B7.3 Further Quantum Theory

Problem Sheet 2

Hilary Term 2020

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There are three types of problems on this sheet. The first problem is revision from Part A (and a small elaboration), and probably doesn't need to be discussed in classes. Of the remaining problems, the two **starred** *problems are to be turned in for marking, while the two* **unstarred** *problems will not be marked. You should try to solve all of the problems and they will all be subjects for discussion in classes.*

2.0 Revision: angular momentum and spherical harmonics

The purpose of this question is to revise the details of the derivation of the structure of irreducible representations of the angular momentum operators in a Hilbert space, and refresh some aspects of the spherical harmonics that arise in the representation of angular momentum operators on wave functions in three dimensions.

Recall the angular momentum commutation relations

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

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

(i) Check that $[J^2, J_i] = 0$ 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 J^2 and J_3 for which J^2 takes a constant value and if $J_3|\psi\rangle = \hbar m|\psi\rangle$ then $J_3|J_\pm\psi\rangle) = \hbar(m \pm 1)|J_\pm\psi\rangle$.

(ii) 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 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 $-j, -j+1, \ldots, j-1, j$.

(iii) 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 realization of *orbital* angular momentum operators L_i acting on wave functions in $\mathbb{R}^3$.

(i) Define $x_\pm = x_1 \pm ix_2 = r\sin\theta \mathrm{e}^{\pm i\phi}$ and $x_3 = r\cos\theta$. The corresponding partial 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 $\partial_\pm x_\mp = 0$. 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

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

(ii) Use the defining relations $L^2\, Y_l^m(\phi,\theta) = \hbar^2 l(l+1)\, Y_l^m(\phi,\theta)$ and $L_3 Y_l^m(\phi,\theta) = m\hbar\, Y_l^m(\phi,\theta)$ to show that $L_- Y_l^{-l} = 0$. Therefore, deduce that $r^l Y_l^{\pm l}$ can be identified with a constant multiple of $x_\pm^l$. Use the raising and lowering operators to find expressions for the *normalized* Y_l^m for $l = 0, 1, 2$.

(iv) Determine the action of the Laplacian on the functions $r^l Y_l^m$. *Don't use spherical coordinates.* Thus infer that the spherical harmonics Y_l^m are (up to normalization) 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_-.

2.1 Bloch waves*

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

(*i*) Using the (discrete) translational symmetry of the potential, show that there will be a basis of (generalized) energy eigenstates for the problem of the form

$$\psi_\theta(x) = \exp\left(\tfrac{i\theta x}{\ell}\right)\varphi(x) ,$$

where $\varphi(x)$ has the same periodicity properties as the potential. Explain why without loss of generality you can take $\theta \in [-\pi, \pi]$.

(*ii*) For an eigenstate with energy E, show that $\varphi(x)$ obeys the second order ODE

$$-\frac{\hbar^2}{2m}\varphi''(x) - \frac{i\hbar^2}{m}\frac{\theta}{\ell}\varphi'(x) + \frac{\hbar^2\theta^2}{2m\ell^2}\varphi(\mathbf{x}) = (E - V(x))\varphi(x) .$$

For what range of x should you solve this equation, and with what boundary conditions?

(*iii*) 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 is 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 you should show that k is implicitly determined by θ according to

$$\cos(\theta) = \cos(k\ell) - \frac{\alpha}{k}\sin(k\ell) ,$$

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.

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

(*v*)* For your own entertainment, think about how you would generalize this story to the case of a three-dimensional lattice of delta functions. The generalization of the choice of $\theta \in [0, 2\pi)$ is now the choice of a point in the *first Brillouin zone* of the lattice.

2.2 Anti-unitarity

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

$$U\exp(-\tfrac{iHt}{\hbar}) = \exp(-\tfrac{iHt}{\hbar})U ,$$

which implies $U^{-1}HU = H$.

(i) If instead U is an anti-unitary operator, show that the above equation implies $U^{-1}HU = -H$, and 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.

(ii) Consider now the anti-unitary operator $\mathcal{T}$ that acts on wave-functions of one real variable 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.

(iii) 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?

2.3 Spin 1/2 and $SU(2)$

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 $\boldsymbol{\sigma} \cdot \mathbf{a} = \sigma_1 a_1 + \sigma_2 a_2 + \sigma_3 a_3$. 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 $\pm|\mathbf{a}|$.

Confirm that the re-scaled matrices $\{\frac{1}{2}\hbar\sigma_1,\ \frac{1}{2}\hbar\sigma_2,\ \frac{1}{2}\hbar\sigma_3\}$ satisfy the angular momentum commutation relations, and further that

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

Check by direct computation that the matrix representing a rotation by angle θ about the axis designated by a unit vector $\mathbf{n}$ is given by

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

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

2.4 Threefold addition of angular momentum*

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

(i) Work out the decomposition of the composite Hilbert space into irreducible representations of the total angular momentum operators.

(ii) Now consider the state[1] $|\frac{1}{2}, \frac{1}{2}\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle$. You can compute this state in two different ways. First, combining the first two spins gives the state $|1, 1\rangle$, and then combining with the third spin gives $\alpha|3/2, 1/2\rangle + \beta|1/2, 1/2\rangle$, 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 $\epsilon|3/2, 1/2\rangle + \zeta|1/2, 1/2\rangle$.

Compute $\alpha, \beta, \gamma, \delta, \epsilon, \zeta$. 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.

(iii) Show that $(J^{(1)} + J^{(2)})^2$ and $(J^{(2)} + J^{(3)})^2$ each separately commute with $(J^{\text{tot}})^2$ and J_3^{tot}, but do not commute with one another. Use this insight to rephrase the resolution of part (*ii*) in terms of two inequivaeltn choices of basis for the triple tensor product of the spin-1/2 representation.

Please send comments and corrections to `christopher.beem@maths.ox.ac.uk`.

[1] Here the convention is as in lectures that (normalized) basis states are written $|j, m\rangle$