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Exotic Hydrogens in Momentum Space

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1 Introduction

When we speak of “hydrogen” we usually mean the simplest atom in which a single electron e^- is bound to a single proton p^+ acting as the nucleus in the center of the atom. The Coulomb attraction between these two particles binds the system into orbits with Bohr “radii”

$$R_B = n^2 \frac{4\pi\epsilon_0 \hbar^2}{\mu Z e^2}. \quad (1)$$

While the size of orbits is seen to increase quadratically with the principal quantum number n , the energy of these states decreases inverse-quadratically with n :

$$E_n = \frac{\mu Z^2 e^4}{2(4\pi\epsilon_0)^2 \hbar^2 n^2}. \quad (2)$$

The μ in these expressions is the electron-proton reduced mass (which is nearly equal to the electron’s mass)

$$\mu = \frac{m_e m_p}{m_e + m_p} \simeq 0.9995 m_e. \quad (3)$$

If we approximate μ by the electron mass in (1) and (2), we obtain the familiar numerical values

$$R_\infty = n^2 \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} = n^2 0.529172^{-10} m, \quad (4)$$

$$E_n = \frac{hc}{n^2 R_\infty} = \frac{13.60569172(53)}{n^2} \text{ eV}. \quad (5)$$

Since the Coulomb attraction between the proton and the electron is responsible for binding in hydrogen, if you replace the electron by some other negatively charged elementary particle you still end up with an atomic bound state. For example, if you replace the electron by a π^- , μ^- or a K^- , you get what is called a form of exotic hydrogen. Actually, since these other elementary particles are much heavier than the electron, (1) tells us that the orbits of exotic hydrogen lie deep within the electronic orbits, in which case there really is no need to replace the electron (the heavy particle just slips in underneath).

Because the orbiting particle in exotic hydrogen decays, these atoms are always unstable and decay with a finite lifetime τ . This finite lifetime means that we cannot be sure of the state’s precise energy and shows itself in the decay spectrum by giving the energy levels a finite width Γ . The uncertainty principle relates the level width and lifetime,

$$\Delta E = \frac{\hbar}{\Delta t}. \quad (6)$$

While at first one might think that a decaying state is quite different from an atom, since these exotic atoms tend to hold together for millions or billions of orbits, they are very much like stable bound states. Because they do eventually decay, exotic atoms are not truly bound states, and so are called *quasi-bound*, *Gamow*, or resonance states.

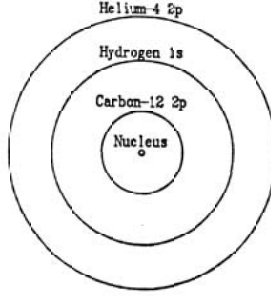


Figure 1: The sizes of various Bohr orbits for various kaonic atoms. The dot at the center is the size of a carbon nucleus (in proportion).

Some of the interesting physics of exotic atoms arises from the fact that the electron's replacement is much heavier than an electron and so orbits much closer to the nucleus, as expected from the inverse proportionality to mass in (1). For example, *kaonic hydrogen* is 633 times smaller than electronic hydrogen:

$$m_{K^-} = 493.699 \text{ MeV}/c^2 \simeq 966 m_e, \quad (7)$$

$$\Rightarrow \mu = \frac{m_K m_p}{m_K + m_p} = 323 \text{ MeV}/c^2 \simeq 633 m_e, \quad (8)$$

$$\Rightarrow R(K^- p) \simeq (0.529172^{-10} m)/633 \simeq 84 \times 10^{-13} \text{ cm} = 84 \text{ Fermi}. \quad (9)$$

Likewise, the ground state energy for kaons is 633 times larger

$$E_{1S}(K^- p) \simeq -8613 \text{ eV} = -8.613 \text{ KeV}. \quad (10)$$

In Fig. 1 we show scaled values for the Bohr radii for various levels in different kaonic atoms as well as the size of a ^{12}C nucleus in proportion (the 1S electron is 51 feet away from the nucleus with this scale). The $1/Z^2$ factor in the Bohr radius makes the orbits for heavier atoms smaller than for hydrogen at the same time as the nucleus tends to grow in size with increasing Z . Since the Bohr radii for kaonic hydrogen are so much smaller than electronic hydrogen, when a kaon is inserted into an ordinary hydrogen atom, it tends to cascade down to an orbit deep within the electronic cloud and is therefore unaffected by the electrons (which just remain in orbit).

