# **Problems Chapter 6**

**Quantum Mechanics** K. Konishi, G. Paffuti

## **Problem 1**

A particle of mass m moves in a radial potential

$$\begin{array}{ll} & \infty \,, & r < R \\ & V[r] = \left\{ \begin{array}{ll} 0 \,, & R \leq r \leq R + a \\ & \infty \,, & r > R + a \end{array} \right. , \end{array}$$

We want to study the spectrum of the system.

- 1. Show that the stationary solutions can be separated in spherical coordinates and write the correct boundary conditions for the radial part of the wave function.
- 2. Find the equation which implicitly determines the energy levels at fixed L (angular momentum).
- **3.** Solve the equation of question 2 for L=0.
- 4. Show that for a « R the first excited state has energy  $\Delta E = \hbar^2 / m R^2$  above the ground state. Explain this result on physical grounds.

#### • Solution

**1** 

The Hamiltonian is rotation invariant, then the angular momentum is conserved and  $L^2$ ,  $L_z$  can be diagonalized with H. The eigenstates of H are written as

$$\psi_{nLm}[\mathbf{r}] = R_{n,L}[\mathbf{r}] Y_{Lm}[\Theta, \varphi].$$
(1.1)

The boundary conditions for  $R_{n\rm L}$  are

chap6prob0eq2

$$R_{nL}[R] = R_{nL}[R + a] = 0.$$
 (1.2)

**■** 2

#### The radial functions satisfy the equation

chap6prob0eq3

$$\frac{d^{2}}{dr^{2}} R_{nL}[r] + \frac{2}{r} \frac{d}{dr} R_{nL}[r] + \left(k^{2} - \frac{L(L+1)}{r^{2}}\right) R_{nL}[r] = 0; \quad R \le r \le R+a.$$
(1.3)

with

$$R_{nL} = 0 \mbox{ for } (r < R \mbox{, } r > R + a) \mbox{, } \mbox{ and } \mbox{ } k = \frac{\sqrt{2\,m\,E}}{\hbar} \mbox{.}$$

Equation (3) is the free particle equation with wave number k and its general solution is

chap6prob0eq4

$$R_{nL}[r] = A j_{L}[kr] + B \eta_{L}[kr].$$
(1.4)

 $j_{L}$  and  $\eta_{L}$  are spherical Bessel functions, regular and singular (resp.ly) at the origin.  $\eta_{L}$  (often donoted as  $n_{L}$ ) is known also as

spherical Neuman functions.

Conditions (2) give

chap6prob0eq5

$$A j_{L}[k R] + B \eta_{L}[k R] = 0; \quad A j_{L}[k (R + a)] + B \eta_{L}[k (R + a)] = 0.$$
(1.5)

The linear system (5) has non trivial solutions if

## 2 Problems\_chap6.nb

chap6prob0eq6

$$det \begin{pmatrix} j_{L}[k R] & \eta_{L}[k R] \\ j_{L}[k (R+a)] & \eta_{L}[k (R+a)] \end{pmatrix} = 0.$$

$$(1.6)$$

This equation is satisfied only for a discrete set of k, which gives the energy eigenvalues with  $E = \hbar^2 k^2 / 2 m$ .

**3** 

For L = 0

$$j_{0}[kr] = \frac{Sin[kr]}{kr}; \quad \eta_{0}[kr] = -\frac{Cos[kr]}{kr}; \quad (1.7)$$

and condition (6) gives

$$Sin[kR] Cos[k(R+a)] - Sin[k(R+a)] Cos[kR] = - Sin[ka] = 0$$
,

with solutions

$$k_{n} = \frac{\pi n}{a}; \quad E_{n} = \frac{\pi^{2} n^{2} \hbar^{2}}{2 m a^{2}}.$$
(1.8)

These solutions are identical to the solutions for a one dimensional well, as could be guessed from the equation (3) by passing to the reduced wave functions.

**4** 

For a  $\ll R$  the centrifugal term in H is almost constant inside the shell R r R+a, therefore its contribution can be regarded as constant. The energy levels are those of L=0 shifted by the centrifugal energy

$$E_{nL} \simeq \frac{\pi^2 n^2 \tilde{h}^2}{2 m a^2} + \frac{\tilde{h}^2 L (L+1)}{2 m R^2}, \quad n = 1, 2, 3, \dots; L = 0, 1, 2, \dots$$
(1.9)

The shifts due to the radial excitations are much higher than angular momentum excitations, as  $a \ll R$ ; the first excited state is (n=1, L=1). The shift with respect to the ground state is

$$\Delta \mathbf{E} = \frac{\hbar^2}{2\,\mathrm{m\,R}^2} = \frac{\hbar^2}{\mathrm{m\,R}^2} \,.$$

The request to have two consecutive zeros for radial functions in a small interval  $a \ll R$  imply that the wave number must be very high,  $k \sim \pi/a$ . The corresponding energy differences are very big and in a first approximation the particle is "frozen" in a radial shell. The energy eigenvalues then must be given by the eigenvalues of a symmetric top, i.e.

$$E \simeq \text{const.} + \frac{\hbar^2 L (L+1)}{2 m R^2}$$

as we have found indeed.

