B7.3 Further Quantum Theory

Sheet 2 — HT21

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2.1 Angular momentum and spherical harmonics (revision, unmarked)

Recall the angular momentum commutation relations

$$[J_i, J_j] = i\hbar \sum_{k=1}^{3} \epsilon_{ijk} J_k \ .$$

Define $\mathbf{J}^2 = J_1^2 + J_2^2 + J_3^2$ and $J_\pm = J_1 \pm iJ_2$.

1. Check that $[\mathbf{J}^2, J_i] = 0$ and $[J_3, J_\pm] = \pm\hbar J_\pm$.

   Deduce that in an irreducible representation of the angular momentum operators, one can find a basis of joint eigenstates of $\mathbf{J}$ and J_3 for which $\mathbf{J}$ takes a constant value and if $J_3|\psi\rangle = \hbar m|\psi\rangle$ then $J_3|J_\pm\psi\rangle) = \hbar(m \pm 1)|J_\pm\psi\rangle$.

2. Compute $\langle J_\pm\psi|J_\pm\psi\rangle$ in terms of $\langle\psi|\psi\rangle$.

   Use this to prove that if we write the $\mathbf{J}^2$ eigenvalue as $\hbar^2 j(j+1)$, then j must be a non-negative half-integer and the possible J_3 eigenvalues can only be of the form $\hbar m$ where m takes values in $-j, -j+1, \ldots, j-1, j$.

3. Explain why in an irreducible representation, each state with a given choice of quantum numbers $|j, m\rangle$ is the unique such state (up to rescaling). Deduce the general structure of the spin-j angular momentum representation.

Now consider the *orbital* angular momentum operators L_i acting on wave functions in $\mathbb{R}^3$. Define $x_\pm = x_1 \pm ix_2 = r\sin\theta \mathrm{e}^{\pm i\phi}$ and $x_3 = r\cos\theta$. The corresponding derivatives are

$$\partial_\pm = \frac{1}{2}\left(\frac{\partial}{\partial x_1} \mp i\frac{\partial}{\partial x_2}\right) \ , \qquad \partial_3 = \frac{\partial}{\partial x_3} \ ,$$

so $\partial_\pm x_\pm = 1$ and $\partial_\pm x_\mp = 0$.

4. Show that with respect to this basis, the components of the orbital angular momentum operators $\mathbf{L} = \mathbf{X} \wedge \mathbf{P} = -i\hbar\, \mathbf{x} \wedge \nabla$ are given by

$$L_\pm \ := \ L_1 \pm iL_2 = \pm\hbar(2x_3\partial_\mp - x_\pm\partial_3) \ , \qquad L_3 = \hbar\left(x_+\partial_+ - x_-\partial_-\right) \ .$$

5. Use the defining relations for spherical harmonics $\mathbf{L}^2\, Y_\ell^m(\phi,\theta) = \hbar^2\ell(\ell+1)\, Y_\ell^m(\phi,\theta)$ and $L_3 Y_\ell^m(\phi,\theta) = \hbar m\, Y_\ell^m(\phi,\theta)$ to show that $L_- Y_\ell^{-\ell} = 0$. Therefore, deduce that $r^\ell Y_\ell^{\pm\ell}$ can be identified with a constant multiple of $x_\pm^\ell$.

   Use the raising and lowering operators to find expressions for the *normalised* Y_ℓ^m for $\ell = 0, 1, 2$.

6. Determine the action of the Laplacian on the functions $r^\ell\, Y_\ell^m(\phi,\theta)$. *Don't use spherical coordinates.*

   Thus infer that the spherical harmonics are, up to normalisation, simply the restriction to the unit sphere of homogeneous, harmonic polynomials of degree ℓ in three variables, with m measuring the power of x_+ minus the power of x_-.