Although it is clear from Fig. 1 that an orbiting kaon is not overlapping much with the nucleus, they are close enough for the nuclear force to perturb the kaon and shift its energy slightly from the Bohr value. In fact, there is also the possibility that the kaon gets captured by the proton and forms a nuclear state from which it never returns, and this may affect the atomic state in an unusual way.

The nuclear reactions between a K^- and a proton are particularly interesting, and for this lab we consider three:

$$K^- p \longrightarrow \left\{ \begin{array}{llll} K^- p & \text{atom} & \text{open} & \text{channel 1,} \\ \Sigma\pi & +100 \text{ MeV} & \text{annihilation} & \text{open channel 2,} \\ \bar{K}^0 n & -5 \text{ MeV} & \text{charge exchange} & \text{closed channel 3.} \end{array} \right. \quad (11)$$

We use a large brace in (11) to indicate that all three reactions are coupled with the probability flux flowing among them. In analogy to the flow of a fluid through canals with open and closed gates, we envision the flow of probability flux through “channels” representing different states of the system. And just like the volume of a fluid is conserved, so the total probability is conserved. When a channel in addition to the entrance channel opens, we envision an additional path for the probability fluid to follow, and so a reduced likelihood of the system remaining in the entrance channel.

The reactions in (11) mean that even though the $K^- p$ system may be in a bound atomic state, enough of the kaon's wave function overlaps with the proton for the $K^- p$ atom to spontaneously

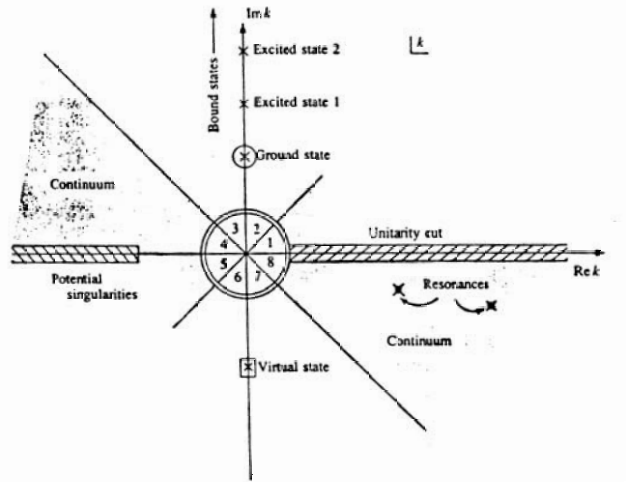


Figure 2: The complex momentum k plane. The upper four octants here correspond to the top complex energy ($E = k^2/2\mu$) sheet, while the lower four octants correspond to the bottom complex energy sheet. The slashed strips represent the unitarity cut (which is where the two energy sheets are joined).

transform into a $\Sigma\pi$ system with the concordant release of 100 MeV. This is a large amount of energy and literally blows the atom apart into Σ and π fragments. Since energy is released into the $\Sigma\pi$ channel, this channel is called “open”; any flux that makes here will flow out. In contrast, the $\overline{K}^0 n$ channel is “closed” since it needs 5 MeV for the reaction to occur there, and the atom does not have that type of energy to spare. So any probability flux that makes it to channel 3 will not flow far. Nevertheless, the existence of a channel that is closed by only 5 MeV has a significant effect on the nuclear interaction, and thus on the level shifts and widths.

1.1 Theory: Relation of Shift and Width to Complex Energy

The nuclear interaction of a kaon in its atomic orbit around a proton shifts and broadens the atomic energy level. The shift occurs because the addition of the nuclear interaction leads to a net force than is more or less attractive than the Coulomb force. The width occurs because the nuclear interaction can remove the kaon from the incident channel, and this is what makes the kaonic atom decay. In fact, this permits one to learn about nuclear forces by studying atomic spectra.

