particle i alone (acting in the Hilbert space of particle i alone) and ignoring the other particle:

$$\hat{S}_{(1+2)} = \hat{S}_1 \otimes \hat{\mathbf{1}}_2 + \hat{\mathbf{1}}_1 \otimes \hat{S}_2 \,.$$

Here, obviously the $\hat{\mathbf{1}}_i$ stand for the identity operator in the Hilbert (spin) space of particle i.

- This notion of two separate Hilbert spaces - one for each particle - of course implies that the respective operators commute:

$$\left[\hat{S}_{1i},\,\hat{S}_{2j}\right] = 0 \quad \text{with } \{i,\,j\} \in \{x,\,y,\,z\}\,.$$

- Within each Hilbert space, however, the original commutators are still valid:

$$\left[\hat{S}_{1i},\,\hat{S}_{1j}\right] = i\hbar\epsilon_{ijk}\hat{S}_{1k} \quad \text{and} \quad \left[\hat{S}_{2i},\,\hat{S}_{2j}\right] = i\hbar\epsilon_{ijk}\hat{S}_{2k}\,.$$

- This implies that for the summed spin operator, the same commutation relations also hold true:

$$\left[\hat{S}_{(1+2)i},\,\hat{S}_{(1+2)j}\right] = i\hbar\epsilon_{ijk}\hat{S}_{(1+2)k}$$

- Therefore, the eigenvalues of various spin operators are given by

$$
\begin{array}{lclclcl}
\underline{\hat{S}}^2_{(1+2)} & = & \left(\underline{\hat{S}}_1 + \underline{\hat{S}}_2\right)^2 & : & s(s+1)\hbar^2 & & \\
\hat{S}_{(1+2)z} & = & \hat{S}_{1z} + \hat{S}_{2z} & : & m\hbar & = & (m_1 + m_2)\hbar \\
\underline{\hat{S}}^2_i & & & : & s_i(s_i+1)\hbar^2 & = & \frac{3}{4}\hbar^2 \\
\hat{S}_{iz} & & & : & m_i & = & \pm\frac{1}{2}
\end{array}
$$

- The natural question now arises on how to go from one set of quantum numbers to another set; in our case at hand we can ask how the state characterised by $|m_1 m_2\rangle$ relates to states characterised by $|sm\rangle$.
  In general,of course, we may want to write these states as $|j_1 j_2; m_1 m_2\rangle$ and $|jm; m_1 m_2\rangle$.

- In the $|m_1 m_2\rangle$ representation we have

$$|m_1 m_2\rangle \ \in \left\{ |\uparrow\uparrow\rangle \ , \ |\uparrow\downarrow\rangle \ , \ |\downarrow\uparrow\rangle \ , \ |\downarrow\downarrow\rangle \right\}$$

while in the $|sm\rangle$ representation the kets are

$$|sm\rangle \ \in \left\{ |11\rangle \ , \ |10\rangle \ , \ |1-1\rangle \ , \ |00\rangle \right\} \, .$$

- Since there are three $s = 1$ but only one $s = 0$ state, they are also denoted as *triplet* and *singlet* states.

- To connect the two representations, first realise that the only way to combine two spin-$\frac{1}{2}$ systems such that they deliver a combinedspin of $+1$ in in z-direction is to have both of them in the $m = +\frac{1}{2}$ state. Therefore

$$|11\rangle = |\uparrow\uparrow\rangle \quad \text{and} \quad |1-1\rangle = |\downarrow\downarrow\rangle$$

- Now, define ladder operators

$$\hat{S}_{(1+2)\pm} = \hat{S}_{1\pm} + \hat{S}_{2\pm} = \left(\hat{S}_{1x} + \hat{S}_{2x}\right) \pm i\left(\hat{S}_{1y} + \hat{S}_{2y}\right) \, .$$

- Acting with $\hat{S}_{(1+2)-}$ on $|11\rangle$ then yields (with $s = m = 1$)

$$\begin{aligned}\hat{S}_{(1+2)-}|11\rangle &= \hbar\sqrt{(1+1)(1-1+1)}\,|10\rangle = \hbar\sqrt{2}\,|10\rangle \\ &= \hbar\sqrt{\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\left(\tfrac{1}{2}-\tfrac{1}{2}+1\right)}\,|{\downarrow\uparrow}\rangle + \hbar\sqrt{\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\left(\tfrac{1}{2}-\tfrac{1}{2}+1\right)}\,|{\uparrow\downarrow}\rangle = \hbar\left[|{\downarrow\uparrow}\rangle + |{\uparrow\downarrow}\rangle\right] \\ &= \left(\hat{S}_{1-}\otimes\hat{\mathbf{1}}_2 + \hat{\mathbf{1}}_1\otimes\hat{S}_{2-}\right)|{\uparrow\uparrow}\rangle\,.\end{aligned}$$

  This results in

$$|10\rangle = \frac{1}{\sqrt{2}}\left[|{\uparrow\downarrow}\rangle + |{\downarrow\uparrow}\rangle\right]$$

- The only configuration of the two spin-$\frac{1}{2}$ left that is orthogonal to all others therefore is

$$|00\rangle = \frac{1}{\sqrt{2}}\left[|{\uparrow\downarrow}\rangle - |{\downarrow\uparrow}\rangle\right]\,.$$

- Taken together, thus

$$
\begin{aligned}
|11\rangle &= |\uparrow\uparrow\rangle \\
|10\rangle &= \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right] \\
|1\,-1\rangle &= |\downarrow\downarrow\rangle \\
|00\rangle &= \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right] \,.
\end{aligned}
$$

- The coefficients on the left hand side are the **Clebsch-Gordan coefficients**, which will be discussed in more detail and for the general case in the next lecture.

Learning outcomes

- Some examples for combined state kets, including spin.
- First trivial example, addition of two spin-$\frac{1}{2}$ systems.

Control questions

17.1 The spin-dependent Hamiltonian of an electron-positron system in the presence of an uniform magnetic field B in the z-direction is given by

$$\hat{H} = A\underline{\hat{S}}^{(-)} \cdot \underline{\hat{S}}^{(+)} + \left(\frac{eB}{mc}\right)\left(\hat{S}_z^{(-)} + \hat{S}_z^{(+)}\right),$$

where A is a real number.
Suppose the spin ket of the system is given by $|\psi\rangle = |\uparrow\rangle^{(-)}|\uparrow\rangle^{(+)}$.

(a) Is this an eigenket of the system, when $A \to 0$ and $eB/(mc) \neq 0$? Is it an eigenket in the opposite case, i.e. $A \neq 0$, $B \to 0$?
(b) What is the expectation value of the energy in this state?
(c) Find the expectation values of the spin operator $\underline{\hat{S}}^{(-)} \cdot \underline{\hat{S}}^{(+)}$ for the triplet and the singlet states of the electron and positron spin.

(Hint: Realise that $\underline{\hat{S}}^{(-)} \cdot \underline{\hat{S}}^{(+)} = \frac{1}{2}(\underline{\hat{S}}^2 - \underline{\hat{S}}^{(+)2} - \underline{\hat{S}}^{(-)2})$.)

17.2 Consider a system containing three spin-$\frac{1}{2}$ particles. By combining the first two particles into triplet and singlet kets, and adding the third spin by hand, construct the Clebsch-Gordon coefficients for the sum of a spin-1 and a spin-$\frac{1}{2}$ system.