These conclusions can be obtained in a more formal way as follows. Put x = k R, y = k a. As discussed above we have to perform the limit  $a \rightarrow 0$  with (k a) fixed. This is also confirmed by the fact that a series expansion in a of the condition (6) gives

$$0 = \frac{a (-a + R)}{k R^3}$$

which has no solutions in k. For large k, x = k R is large, then we can use asymptotic expansion of spherical Bessel functions:

$$\mathbf{j}_{\mathrm{L}}[\mathbf{x}] \sim \sqrt{\frac{\pi}{2}} \left( \frac{\left(\mathbf{L} + \mathbf{L}^{2}\right) \operatorname{Cos}\left[\frac{\mathbf{L}\pi}{2} - \mathbf{x}\right]}{\sqrt{2\pi} \mathbf{x}^{2}} - \frac{\sqrt{\frac{2}{\pi}} \operatorname{Sin}\left[\frac{\mathbf{L}\pi}{2} - \mathbf{x}\right]}{\mathbf{x}} \right);$$
$$\eta_{\mathrm{L}}[\mathbf{x}] \sim \sqrt{\frac{\pi}{2}} \left( -\frac{\sqrt{\frac{2}{\pi}} \operatorname{Cos}\left[\frac{\mathbf{L}\pi}{2} - \mathbf{x}\right]}{\mathbf{x}} - \frac{\left(\mathbf{L} + \mathbf{L}^{2}\right) \operatorname{Sin}\left[\frac{\mathbf{L}\pi}{2} - \mathbf{x}\right]}{\sqrt{2\pi} \mathbf{x}^{2}} \right)$$

Substitution in (6) gives

$$\frac{-2 L (1 + L) Y Cos[Y] + (L^{2} (1 + L)^{2} + 4 x (x + Y)) Sin[Y]}{4 x^{2} (x + Y)^{2}} = 0.$$

The leading solution  $y = n \pi$  corresponds to the eigenvalues of the one dimensional shell. Writing  $y = n \pi + \xi$ , x = y R/a, and expanding  $\xi$  we can easily get

$$\xi = \frac{a^2 L (1 + L)}{2 n \pi R^2};$$

The eigenvalues follow

$$k = \frac{1}{a} \left( n \pi + \frac{a^2 L (1 + L)}{2 n \pi R^2} \right); \quad E = \frac{\hbar^2}{2 m} k^2 \simeq \frac{n^2 \pi^2}{2 m a^2} + \frac{L (L + 1)}{2 m R^2} + O[a]^2$$

in agreement with previous results. As already noted, the first two terms have simple physical interpretations. The first term represents the radial excitations, which are just those inside a one-dimensional infinite well of width a. The second term represents rotational modes at fixed radius R, which are given by the centrifugal energy only.

## prob1nInfinity

## Problem 2

*Compute the limit of radial hydrogen wavefunctions as*  $n \rightarrow \infty$ *.* 

#### Solution

We work in atomic units. Radial eigenfunctions are given by (we use Mathematica notation for Laguerre polynomials)

prob1radialeq

$$R[n, L, r] = Z^{3/2} \frac{2}{n^2} \sqrt{\frac{(n-L-1)!}{(n+L)!}} \left(\frac{2 Z r}{n}\right)^L e^{-\frac{r}{n}} LaguerreL[n-L-1, 2L+1, \frac{2 Z r}{n}]$$
(2.1)

They satisfy the radial Schrödinger equation

prob1radialequation

$$\frac{d^{2}R}{dr^{2}} + \frac{2}{r}\frac{dR}{dr} - \frac{L(L+1)}{r^{2}}R + 2\left(E_{n} + \frac{Z}{r}\right)R = 0; \quad E_{n} = -\frac{1}{2n^{2}}.$$
(2.2)

We see that the large n limit of (1),  $R_{as}$  must be a regular solution of (2) with E =0, the large n limit of the eigenvalues:

prob1radialequationas

$$\frac{d^{2} R_{as}}{dr^{2}} + \frac{2}{r} \frac{d R_{as}}{dr} - \frac{L (L+1)}{r^{2}} R_{as} + \frac{2}{r} R_{as} = 0.$$
(2.3)