2.2 Spin $1/2$ and $\mathrm{SU}(2)$ (unmarked)

Here you should work through for yourself some of the discussion of the spin 1/2 projective representation of the rotation group. The Pauli spin matrices are defined by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For a vector $\mathbf{a}$, we define $\boldsymbol{\sigma}\cdot\mathbf{a} = \sigma_1 a_1 + \sigma_2 a_2 + \sigma_3 a_3$. This is the observable associated with measuring spin alon gthe $\mathbf{a}$ axis.

1. Derive the following relation:

$$(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b}\, I_{2\times 2} + i\boldsymbol{\sigma}\cdot(\mathbf{a}\wedge\mathbf{b})$$

   and thus deduce that the eigenvalues of $\boldsymbol{\sigma}\cdot\mathbf{a}$ are $\pm|\mathbf{a}|$.

2. Check by direct computation that the matrix representing a rotation by angle θ about the axis designated by a unit vector $\mathbf{n}$ takes the form

$$\exp\left(-\frac{i\theta}{2}\boldsymbol{\sigma}\cdot\mathbf{n}\right) = \cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)\boldsymbol{\sigma}\cdot\mathbf{n}\,.$$

3. Argue that a two-by-two matrix of this form is the most general two-by-two *unitary* matrix with determinant one, and so this representation gives a two-to-one identification of elements of $\mathrm{SU}(2)$ with those of $\mathrm{SO}(3)$.

   (If you are interested, you might try to visualise that this presentation of $\mathrm{SU}(2)$ *allows us to identify it topologically with the three-sphere* S^3*, while the rotation group is realised as a quotient* $\mathrm{SO}(3) \cong S^3/\mathbb{Z}_2$*.)*

2.3 Lattice translations and Bloch waves

Consider a particle moving in one dimension with potential given by a periodic function $V(x) = V(x+\ell)$ for some real $\ell > 0$.

1. Using the (discrete) translational symmetry of the potential, show that there will be a basis of (generalised) energy eigenstates for the problem of the form
$$\psi_\theta(x) = \exp\left(\frac{i\theta x}{\ell}\right)\varphi(x) ,$$
where $\varphi(x)$ has the same periodicity properties as the potential. Explain why without loss of generality you can take $\theta \in [-\pi, \pi]$.

2. For an (generalised) eigenstate with energy E, show that $\varphi(x)$ obeys the second order ODE,
$$-\frac{\hbar^2}{2m}\varphi''(x) - \frac{i\hbar^2}{m}\frac{\theta}{\ell}\varphi'(x) + \frac{\hbar^2\theta^2}{2m\ell^2}\varphi(x) = (E - V(x))\,\varphi(x) .$$
For what range of x should you solve this equation, and with what boundary conditions?

3. Now suppose that the potential is a lattice of *delta functions*,
$$V(\mathbf{x}) = -\lambda\sum_n \delta(x - n\ell) , \qquad \lambda > 0 .$$
This can be thought of as a model for a one-dimensional *crystal*, where at the locations of the atoms in the crystal a particle experiences an ultralocal attractive interaction.

   Solve the ODE from the previous part of the question in this case for $E > 0$. You should leave the expression in terms of the energy E (or better, k where $k^2 = 2mE/\hbar^2$), where k is implicitly determined by θ according to (show this!)
$$\cos(\theta) = \cos(k\ell) - \frac{\alpha}{k}\sin(k\ell) ,$$
for a constant α that you determine.

   [You may want to consider your freedom to choose an appropriate range of values of x for which to write your solution. You can make a choice, for example, so the delta function appears in the middle of your interval.]

4. Give a qualitative description of the allowed energy levels of the crystal. It will be useful to do some investigations in a computational environment like Matlab or Mathematica. You will discover the phenomenon of "electronic band structure".

5. **[Unmarked]** For your own entertainment, think about how you would generalise this story to the case of a three-dimensional lattice of delta functions. The generalisation of the choice of $\theta \in [0, 2\pi)$ is now the choice of a point in what's called the *first Brillouin zone* of the lattice.

