Prof. Dr. Hans Peter Büchler Institut für Theoretische Physik III, Universität Stuttgart 20. Dezember 2016 WS 2016/17

## Exercise 1: Spherical oscillator (Written, 8 Pts.)

In this exercise we diagonalize the three dimensional, isotropic harmonic oscillator, given by the Hamiltonian

$$H_{\rm 3D} = \frac{\mathbf{p}^2}{2m} + \frac{m\omega^2}{2} \mathbf{x}^2, \qquad (1)$$

in two ways. Here, **x** and **p** obey canonical commutation relations:  $[x_i, p_j] = i\hbar \delta_{ij}$ .

The simplest method to diagonalize  $H_{3D}$  is the following:

a) Show that  $H_{3D}$  can be decomposed into the sum of three one-dimensional harmonic oscillators. Thereby derive the eigenvectors and eigenvalues of  $H_{3D}$  and comment on the degeneracy of energy levels.

In the remainder of this exercise, we follow an alternative route to diagonalize  $H_{3D}$  in analogy to the Hydrogen atom (known from the lecture):

- b) Show that  $[\mathbf{L}^2, H] = 0 = [L_z, H]$ . Similarly to the derivation of the Hydrogen atom, show that angular and radial dependence can be separated and write  $H_{3D}$  in spherical coordinates with angular momentum operators.
- c) Make the ansatz

$$\Psi(\mathbf{r}) = \frac{x_l(r)}{r} Y_{lm}(\phi, \theta) \tag{2}$$

for the eigenfunctions and derive a differential equation for the radial component  $x_l(r)$ . Here,  $Y_{lm}(\phi, \theta)$  are the spherical harmonics that were introduced in the lecture.

d) Define  $\rho \equiv \sqrt{m\omega/\hbar r}$  and  $\varepsilon \equiv 2E/\hbar\omega$  and show that the DGL takes the form

$$-\partial_{\rho}^{2}x_{l} + \left[\frac{l(l+1)}{\rho^{2}} + \rho^{2}\right]x_{l} = \varepsilon x_{l}.$$
(3)

Consider the asymptotic behaviour of the latter for  $\rho \to \infty$  and  $\rho \to 0$  and show that this suggests the ansatz

$$x_l(\rho) = e^{-\rho^2/2} \rho^{l+1} \sum_{n=0}^{\infty} a_n \rho^n \,.$$
(4)

Show that the recursion relation for the coefficients  $a_n$  reads

$$a_{n+2} = \frac{2(n+l+1) - (\varepsilon - 1)}{(n+l+3)(n+l+2) - l(l+1)} a_n$$
(5)

and explain why  $a_n = 0$  for odd n.

Finally, determine the eigenvalues of  $H_{3D}$  and comment on the degeneracy. Compare your result with a).

## Exercise 2: Runge-Lenz vector (Written, 6 Pts. + 2 Bonus Pts.)

In classical mechanics, Kepler problems<sup>1</sup> feature an additional conserved quantity ("integral of motion") called the *Runge-Lenz vector*  $\mathbf{M}_{cl}$ . The latter lies within the plane of motion and is parallel to the major axis of the elliptical orbit. *Classically* one finds

$$\mathbf{M}_{\rm cl} = \frac{1}{me^2} \mathbf{L} \wedge \mathbf{P} + \frac{\mathbf{Q}}{Q} \qquad \text{with the Hamiltonian} \qquad H_{\rm cl} = \frac{\mathbf{P}^2}{2m} - \frac{e^2}{Q} \tag{6}$$

where  $\mathbf{P}$  and  $Q = \|\mathbf{Q}\|$  are relative momenta and coordinates of the two constituents. If the theory is quantized,  $\mathbf{P}$  and  $\mathbf{Q}$  become operators with canonical commutation relations:  $[Q_i, P_j] = i\hbar\delta_{ij}$ . This yields the Hamiltonian of the Hydrogen atom known from the lecture:

$$H = \frac{\mathbf{P}^2}{2m} - \frac{e^2}{Q} \tag{7}$$

There is, however, a subtlety in quantizing the Runge-Lenz vector  $\mathbf{M}_{cl}$ : Simply replacing  $\mathbf{P}$ ,  $\mathbf{L}$  and  $\mathbf{Q}$  by operators in  $\mathbf{M}_{cl}$  yields a non-hermitian operator,  $\mathbf{M}_{cl}^{\dagger} \neq \mathbf{M}_{cl}$  (Why?). This clashes with the requirement of a *measurable* conserved quantity.