The general solution of this equation is

$$C_{1} \frac{\text{BesselJ} \left[1+2 \text{L}, 2 \sqrt{2 \text{Zr}}\right]}{\sqrt{2 \text{Zr}}} + C_{2} \frac{\text{BesselY} \left[+1+2 \text{L}, 2 \sqrt{2 \text{Zr}}\right]}{\sqrt{2 \text{Zr}}}$$

as the reader can check using DSolve in *Mathematica* or by making the substitution  $r = x^2/(8Z)$ , R = f[x]/x in (2). Regularity at origin imply  $C_2 = 0$ . To fix  $C_1$  we have to match the normalization of equation (1). From the definition of Laguerre polynomials, see notebook [\*], it follows

$$L_n^{\lambda}(0) = \binom{n}{\lambda}$$

then, as  $r \rightarrow 0$ 

$$R[n, L, r] \rightarrow Z^{3/2} \frac{2}{n^2} \sqrt{\frac{(n-L-1)!}{(n+L)!}} \left(\frac{2 Z r}{n}\right)^L \frac{(n-L-1)!}{(2 L+1)! (n-3 L-2)!}$$

For large n the Stirling formula gives

$$\frac{(n-L-1)!}{(n+L)!} \rightarrow \left(\frac{1}{n}\right)^{1+2L}; \quad \frac{(n-L-1)!}{(n-3L-2)!} \rightarrow \left(\frac{1}{n}\right)^{-1-2L};$$

thus for small r and large n

$$R[n, L, r] \rightarrow \frac{2 Z^{3/2}}{n^{3/2}} \frac{(2r)^{L}}{(2L+1)!}$$

## 4 Problems\_chap6.nb

The Taylor expansion of the Bessel function starts with

$$\frac{\text{BesselJ}\left[1+2\text{L}, 2\sqrt{2\text{Z}\text{r}}\right]}{\sqrt{2\text{Z}\text{r}}} \rightarrow \frac{1}{\sqrt{2\text{Z}\text{r}}} \left(\sqrt{2\text{Z}\text{r}}\right)^{2\text{L}+1} \frac{1}{(2\text{L}+1)!} = \frac{(2\text{Z}\text{r})^{\text{L}}}{(2\text{L}+1)!};$$

from which we have finally

$$C_{1} = \frac{2 z^{3/2}}{n^{3/2}}; \qquad R_{as}[n, L, r] = \frac{2 z^{3/2}}{n^{3/2}} \frac{\text{BesselJ}\left[1 + 2 L, 2 \sqrt{2 Z r}\right]}{\sqrt{2 Z r}}$$
(2.4)

In terms of Laguerre's polynomials what we have proved can be stated as (see also [1]):

$$L\left[n, \alpha, \frac{x}{n}\right] \xrightarrow[n \to \infty]{} n^{\alpha} x^{-\alpha/2} J_{\alpha}\left[2 \sqrt{x}\right]$$
(2.5)

## • References

prob15ref1

[1] I.S. Gradshteyn, I.M. Ryzhik: Table of integrals series and products, Academic Press; (1965).

#### prob1nInfinity

## **Problem 3**

Explain the n<sup>2</sup> degeneracy of the Hydrogen energy levels, by making use of the fact that the Lenz vector

$$\mathbf{A} = \frac{\mathbf{r}}{\mathbf{r}} - \frac{1}{\mathbf{z}} \frac{1}{\mathbf{z}} (\mathbf{p} \wedge \mathbf{L} - \mathbf{L} \wedge \mathbf{p})$$

commutes with H.

#### Solution

The degeneracy  $n^2$  is due to a higher symmetry peculiar to the Coulomb interaction. The additional conserved quantity is known from classical mechanics, and is called Lenz vector [1]. In atomic units:

$$\mathbf{A} = \frac{\mathbf{r}}{r} - \frac{1}{Z} \frac{1}{2} (\mathbf{p} \wedge \mathbf{L} - \mathbf{L} \wedge \mathbf{p})$$
(3.1)

A is hermitian:

$$(\varepsilon_{ijk} p_j L_k)^* = \varepsilon_{ijk} L_k p_j = -\varepsilon_{ikj} L_k p_j = -(\mathbf{p} \wedge \mathbf{L})_i$$

Let us also note the identity

$$\varepsilon_{ijk} L_j p_k = \varepsilon_{ijk} p_k L_j + i \varepsilon_{ijk} \varepsilon_{jka} p_a = -(\mathbf{p} \wedge \mathbf{L})_i + 2i p_i \Rightarrow \mathbf{A} = \frac{\mathbf{r}}{\mathbf{r}} - \frac{1}{\mathbf{Z}} (\mathbf{p} \wedge \mathbf{L} - i\mathbf{p}).$$