By convention, the atomic level shift ϵ is defines as the increase in binding relative to the Bohr value E_n :

$$\epsilon = E_n - E_{atom}. \quad (12)$$

The values of ϵ for heavy kaonic atoms are approximately $-(100-1000)\text{eV}$'s, that is, uniformly to the *less bound* (upwards). The value for hydrogen has been very hard to measure and the results have been controversial; this was the motivation for the original research upon which the lab is based.

While conventional wisdom leads us to believe that a nuclear potential whose addition diminishes the atomic binding must be repulsive, there is some unusual physics here. The existence of the open channels in (11) means that any kaon that gets close to the proton will be annihilate and flow into the open channel. This strong absorption of the wave function near the origin reduced the value of the wave function there, much like would a repulsive force, and so even though the nuclear force is attractive, the strong absorption produces the same shift to the less bound as would a repulsive force.

As we indicated above, decaying bound states require an extension of the usual ideas of quantum mechanics, specifically in regards to the time dependence of decaying bound states (Gamow, 1928;

Blatt and Weisskopf, 1952; Kapur and Peirles, 1938; Kwon and Tabakin, 1978; Hernandez and Mondragon, 1984; Landau, 1983). We know that a stationary state (quantum eigenstate) has the time dependence

$$\Psi_n(x, t) \propto \exp(-iE_n t)\psi(x). \quad (13)$$

We also know that a decaying state with lifetime τ has the time dependence

$$\Psi_n(x, t) \propto \exp(-t/\tau) \exp(-iE_n t)\psi(x). \quad (14)$$

We combine these two notions by postulating that a decaying state can be thought of as an generalization of a stationary state to a complex energy

$$E = E_n - i\Gamma/2, \quad (15)$$

$$E_I = -\Gamma/2, \quad E_R = E_n. \quad (16)$$

The wave function Ψ and probability density $|\Psi|^2$ for a state with complex energy theqwn have the time dependences:

$$\Psi \propto e^{-iEt} = e^{-iE_n t} e^{-\Gamma t/2}, \quad (17)$$

$$|\Psi|^2 \propto e^{-\Gamma t} = e^{-t/\tau}. \quad (18)$$

As desired, the probability density of a resonance decays exponentially in time with a time constant or lifetime

$$\tau = \frac{1}{\Gamma} \equiv \frac{\hbar}{\Gamma}. \quad (19)$$

Decaying states were introduced into quantum mechanics by Gamow in 1928 while developing a model for alpha-particle emission from nuclei. The equivalent concept of resonant states having a complex energy was further developed by Kapur and Peirles in 1938. Both models envision a confined state which decays slowly in time by emitting particles. Since this state is radiating probability, for large r it must look like an *outgoing wave* e^{ikr} in space. In fact, since only certain energies will produce outgoing waves for a given potential, it is this extra outgoing-wave constraint that turns this into an eigenvalue problem with discrete, complex energies. (Equivalently, a complex potential might also produce complex eigenvalues.)

The combined requirements that a solution of the Schrödinger equation decay in time as $e^{-\Gamma t}$ and radiate in space like e^{ikr} for large r is hard to meet. For a state to decay exponentially in time, that is, be described by (17) with $\Gamma > 0$, we must have the imaginary part of the energy negative. This, in turn, requires the k which appears in the outgoing wave e^{ikr} be complex:

$$k^2 = 2\mu E = (k_R^2 - k_I^2) + 2ik_R k_I, \quad (20)$$

$$\Rightarrow k_R > 0, k_I < 0, \quad \text{or} \quad k_R < 0, k_I > 0. \quad (21)$$

For a given energy there are usually two solutions (here in the large r region), one corresponding to a resonance, and the other to a bound state:

$$\psi = \begin{cases} \psi_{res} \sim e^{ik_R r} e^{|k_I| r}, & \text{with } k_R > 0, k_I < 0, \\ \psi_{bs} \sim e^{-i|k_R| r} e^{-k_I r}, & \text{with } k_R < 0, k_I > 0. \end{cases} \quad (22)$$

We identify the outgoing wave state ψ_{res} as a *resonant* state if its momentum is in the eighth octant of the complex-momentum plane in Fig. 2 and close to the real axis. We identify the incoming wave state ψ_{bs} containing a decaying exponential in space, as an *unstable bound state* if its momentum is in the third octant of the complex-momentum plane and close to the imaginary axis. Notice that the bound state wave function is normalizable, but that a resonance wave function is not.