2.4 Anti-unitarity

For a symmetry represented by a unitary operator U to be a dynamical symmetry, we require the condition

$$U \exp\left(-\frac{iHt}{\hbar}\right) = \exp\left(-\frac{iHt}{\hbar}\right) U \ ,$$

which implies $UHU^* = H$.

1. If instead U is an anti-unitary operator, show that the above equation would imply that $UHU^* = -H$.

   Explain why this means that a system with such a dynamical, anti-unitary symmetry would have negative energy states with energy $-E$ for every positive energy state with energy E.

2. Consider now the anti-unitary operator $\mathcal{T}$ that acts on wave functions in $L^2(\mathbb{R})$ by complex conjugation:

   $$\mathcal{T}(\psi(x)) = \overline{\psi(x)} \ .$$

   Explain how this evades the above issue in the case of, say, the harmonic oscillator Hamiltonian, for which $\mathcal{T}$ is a true symmetry (sending energy eigenstates to energy eigenstates).

3. Consider a single particle in $\mathbb{R}^3$ subject to the Hamiltonian

   $$H = \frac{\mathbf{P}^2}{2m} + \mathbf{L} \cdot \mathbf{V} \ ,$$

   where $\mathbf{L}$ is the orbital angular momentum operator and $\mathbf{V}$ is a fixed (constant) vector. Is this system $\mathcal{T}$-symmetric?

   Formulate a general condition for a Hamiltonian of a single-particle system (written in terms of $\mathbf{X}$ and $\mathbf{P}$ operators) to respect $\mathcal{T}$ symmetry.

   Can you explain why this condition should hold intuitively?

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2.5 Threefold addition of angular momentum

Consider three (distinguishable) spin-1/2 systems with angular momentum operators $J_i^{(1)}$, $J_i^{(2)}$, $J_i^{(3)}$, respectively, all with the usual commutation relations. The total angular momentum operators $J_i^{(\mathrm{tot})} = J_i^{(1)} + J_i^{(2)} + J_i^{(3)}$ act on the tensor product of the Hilbert spaces.

1. Work out the decomposition of the composite Hilbert space into irreducible representations of the total angular momentum operators in terms of what irreducible representations appear.

2. Consider the state $\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle$. (Here the convention is as in lectures that (normalised) basis states are written $|j,m\rangle$.) You can determine how this state is expressed in terms of representations of the total angular momentum operators in two different ways.

   - First, combining the first two spins gives the state $|1,1\rangle$, and then combining with the third spin gives $\alpha\left|\frac{3}{2},\frac{1}{2}\right\rangle + \beta\left|\frac{1}{2},\frac{1}{2}\right\rangle$, for some numbers α and β.
   - On the other hand, combining the second and third spin in the first instance gives $\gamma|0,0\rangle + \delta|1,0\rangle$, whereupon taking the further tensor product with the first spin gives $\epsilon\left|\frac{3}{2},\frac{1}{2}\right\rangle + \zeta\left|\frac{1}{2},\frac{1}{2}\right\rangle$.

   Compute $\alpha,\beta,\gamma,\delta,\epsilon,\zeta$ (you may use values of Clebsch-Gordan coefficients given in textbooks if you wish).

   If you've followed the instructions, you have probably most likely $\beta \neq \zeta$. Explain what went wrong, and identify the true answer for the resultant state.

3. Show that $\left(\mathbf{J}^{(1)} + \mathbf{J}^{(2)}\right)^2$ and $\left(\mathbf{J}^{(2)} + \mathbf{J}^{(3)}\right)^2$ each separately commute with $\left(\mathbf{J}^{(\mathrm{tot})}\right)^2$ and $J_3^{(\mathrm{tot})}$, but do not commute with one another.

   Use this insight to rephrase the resolution of part two of this question in terms of two inequivalent choices of basis for the triple tensor product of the spin-$\frac{1}{2}$ representation.