By a systematic use of the identity [A B,C] = A[B,C] + [A,C]B it is simple to find

$$\frac{1}{2} \left( \mathbf{p} \wedge \mathbf{L} - \mathbf{L} \wedge \mathbf{p} \right), \frac{1}{r} \right] = i \left( \frac{\mathbf{r}}{r^3} \left( \mathbf{r} \cdot \mathbf{p} \right) - \frac{1}{r} \mathbf{p} \right) + \frac{\mathbf{r}}{r^3};$$
$$\left[ \frac{\mathbf{r}}{r}, \frac{\mathbf{p}^2}{2} \right] = i \left( -\frac{\mathbf{r}}{r^3} \left( \mathbf{r} \cdot \mathbf{p} \right) + \frac{1}{r} \mathbf{p} \right) - \frac{\mathbf{r}}{r^3}$$

From which the conservation of A for a Coulomb potential with charge Z follows:

$$[\mathbf{A}, \mathbf{H}] = \left[\mathbf{A}, \frac{\mathbf{p}^2}{2} - \frac{\mathbf{Z}}{\mathbf{r}}\right] = \mathbf{0}.$$

With some more work with commutators one can verify the correct commutation relations with angular momentum (as any vector) and the commutation relations among different **A** components:

AlgebraVettoreLenz

$$\begin{bmatrix} L_{i}, A_{j} \end{bmatrix} = i \varepsilon_{ijk} A_{k}; \quad \begin{bmatrix} A_{i}, A_{j} \end{bmatrix} = \begin{pmatrix} -\frac{2H}{Z^{2}} \end{pmatrix} i \varepsilon_{ijk} L_{k}$$
(3.2)

Consider now the subspaces of the Hilbert space with fixed energy. In this subspace we can diagonalize simultaneously, for example,  $L^2$  and  $L_z$ , as

usually done in any central potential, or  $L_z$  and  $A_z$ . But  $A_z$  and  $L^2$  do not commute so, for fixed  $L_z$  there must be a degeneracy. A complete set of commuting variables is given by H,  $L_z$ ,  $A_z$ .

Starting from algebra (2) it is easy to find the negative energy spectrum. Defining  $\mathbf{u} = \mathbf{A} Z/\sqrt{-2 E}$  we have

$$\begin{bmatrix} \mathbf{L}_{i}, \mathbf{L}_{j} \end{bmatrix} = \mathbf{i} \, \varepsilon_{ijk} \, \mathbf{L}_{k}; \quad \begin{bmatrix} \mathbf{L}_{i}, \mathbf{u}_{j} \end{bmatrix} = \mathbf{i} \, \varepsilon_{ijk} \, \mathbf{u}_{k}; \quad \begin{bmatrix} \mathbf{u}_{i}, \mathbf{u}_{j} \end{bmatrix} = \mathbf{i} \, \varepsilon_{ijk} \, \mathbf{L}_{k}$$

This is the algebra of the group  $SU(2) \otimes SU(2)$  as is evident introducing

$$\mathbf{j}_1 = \frac{1}{2} (\mathbf{L} + \mathbf{u}) \mathbf{i} \quad \mathbf{j}_2 = \frac{1}{2} (\mathbf{L} - \mathbf{u})$$

which, from previous relations, satisfy

$$\left[\mathbf{j}_{1,i} \mathbf{j}_{1,j}\right] = \mathbf{i} \varepsilon_{ijk} \mathbf{j}_{1,k}; \quad \left[\mathbf{j}_{2,i} \mathbf{j}_{2,j}\right] = \mathbf{i} \varepsilon_{ijk} \mathbf{j}_{2,k}; \quad \left[\mathbf{j}_{1,i} \mathbf{j}_{2,j}\right] = \mathbf{0}.$$

The irreducibles representations are well known and we have

$${ j } _{1}^{2} = { j } _{1} \ ( { j } _{1} + 1 ) \ { ; } \ \ { j } _{2}^{2} = { j } _{2} \ ( { j } _{2} + 1 ) \ { ; } \ \ { j } _{1} \ { , } \ { j } _{2} \in \ \mathbb{N} \ / \ 2 \$$

Using

$$\mathbf{L} \cdot \mathbf{u} = \mathbf{u} \cdot \mathbf{L} = 0$$
;  $\Rightarrow$   $\mathbf{j}_1^2 = \mathbf{j}_2^2 = \mathbf{L}^2 + \mathbf{u}^2 = -1 - \frac{\mathbf{Z}^2}{2\mathbf{E}}$ 

and denoting by j the common semi-integer value  $j_1 = j_2$  it follows

$$E = -\frac{Z^2}{2(2j+1)^2} = -\frac{Z^2}{2n^2}; n = 2j+1 = 1, 2, \dots$$

i.e. the known spectrum. The degeneracy is given by the eigenvalues of  $j_{1,z}$ ,  $j_{2,z}$ , i.e.

$$(2 j_1 + 1) (2 j_2 + 1) = (2 j + 1)^2 = n^2;$$

as expected.