The program you run in this lab searches throughout the complex momentum and energy space for complex energy eigenstates. There can be many such solutions. After the solution is found, we must be careful to ensure that it is a physically significant state by checking that all these conditions have been met.

1.2 Theory: Gamow States Momentum Spaces

Since we will deal with nonnormalizable quasi-bound states, we do not have the standard eigenvalue problem to solve. Instead, we use the Lippmann-Schwinger equation, a form of the Schrödinger equation usually used to describe scattering[14], and then search for the poles of the scattering matrix T . Actually, this makes some sense because these exotic atomic states are resonances in the scattering part of the spectrum. The Lippmann-Schwinger equation for our problem has the form

$$T(k', k; E) = V(k', k) + \frac{2}{\pi} \int_0^\infty dp p^2 V(k', p) G_E(p) T(p, k; E), \quad (23)$$

where $T(k', k; E)$ is the transition matrix, $V(k', k)$ is the potential matrix,

$$G_E(p) = \frac{1}{E - H_0(p)} \quad (24)$$

is the Green's function, and all these operators are evaluated in the momentum representation. The coupled-channels physics described by (11) is included by making T , V and G super matrices composed of submatrices for each channel:

$$V \equiv \begin{bmatrix} V_{11} & V_{12} & V_{13} \\ V_{21} & V_{22} & V_{23} \\ V_{31} & V_{32} & V_{33} \end{bmatrix}, \quad T \equiv \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}, \quad (25)$$

$$G = \begin{bmatrix} [E - E_1(p)]^{-1} & 0 & 0 \\ 0 & [E + i\epsilon + \Delta M_{12} - E_2(p)]^{-1} & 0 \\ 0 & 0 & [E + \Delta M_{13} - E_3(p)]^{-1} \end{bmatrix}. \quad (26)$$

Here ΔM_{ij} is the mass difference between channels [the energies listed in (11)], and the $i\epsilon$ in the channel 2 part of G guarantee outgoing-wave boundary conditions in that open channel, and leads to the energies having imaginary parts.

The connection between these integral equations and exotic atom states follows from examining the operator (equivalent to matrix) form of the Lippmann Schwinger equation (23)

$$T = V + VG_E T. \quad (27)$$

As you have seen in linear algebra, this equation has the formal solution

$$T = (1 - VG_E)^{-1} V. \quad (28)$$

As is known from scattering theory[14], the condition for a Hamiltonian to have a bound state at some energy is the same as for the scattering or T matrix to have a pole at that energy. We see that (28) has poles when the denominator vanishes, and for this matrix problem, that is equivalent to

$$\det(1 - VG_E) = 0. \quad (29)$$

We can make a connection here with the more familiar eigenvalue form of the Schrödinger equation, by writing the Schrödinger equation in terms of bras and operators:

$$\langle \psi | (E - H_0) = \langle \psi | V. \quad (30)$$

If we right multiply by $G_E = (E - H_0)^{-1}$, we obtain Schrödinger equation as

$$\langle \psi | (E - H_0)(E - H_0)^{-1} = \langle \psi | VG_E \quad (31)$$

$$\langle \psi | \tilde{1} = \langle \psi | VG_E \quad (32)$$

$$\Rightarrow \langle \psi | (\tilde{1} - VG_E) = 0. \quad (33)$$

Yet for this to make sense, either we have the trivial solution $\langle \psi | = 0$, or the inverse operator we used does not exist (i.e., we divided by zero). The condition for the inverse operator not to exist is just (29), the condition for a bound state.

