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Problem 8.1: Bound states of a spherical potential well **[Oral] (3 pts.)**

↪ ID: ex_bound_states_spherical_potential_well:qm2122

> **Learning objective**
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> Here you derive the bound states of a spherically symmetric potential well. To do so, you exploit the rotation symmetry of the problem and show that the radial solutions are given by *spherical Bessel functions*. You explicitly derive the transcendental equation that determines the eigenenergies for bound states with angular momentum $l = 0$.

Consider the Hamiltonian of a particle in three dimensions

$$H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r}) \tag{1}$$

with the spherically symmetric and piecewise constant potential

$$V(\boldsymbol{r}) = V(r) = \begin{cases} 0 & r > R \\ V_0 & r \leq R \end{cases} \tag{2}$$

with $r = |\boldsymbol{r}|$, $R > 0$ the radius of the potential well and $V_0 < 0$ the potential depth.

Your goal is to find the bound states and eigenenergies of this system and the conditions that are necessary for their existence.

a) Make the separation ansatz $\Psi(\boldsymbol{r}) = R_l(r) \cdot Y_{lm}(\theta, \varphi)$ with spherical harmonics Y_{lm} and show that the eigenvalue problem reduces to

$$\left[\rho^2 \partial_\rho^2 + 2\rho\partial_\rho + \rho^2 - l(l+1)\right] \tilde{R}_l(\rho) = 0 \tag{3}$$

with $\rho \equiv K_r r$ and $\tilde{R}_l(\rho) \equiv R_l(r)$ where $K_r \equiv \sqrt{\frac{2m(E-V(r))}{\hbar^2}}$.

b) Write down the general solution of the radial problem in the two regions $r > R$ and $r \leq R$ for a given angular momentum l and formulate the continuity and boundary conditions that the eigenstates must satisfy.

Hint: Use that the solutions of the differential equation

$$\left[x^2 \partial_x^2 + 2x\partial_x + x^2 - l(l+1)\right] y(x) = 0 \tag{4}$$

are given by the *spherical Bessel functions*

$$j_l(x) = (-x)^l \left(\frac{1}{x}\partial_x\right)^l \frac{\sin(x)}{x} \quad \text{and} \quad y_l(x) = -(-x)^l \left(\frac{1}{x}\partial_x\right)^l \frac{\cos(x)}{x} \tag{5}$$

for $l \in \mathbb{N}_0$. (The functions y_l are sometimes denoted n_l and referred to as *spherical Neumann functions*.) Write the eigenstates in terms of these functions.

c) Consider the simplest case for $l = 0$. Find explicit expressions for the bound states and derive a transcendental equation to determine their eigenenergies. At which potential depth V_0 appears the first bound state?

Hint: Use your knowledge of the one-dimensional potential well to analyze the transcendental equation.

Problem 8.2: Bound state of a pseudo potential in three dimensions [Oral] (3 pts.)

↪ ID: ex_bound_state_pseudo_potential_three_dimensions:qm2122

Learning objective

In a previous exercise you derived the bound state of a delta potential in one dimension. Here you show that a delta potential in *three* dimensions leads to inconsistencies. To allow for bound state solutions that are singular at the origin, the delta potential must be modified to a so called *pseudo potential*. Your goal is then to derive the bound state and its energy of this pseudo potential.

We are interested in the bound states of the Hamiltonian in three dimensions

$$\tilde{H} = \frac{\boldsymbol{p}^2}{2m} + \tilde{V}(\boldsymbol{r}) \quad \text{with} \quad \tilde{V}(\boldsymbol{r}) = g\,\delta^{(3)}(\boldsymbol{r})\,\partial_r r\,. \tag{6}$$

Here $\delta^{(3)}(\boldsymbol{r})$ is the delta distribution in three dimensions and $r = |\boldsymbol{r}|$; $\tilde{V}(\boldsymbol{r})$ is known as a *pseudo potential* (note that $\tilde{V}$ acts as a *differential operator* on the wave function) with coupling strength $g \in \mathbb{R}$.

a) To understand the necessity for $\tilde{V}$, consider instead the true delta potential $V(\boldsymbol{r}) = g\,\delta^{(3)}(\boldsymbol{r})$ in three dimensions (and the corresponding Hamiltonian H). Show that solving for bound states leads to inconsistencies.

What happens in one dimension? Compare your results to the bound state energy derived in Problem 5.2. What is the condition on the coupling g for the bound state to exist?