It is possible to show that eigenvalues of  $j_{1,z}$  and  $j_{2,z}$  are exactly related to parabolic quantum numbers  $n_1$  and  $n_2$ 

$$j_{1,z} = \frac{1}{2} (m + n_1 - n_2); \quad j_{1,z} = \frac{1}{2} (m - n_1 + n_2); \quad \Rightarrow \quad u_z = n_1 - n_2 \Rightarrow A_z = \frac{n_1 - n_2}{n}.$$

While energy is related to the sum  $(n_1 + n_2 + |m| + 1)$  the eigenvalues of Lenz vector is related to the difference of  $n_1$  and  $n_2$ .

#### References

ref1Parabolic

[1] One of the first deductions of the spectrum ot the hydrogen atom within Quantum Mechanics was due to Pauli, which used exactly the algebraic relations used in this section, W.Pauli: Zs. f. Phys. 36, (1926) 336. For a more recent review see for example D.Park, Z. Phys. 159, (1960), 155.

## Problem 4

Solve the Coulomb problem in parabolic coordinates  $(\xi, \eta, \varphi)$  defined by

$$\mathbf{x} = \sqrt{\xi \eta} \operatorname{Cos}[\varphi]; \mathbf{y} = \sqrt{\xi \eta} \operatorname{Sin}[\varphi]; \mathbf{z} = \frac{1}{2} (\xi - \eta);$$

## Solution

#### Definitions

Parabolic coordinates  $(\xi, \eta, \varphi)$  are defined by

$$\mathbf{x} = \sqrt{\xi \eta} \operatorname{Cos}[\varphi]; \mathbf{y} = \sqrt{\xi \eta} \operatorname{Sin}[\varphi]; \mathbf{z} = \frac{1}{2} (\xi - \eta);$$
$$\xi = \mathbf{r} + \mathbf{z}; \eta = \mathbf{r} - \mathbf{z}; \varphi = \operatorname{ArcTan}\left[\frac{\mathbf{y}}{\mathbf{x}}\right]; \mathbf{r} = \frac{1}{2} (\xi + \eta);$$

x,y,z are Cartesian coordinates, r and  $\varphi$  radius and azimuthal angle (rotation around z axis). Line element and Jacobian between parabolic and cartesian coordinates are easily seen to be

$$ds^{2} = h_{1}^{2} d\xi^{2} + h_{2}^{2} d\eta^{2} + h_{3}^{2} d\varphi^{2} = \frac{\xi + \eta}{4\xi} d\xi^{2} + \frac{\xi + \eta}{4\eta} d\eta^{2} + \xi \eta d\varphi^{2};$$
$$J = \sqrt{g} = h_{1} h_{2} h_{3} = \frac{\xi + \eta}{4};$$

From the general expression for laplacian in a curvilinear orthogonal system  $(u_1, u_2, u_3)$ 

$$\Delta f = \frac{1}{h_1 h_2 h_3} \sum \frac{\partial}{\partial u_1} \left( \frac{h_2 h_3}{h_1} \frac{\partial f}{\partial u_1} \right);$$

it follows that

$$\Delta = \frac{4}{\xi + \eta} \frac{\partial}{\partial \xi} \left( \xi \frac{\partial}{\partial \xi} \right) + \frac{4}{\xi + \eta} \frac{\partial}{\partial \eta} \left( \eta \frac{\partial}{\partial \eta} \right) + \frac{1}{\xi \eta} \frac{\partial^2}{\partial \varphi^2}$$

The range for these coordinates is

 $0 \leq (\xi, \eta) \leq \infty; \quad 0 \leq \varphi \leq 2\pi$ 

#### The Schrödinger equation

The Schrödinger equation for a Coulombic system (a nucleus of charge Ze and an electron of charge -e) in atomic units ( $\hbar = m = e = 1$ ) is

$$-\frac{1}{2}\left(\frac{4}{\xi+\eta}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right)+\frac{4}{\xi+\eta}\frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right)+\frac{1}{\xi\eta}\frac{\partial^{2}}{\partial\varphi^{2}}\right)\psi-\frac{2Z}{\xi+\eta}\psi=\mathbf{E}\psi,$$

or

$$\left(\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right) + \frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right) + \frac{\xi+\eta}{4\,\xi\,\eta}\frac{\partial^2}{\partial\varphi^2}\right)\psi + \left(\mathbf{Z} + \frac{\xi+\eta}{2}\mathbf{E}\right)\psi = \mathbf{0}\,.$$