Thus one defines the symmetrized version

$$\mathbf{M} := \frac{1}{2me^2} \left( \mathbf{L} \wedge \mathbf{P} - \mathbf{P} \wedge \mathbf{L} \right) + \frac{\mathbf{Q}}{Q}$$
(8)

of the Runge-Lenz vector (operator) with  $\mathbf{M}^{\dagger} = \mathbf{M}$  (Why?) and square

$$\mathbf{M}^2 = \frac{2}{me^4} H\left(\mathbf{L}^2 + \hbar^2 \mathbb{1}\right) + \mathbb{1} .$$
(9)

a) Show the following:

$$\mathbf{M} \cdot \mathbf{L} = 0 \tag{10a}$$

$$\left[\mathbf{L}^2, \mathbf{M}^2\right] = 0 \tag{10b}$$

$$\left[L_z, \mathbf{M}^2\right] = 0 \tag{10c}$$

$$[L_i, M_j] = i\hbar \varepsilon_{ijk} M_k \tag{10d}$$

$$[H, \mathbf{M}] = 0 \tag{10e}$$

In conclusion, we found that H,  $L^2$ ,  $L_z$ , and  $M^2$  define a set of pairwise commuting observables, i.e., there is a basis in which all four operators are diagonal.

Hints: The following may be useful:

- Write  $(\mathbf{v} \wedge \mathbf{w})_i = \varepsilon_{ijk} v_j w_k$  in terms of the Levi-Civita symbol  $\varepsilon_{ijk}$ .
- Use the relation  $\varepsilon_{ijk}\varepsilon_{ilm} = \delta_{jl}\delta_{km} \delta_{jm}\delta_{kl}$  where Einstein notation is used.

<sup>&</sup>lt;sup>1</sup>Two bodies interacting via a radially symmetric inverse square-law force. For instance: planetary motion ruled by gravitation, the Hydrogen atom with the Coulomb force, etc..

- Use that  $[L_i, V_j] = i\hbar\varepsilon_{ijk} V_k$  if **V** is a vector operator.
- Derive and use the commutator  $[1/Q, P_k] = -i\hbar \frac{Q_k}{Q^3}$ .

b\*) Desperately looking for more commutators to evaluate? Then show that

$$[M_i, M_j] = -\frac{2i\hbar}{me^4} \varepsilon_{ijk} H L_k \,. \tag{11}$$

**Hint:** Prove and use the relation  $(\mathbf{L} \wedge \mathbf{P})_j = -(\mathbf{P} \wedge \mathbf{L})_j + 2i\hbar P_j$ . Relations derived in a) and given in the previous hint may also be useful.

## Exercise 3: Hydrogen Atom – An algebraic approach (Oral)

We now bring in the harvest of the (technical) previous task with a derivation of the Hydrogen atom energy levels (i.e., the spectrum of H) by purely algebraic means. Historically, this was first achieved by WOLFGANG PAULI even *before* ERWIN SCHRÖDINGER published his famous equation.

a) Let  $\mathbf{N} := \mathbf{M}/\sqrt{\lambda}$  with  $\lambda \in \mathbb{R}_+$ . Determine  $\lambda$  such that the following algebra is satisfied:

$$[L_i, L_j] = i\hbar \varepsilon_{ijk} L_k \tag{12a}$$

$$[L_i, N_j] = i\hbar \varepsilon_{ijk} N_k \tag{12b}$$

$$[N_i, N_j] = i\hbar \varepsilon_{ijk} L_k \tag{12c}$$

**Hint**: Use Eq. (11) and that H commutes with all operators  $N_i$  and  $L_i$  and therefore can be replaced by its eigenvalue.

b) Define the new operators

$$\mathbf{A} := \frac{1}{2} \left( \mathbf{L} + \mathbf{N} \right) \quad \text{and} \quad \mathbf{B} := \frac{1}{2} \left( \mathbf{L} - \mathbf{N} \right)$$
(13)

and derive their commutator algebra.

- c) Derive the eigenvalues<sup>2</sup> of  $A^2$  and  $B^2$  by comparison with the known angular momentum algebra.
- d) Define the new operators<sup>3</sup>

$$C_1 := \mathbf{A}^2 + \mathbf{B}^2 \qquad \text{and} \qquad C_2 := \mathbf{A}^2 - \mathbf{B}^2 \tag{14}$$

and show that  $C_1 = \frac{1}{2} (\mathbf{L}^2 + \mathbf{N}^2)$  and  $C_2 = 0$ . Conclude that the eigenvalues of  $\mathbf{A}^2$  and  $\mathbf{B}^2$  coincide.

e) Use Eq. (9) to derive a relation between H and  $\mathbf{L}^2$ ,  $\mathbf{N}^2$  and solve it for H. Finally, derive the eigenvalues of H from the eigenvalues of  $\mathbf{L}^2 + \mathbf{N}^2$  and compare them with the results from the lecture. Be happy.

 $<sup>^{2}...</sup>$  for irreducible representations.

<sup>&</sup>lt;sup>3</sup>In the theory of Lie algebras, those are known as *Casimir operators*. The Casimir operator of the angular momentum algebra is  $\mathbf{L}^2$  and characterized by  $[L_i, \mathbf{L}^2] = 0$  for all *i*.

Our christmas present for you:

There are no exercises on this page!

