Prof: Björn Garbrecht
TA: Juan S. Cruz*

Technische Universität München
November 20, 2019

Group Theory in Physics WS 2019/2020
Exercise Sheet 5

Problems will be discussed in the tutorial sessions every Friday at 2:00p.m. in the Minkowski Room

1 The "Stark" hydrogen atom

Let us consider the time independent Schrödinger equation at a fixed energy level E. The Hamiltonian is then given by:

$$H = \frac{p^2}{2m} - \frac{e^2}{r} \tag{1}$$

where H, p and r are to be understood as operators, I will reserve hats for unit vectors. We know the square of the vector operator of angular momentum defined according to $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, commutes with H and therefore allows us to label eigenstates according its energy level, E_n or just n and angular momentum number, ℓ. This is known from generic central potentials, however one can define an extra set of operators which also commute with H and thus help us to realize the full symmetry of the hydrogen atom. Drawing some intuition from planetary systems, where the Runge-Lenz vector is $\mathbf{p} \times \mathbf{L} - me^2\hat{\mathbf{r}}$, define its quantum version as

$$\mathbf{A} = \frac{1}{2}\left(\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}\right) - e^2\hat{\mathbf{r}} \tag{2}$$

where $\hat{\mathbf{r}} = \mathbf{r}/r$.

a) Prove that $\mathbf{A}$ commutes with H and obtain the commutation relations for all the components of $\mathbf{L}$ and $\mathbf{A}$. Realize that this is the $\mathfrak{so}(4)$ algebra (redefining A through a constant). Also show that $\mathbf{A} \cdot \mathbf{L} = 0$ and compute $\mathbf{A}^2$ and $\mathbf{A} \times \mathbf{A}$.

b) Let us define a new basis for the algebra through

$$\mathbf{J}_1 = \frac{1}{2}\mathbf{L} + q\mathbf{A} \quad \text{and} \quad \mathbf{J_2} = \frac{1}{2}\mathbf{L} - q\mathbf{A}.. \tag{3}$$

First verify that these follow the usual $\mathfrak{so}(3) \cong \mathfrak{su}(2)$ commutation relations, (that is they can be thought as angular momentum), if q is picked appropriately.

We have now two basis for the same algebra , $\mathfrak{so}(4)$, consider labeling states by $|n\ell m\rangle$ according to the eigenvalues of $\mathbf{L}^2$ and L_z and a second set of eigenstates labeled according to the eigenvalues of $(\mathbf{J_1} + \mathbf{J_2})^2, J_{1z}, J_{2z}$. Let us now fix $E < 0$ and define $\mathbf{A}_n = q\mathbf{A}$ found in b).

c) Express $\mathbf{A} \cdot \mathbf{L}$ in terms of the new basis and conclude that for hydrogen, fixing an energy level means the eigenstate subspace must be described by the same eigenvalue for $\mathbf{J}_1$ and $\mathbf{J}_2$, so that the labeling $|nfg\rangle$ for the second base makes sense for f, g being the possible eigenvalues of J_{1z} and J_{2z}.

*Responsible for the sheet: Juan S. Cruz, Office 1112, juan.cruz@tum.de

For this case of angular momentum, the Wigner-Eckart theorem applied to a spherical rank 1 (vector) operator $\mathbf{V}$, with components $V_0, V_{\pm 1}$ such that

$$[\mathbf{L}, V_0] = 0 \tag{4}$$

$$[L_{\pm 1}, V_m] \propto V_{m\pm 1} \tag{5}$$

reduces to

$$\langle n\ell m|V_M|n'\ell' m'\rangle = \frac{\delta_{m,m'+M}}{\sqrt{2\ell+1}}\langle n\ell||\mathbf{V}||n'\ell'\rangle\langle \ell'\, m'\, 1\, m\, |\ell'\, 1\, \ell\, m+m'\,\rangle \tag{6}$$

where the first factor are the reduced matrix elements of $\mathbf{V}$ and the last factor are the Clebsch-Gordan coefficients, which in the case of angular momenta are fully known and are given by:

$$\langle j_1, j_2; m_1, m_2|j_1, j_2; J, M\rangle = \delta_{M,m_1+m_2}\sqrt{\frac{(2J+1)(J+j_1-j_2)!(J-j_1+j_2)!(j_1+j_2-J)!}{(j_1+j_2+J+1)!}} \times$$
$$\sqrt{(J+M)!(J-M)!(j_1-m_1)!(j_1+m_1)!(j_2-m_2)!(j_2+m_2)!} \times$$
$$\sum_k \frac{(-1)^k}{k!(j_1+j_2-J-k)!(j_1-m_1-k)!(j_2+m_2-k)!(J-j_2+m_1+k)!(J-j_1-m_2+k)!}. \tag{7}$$

d) Prove that A_{nz} is diagonal in the $|nfg\rangle$ basis and conclude using the Wigner-Eckart theorem that the reduced matrix element $\langle n\ell||\mathbf{A}||n'\ell'\rangle$ is proportional to $\delta_{nn'}$.

e) In order to compute $\langle n\ell||\mathbf{A}_n||n\ell'\rangle$, we will use the relation $\mathbf{A} = 2\mathbf{J}_1 - \mathbf{L}$. Take $\mathbf{V} = \mathbf{L}, \mathbf{J}_1$ to obtain the reduced matrix elements for $\mathbf{L}$ and $\mathbf{J}_1$.

Now let us relate what we have done to a dipolar interaction. That is let us add a term to our Hamiltonian proportional to $\mathbf{r}\cdot\mathbf{E}$ coupled to some external electric field

f) The operator $\mathbf{r}$ is also a vector (spherical) operator so the Wigner-Eckart theorem can be applied directly if we now its reduced matrix element. For that, consider the auxiliary operator

$$\mathbf{B} = -2\mathbf{r} - i(\mathbf{r}(\mathbf{r}\cdot\mathbf{p}) - 2r^2\mathbf{p}) \tag{8}$$

and compute its commutator with H (without the new term).

g) By taking the expectation values of the result in f) with states at the same energy level (same n) but otherwise arbitrary, find a relation between the reduce matrix elements of $\mathbf{A}$ and $\mathbf{r}$.

h) Treating the dipole term as a perturbation, the shift in eigenvalues will be proportional to the expectation values just computed, write down a generic transition given by this interaction collecting the results and using the Wigner-Eckart theorem Eq. (6)