The system is invariant under rotations around z axis, so eigenstates are of the form  $F[\xi,\eta] \operatorname{Exp}[i \mod \varphi]$ . We look for a solution by separation of variables

$$\psi = \mathbf{f}_1[\xi] \mathbf{f}_2[\eta] \operatorname{Exp}[\mathfrak{im} \varphi]$$

By substitution, after division by  $\psi$ , we have

$$\frac{1}{f_1} \left( \frac{d}{d\xi} \left( \xi \frac{df_1}{d\xi} \right) - \frac{m^2}{4\xi} f_1 + \frac{E}{2} \xi f_1 \right) + \frac{1}{f_2} \left( \frac{d}{d\eta} \left( \eta \frac{df_2}{d\eta} \right) - \frac{m^2}{4\eta} f_2 + \frac{E}{2} \eta f_2 \right) + Z = 0.$$

The first term depends only on  $\xi$ , the second only on  $\eta$ , since their sum is constant there must be two constant  $Z_1$  and  $Z_2$  such that

HydrogenParabolic1

$$\frac{\mathrm{d}}{\mathrm{d}\,\varepsilon} \left( \varepsilon \, \frac{\mathrm{d}\mathbf{f}_1}{\mathrm{d}\,\varepsilon} \right) + \left( \frac{\mathrm{E}}{2} \, \varepsilon - \frac{\mathrm{m}^2}{4 \, \varepsilon} + \mathbf{Z}_1 \right) \, \mathbf{f}_1 = 0;$$

$$\frac{\mathrm{d}}{\mathrm{d}\,\eta} \left( \eta \, \frac{\mathrm{d}\mathbf{f}_2}{\mathrm{d}\,\eta} \right) + \left( \frac{\mathrm{E}}{2} \, \eta - \frac{\mathrm{m}^2}{4 \, \eta} + \mathbf{Z}_2 \right) \, \mathbf{f}_2 = 0;$$

$$\mathbf{Z}_1 + \mathbf{Z}_2 = \mathbf{Z}.$$
(4.1)

If we look for normalizable solutions, the two differential equations (1) are eigenvalue equations with eigenvalues  $Z_{i}$ . These eigenvalues depend parametrically on E (changing E the equations change), The last constraint fixes E.

The two equations have the same structure, so let us consider only the first. We look for a regular solution as  $\xi \rightarrow 0$ , of the form  $\xi^{\alpha}$ . The term linear in  $\xi$  and the constant are negligible in this range:

$$0 \simeq \xi \mathbf{f}_1^{''} + \mathbf{f}_1^{'} - \frac{\mathbf{m}^2}{4 \xi} \mathbf{f}_1 \Rightarrow \alpha (\alpha - 1) + \alpha - \frac{\mathbf{m}^2}{4} = 0 \Rightarrow \alpha = |\mathbf{m}| / 2.$$

For large  $\xi$ , for an exponential depressed function, the dominant terms are

$$0 \simeq \xi \mathbf{f}_{1}' = \frac{\mathbf{E}}{2} \xi \mathbf{f}_{1} \Rightarrow \mathbf{f}_{1} = \exp\left[-\sqrt{-2 \mathbf{E}} \xi / 2\right].$$

As expected bounded solutions only exist for E < 0. Previous asymptotic behavior suggests the change of variables

$$f_1[\xi] = \xi^{|\mathfrak{m}|/2} \operatorname{Exp}[-\varepsilon \xi/2] \operatorname{F}[\xi]; \quad \text{with}: \quad \varepsilon = \sqrt{-2 \operatorname{E}} \ .$$

Substitution in (1) gives

$$\xi \frac{d^2 F}{d\xi^2} + (|m|+1 - \epsilon \xi) \frac{dF}{d\xi} + \left( Z_1 - \frac{|m|+1}{2} \epsilon \right) F = 0.$$

or, with  $z = \epsilon \xi$ 

hydrogenParabolic2

$$z \frac{d^{2} F}{d z^{2}} + (|m|+1-z) \frac{dF}{d z} + \left(\frac{Z_{1}}{\epsilon} - \frac{|m|+1}{2}\right) F = 0.$$
 (4.2)

This equation is of hypergeometric type, its solutions are confluent hypergeometric functions. The only solution regular at the origin and bounded not growing to fast at infinity (in such a way that  $\exp[-\epsilon \xi/2]$  F is bounded) corresponds to integer numbers for the second parenthesis.

$$\frac{\mathbb{Z}_1}{\varepsilon} - \frac{|\mathfrak{m}| + 1}{2} = \mathfrak{n}_1; \quad 0 \le \mathfrak{n}_1 \in \mathbb{N}.$$

$$(4.3)$$

In this case (2) is the defining equation for generalized Laguerre polynomials  $L_{n_1}^m(z)$ .