Hint: Fourier transform the stationary Schrödinger equation and solve it. Then invert the Fourier transform to find an expression for the candidate bound state and set $\boldsymbol{r} = \boldsymbol{0}$ to derive an equation for the eigenenergy.

b) Show that the modification $V \mapsto \tilde{V}$ does not alter the action of H on non-singular wave functions $\psi(\boldsymbol{r})$, i.e., show that $H\psi = \tilde{H}\psi$.

c) Show that the pseudo potential Hamiltonian $\tilde{H}$ has a bound state and determine its energy as a function of g and m. Comment on the sign of the coupling g that is necessary for the bound state to exist and compare this to the result in one dimension (for the true delta potential).

Hint: Use that the Green's function of the Helmholtz equation, i.e., the solution of the differential equation

$$\left[\Delta + k^2\right] G(\boldsymbol{r}) = -\delta^{(3)}(\boldsymbol{r}) \tag{7}$$

with the boundary condition $\lim_{|\boldsymbol{r}|\to\infty} G(\boldsymbol{r}) = 0$, is given by $G(\boldsymbol{r}) = \frac{e^{ikr}}{4\pi r}$ with $r = |\boldsymbol{r}|$.

Problem 8.3: Runge-Lenz vector **[Written] (5 pts.)**

↪ ID: ex_runge_lenz_vector:qm2122

Learning objective

You have learned that H, $\boldsymbol{L}^2$, and L_z are conserved quantities of a particle in a three-dimensional, rotational symmetric potential. In this exercise, you show that if the potential behaves as $V(r) \propto \frac{1}{r}$, there is an additional conserved quantity $\boldsymbol{M}^2$ where $\boldsymbol{M}$ is the quantized *Runge-Lenz vector.*

In classical mechanics, Kepler problems[1] feature a conserved quantity ("integral of motion") called the *Runge-Lenz vector* $\boldsymbol{M}_{\text{cl}}$. The latter lies within the plane of motion and is parallel to the major axis of the elliptical orbit. *Classically* one finds

$$\boldsymbol{M}_{\text{cl}} = \frac{1}{me^2}\boldsymbol{L}\times\boldsymbol{p} + \frac{\boldsymbol{q}}{q} \qquad \text{with the Hamiltonian} \qquad H_{\text{cl}} = \frac{\boldsymbol{p}^2}{2m} - \frac{e^2}{q} \tag{8}$$

where $\boldsymbol{p}$ and $q = \|\boldsymbol{q}\|$ are relative momenta and coordinates of the two constituents. If the theory is quantized, $\boldsymbol{p}$ and $\boldsymbol{q}$ 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:

$$H = \frac{\boldsymbol{p}^2}{2m} - \frac{e^2}{q}\,. \tag{9}$$

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

Thus one defines the symmetrized version

$$\boldsymbol{M} := \frac{1}{2me^2}\left(\boldsymbol{L}\times\boldsymbol{p} - \boldsymbol{p}\times\boldsymbol{L}\right) + \frac{\boldsymbol{q}}{q} \tag{10}$$

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

$$\boldsymbol{M}^2 = \frac{2}{me^4}\,H\left(\boldsymbol{L}^2 + \hbar^2\mathbb{1}\right) + \mathbb{1}\,. \tag{11}$$

a) Show the following commutation relations:

$$\begin{aligned} \boldsymbol{M}\cdot\boldsymbol{L} &= 0 && \text{(12a)}\\ \left[\boldsymbol{L}^2, \boldsymbol{M}^2\right] &= 0 && \text{(12b)}\\ \left[L_z, \boldsymbol{M}^2\right] &= 0 && \text{(12c)}\\ \left[L_i, M_j\right] &= i\hbar\,\varepsilon_{ijk}M_k && \text{(12d)}\\ \left[H, \boldsymbol{M}\right] &= 0 && \text{(12e)} \end{aligned}$$

In conclusion, we found that H, $\boldsymbol{L}^2$, L_z, and $\boldsymbol{M}^2$ 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:

[1] 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.

- Write $(\boldsymbol{v} \times \boldsymbol{w})_i = \varepsilon_{ijk} v_j w_k$ in terms of the Levi-Civita symbol ε_{ijk}.
- Use the relation $\varepsilon_{ijk}\varepsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$ where Einstein notation is used.
- Use that $[L_i, V_j] = i\hbar\varepsilon_{ijk} V_k$ if $\boldsymbol{V}$ 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

$$[M_i, M_j] = -\frac{2i\hbar}{me^4}\,\varepsilon_{ijk} H L_k\,. \tag{13}$$

Hint: Prove and use the relation $(\boldsymbol{L} \times \boldsymbol{p})_j = -(\boldsymbol{p} \times \boldsymbol{L})_j + 2i\hbar p_j$. Relations derived in a) and given in the previous hint may also be useful.