Exactly the same conclusions can be drawn from equation for  $\eta$ , obtaining

$$\frac{Z_2}{\epsilon} - \frac{\mid \mathfrak{m} \mid +1}{2} = \mathfrak{n}_2; \quad 0 \le \mathfrak{n}_2 \in \mathbb{N}.$$
(4.4)

The last constraint in (1) implies

$$\begin{array}{c} Z\\ -=\\ \epsilon \end{array} \mid \mathfrak{m} \mid +1 + \mathfrak{n}_1 + \mathfrak{n}_2 \equiv \mathfrak{n} \geq 1; \quad \Rightarrow \quad -\frac{Z^2}{2E} = \mathfrak{n}^2. \end{array}$$

$$(4.5)$$

For a fixed value of n clearly -(n-1) m (n-1), as  $n_1$  and  $n_2$  are nonnegative. The number of ways in which the sum of two non negative integers numbers (here  $n_1$  and  $n_2$ ) can give a fixed number k is N[k] = k+1. The number of states for fixed n, i.e. the degeneracy of the level is (we separate m=0 from m 0, in the last case  $\pm$  m gives the same contribution)

$$deg[n] = N[n-1] + 2\sum_{m=1}^{n-1} N[n-1-m] = n + 2\sum_{m=1}^{n-1} (n-m) = n^{2}$$

as expected.

The normalized wave functions are

HydrogenParabolicWaveFunctions

$$\psi_{n_{1}n_{2}m}[\xi, \eta, \varphi] := f_{n_{1}m}[\xi] f_{n_{2}m}[\eta] \frac{e^{im\varphi}}{\sqrt{2\pi}};$$

$$f_{n_{1}m}[\xi] = 2^{1/4} \varepsilon \sqrt{\frac{n!}{(n+|m|)!}} (\varepsilon \xi)^{|m|/2} e^{-\varepsilon \xi/2} L_{n}^{|m|}(\varepsilon \xi)$$
(4.6)

where, as before,  $\varepsilon = 1/(n_1 + n_2 + m + 1)$  and the scalar product is

$$\int \psi_{\mathbf{n}_1 \, \mathbf{n}_2 \, \mathfrak{m}} \star \psi_{\mathbf{k}_1 \, \mathbf{k}_2 \, \mathfrak{m}'} \; \; \frac{\xi + \eta}{4} \; \mathrm{d} \xi \; \mathrm{d} \eta \; \; \mathrm{d} \varphi \; = \; \delta_{\mathbf{n}_1 \, \mathbf{k}_1} \; \delta_{\mathbf{n}_2 \, \mathbf{k}_2} \; \delta_{\mathbf{m} \, \mathfrak{m}'}$$

The normalization constant in (6) is easily computed remembering that the functions

$$\sqrt{ \frac{n!}{(n+\mid m \mid) !}} (\mathbf{x})^{\mid m \mid / 2} e^{-\mathbf{x}/2} \mathbf{L}_{n}^{\mid m \mid} (\mathbf{x})$$

are an orthonormal set and using the recurrence relation for Laguerre polynomials

$$x L_n^{\alpha}(x) = -(n+\alpha) L_{n-1}^{\alpha}(x) - (n+1) L_{n+1}^{\alpha}(x) + (2n+\alpha+1) L_n^{\alpha}(x).$$

## **Problem 5**

A particle of mass m moves in a radial potential  $g_0 \delta(r - R)/4\pi R^2$ . Compute for small R the continuum eigenstates and the possible bound states.

#### Solution

We use natural units  $\hbar = m = 1$ . The Schrödinger equation for the reduced radial wave functions  $\varphi$  is

chap5prodeltaeq1

$$-\frac{1}{2}\frac{d^{2}}{dr^{2}}\varphi + \left(\frac{g_{0}}{4\pi R^{2}}\delta(r-R) + \frac{L(L+1)}{2r^{2}}\right)\varphi[r] = \frac{k^{2}}{2}\varphi[r].$$
(5.1)

Where  $E = k^2 / 2$ . We look for continuum solutions corresponding to scattering states, i.e. regular solutions with asymptotic behavior

$$\varphi \sim \operatorname{Sin}\left[\operatorname{kr} - \operatorname{L} \frac{\pi}{2} + \delta_{\operatorname{L}}\right]$$

For small R only s-waves (L=0) are involved in the scattering process so we limit ourselves to this case.

In the region r > R and r < R the solution can be conveniently written

chap5prodeltaeq2

$$\varphi_{+}[\mathbf{r}] = \mathbf{A} \left( \operatorname{Sin}[\mathbf{k}\mathbf{r}] + \operatorname{Tan}[\delta] \operatorname{Cos}[\mathbf{k}\mathbf{r}] \right); \quad \varphi_{-} = \mathbf{B} \operatorname{Sin}[\mathbf{k}\mathbf{r}].$$
(5.2)

Continuity and integration of (1) in a small region around r~R gives the condition

$$\frac{1}{2} \left( \frac{\varphi'_{+}[R]}{\varphi_{+}[R]} - \frac{\varphi'_{-}[R]}{\varphi_{-}[R]} \right) = \frac{g_{0}}{4 \pi R^{2}}, \quad \Rightarrow \ k \left( \frac{\operatorname{Cos}[k R] + \operatorname{Tan}[\delta] \operatorname{Sin}[k R]}{\operatorname{Sin}[k R] + \operatorname{Tan}[\delta] \operatorname{Cos}[k R]} - \frac{\operatorname{Cos}[k R]}{\operatorname{Sin}[k R]} \right) = \frac{g_{0}}{2 \pi R^{2}}.$$

Expanding for small R

$$\frac{1}{g_0} = -\frac{1}{2\pi R} - \frac{k \operatorname{Cot}[\delta]}{2\pi}$$

To define a sensible theory we can define a renormalized coupling (see complement of this chapter):

chap5prodeltaeq3

$$\frac{1}{g_0} + \frac{1}{2\pi R} = \frac{1}{g}.$$
 (5.3)

In terms of this coupling

$$\operatorname{Tan}[\delta] = -\frac{\mathrm{k}\,\mathrm{g}}{2\,\pi}.\tag{5.4}$$

#### Bound states

With E =  $-\mu^2/2$  the Schrödinger equation has a regular solution (bounded at infinity):

$$\varphi_{+}[\mathbf{r}] = \mathbf{A} \, \mathrm{e}^{-\mu \, \mathbf{r}} \, \mathbf{i} \quad \varphi_{-} = \mathbf{B} \, \mathrm{Sinh}[\mu \, \mathbf{r}] \, . \tag{5.5}$$

Condition (2) gives

$$\left(-\mu - \mu \frac{\operatorname{Cosh}[\mu R]}{\operatorname{Sinh}[\mu R]}\right) = \frac{\mathbf{v}}{2 \pi R^2}.$$

The expansion for small R gives

$$\frac{1}{v} = -\frac{1}{2\pi R} + \frac{\mu}{2\pi}$$

and the same renormalization (3) gives

$$\mu = \frac{2\pi}{g}.$$
 (5.6)

A bound state exists only for g > 0.

Let us note that the normalized wave function in the region r > R is

$$\varphi_+[r] = \sqrt{2\mu} \operatorname{Exp}[-\mu r].$$

By continuity the inner part of the wave function is

$$\varphi_{-}[\mathbf{r}] = \sqrt{2\mu} \operatorname{Exp}[-\mu R] \frac{\operatorname{Sinh}[\mu r]}{\operatorname{Sinh}[\mu R]} \leq \sqrt{2\mu} \operatorname{Exp}[-\mu R]; \quad \mathbf{r} \leq R.$$

The contribution to the norm  $% \left( {{\mathbf{T}}_{R}} \right)$  of this part goes to 0 as  $R \rightarrow 0$ 

$$\int_{0}^{\mathbb{R}} \left| \varphi_{-}[r] \right|^{2} dr \leq \left( 2 \mu e^{-2 \mu R} \right) R$$

This means that for small R the wave function  $\phi_+$  is correctly normalized and the system does not depend on any unrenormalized parameter.

These results, both for the scattering phase amplitude and for the bound state, reproduce the results obtained in Complement Section 20.12 with a cut off in the momentum space, after identifying  $\Lambda = \frac{1}{R}$ .  $g_0$  represents the "bare" or "unrenormalized" coupling constant; g is the renormalized

coupling constant, in terms of which physical quantities are expressed. The cutoff  $(\Lambda, \frac{1}{R})$  and bare quantities disappears from the theory at the end. These are typical characteristics of renormalizable quantum field theories in four dimensions, used to describe the elementary particles.

#### • Reference

R. Jackiw, "Delta-function potentials in two- and three-dimensional quantum mechanics", Beg Memorial Volume, eds. A. Ali and P. Hoodbhoy (WorldScientific, Singapore, 1991).