2 Computation

Our computational problem is to search for complex energies (momenta) that solve (29) with V a large, complex, momentum-space matrix. The particular version given here looks only for S ($l = 0$) states, with no restriction on the n value. When these momenta are on the positive imaginary k axis they are conventional bound states. When the energies are complex, we view as the energies of Gamow states with widths Γ given by (16). Whether these poles are “bound states” or “resonances” depends on its location on the complex energy sheets. States with negative imaginary energies (positive lifetimes), are always be in the lower half of the energy planes. They are resonances if their home is on the second sheet, and bound states if their home is on the first energy sheet.

Below we outline the theory upon which the code is based. Most of this is explained in some detail in QMII[14], and we recommend you look there for a more thorough treatment.

To handle the nonlocal nature of the nuclear potential, we need to solve the dynamical equations in momentum space. Yet handling the Coulomb potential there is a problem since the long range of the potential in coordinate space translates into a momentum-space singularity at $k = k'$:

$$\langle \vec{k} | V^C | \vec{k}' \rangle = \frac{-Ze^2}{2\pi^2(\vec{k} - \vec{k}')^2}, \quad (34)$$

$$V_{l=0}^C(k', k) = -\frac{Ze^2}{2kk'} \ln \left| \frac{k+k'}{k-k'} \right|, \quad (35)$$

where the second form is in the partial-wave basis.

Way back in 1935, Fock[5] was able to solve the momentum-space Schrödinger equation directly for hydrogen. He found that the 1S wave function has the form (with $\hbar = c = 1$)

$$\psi_{1S}(p) = \frac{1}{(p^2 R_B^2 + 1)^2}. \quad (36)$$

Although we will solve for a mixed Coulomb plus nuclear state, and thus have a more complicated wave function than this, the form will be similar. On the one hand, we see that the Coulomb wave function decays rather slowly in momentum space; for this reason we will have to have our integration points cover a large region of momentum space. On the other hand, we note that the wave function has a pole when

$$p^2 = -\frac{1}{R_B^2}, \quad \Rightarrow p = \frac{+i}{R_B} \text{ (bound state), } \quad p = \frac{-i}{R_B} \text{ (virtual bound state)}. \quad (37)$$

This is just the bound state pole we have been talking about, and, as expected, it occurs at the Bohr energy.

To solve an integral equation numerically, we must remove the logarithmic singularity in the Coulomb potential V^C . We do that[2, 6, 7] by subtracting off the singularity in the Coulomb potential while simultaneously solving the integral equation:

$$T(k', k) = V^C(k', k) + \frac{2}{\pi} \int dp V^C(k', p) \left[p^2 G_E(p) T(p, k) - \frac{k'^2 G(k') T(k', k; E)}{P_l(z_{k'p})} \right] + \frac{2}{\pi} k'^2 G_E(k') T(k', k) S(k') \quad (38)$$

$$S(k') = \int_0^\infty \frac{V^C(k', p)}{P_l(z_{k'p})} dp, \quad z_{k'p} = (k'^2 + p^2)/2k'p. \quad (39)$$

Here P_l is the Legendre polynomial of the first kind, the subtracted term in square brackets makes the integrand nonsingular, and the GTS term corrects for the subtraction. With 40 integration points, we obtain six-place accuracy for the analytically-known pure Coulomb E_{1S} for K^-p .

The Green's function G_E for an open channel also has a singularity since the channel is open, and that too must be modified to permit a numerical solution. We make that singularity computable by

separating the integral of $VGE T$ into delta function and principal value parts, and then evaluating the principal value part with a subtraction[8]

$$\begin{aligned} \int dpp^2 \frac{V(k', p)T(p, k)}{E + i\epsilon - E(p)} &= P \int dpp^2 \frac{V(k', p)T(p, k)}{E - E(p)} - i\pi\mu k_0 V(k', k_0)T(k_0, k) \quad (40) \\ &= \int dp \left[p^2 \frac{V(k', p)T(p, k)}{E - E(p)} - k_0^2 \frac{V(k', k_0)T(k_0, k)}{\frac{k_0^2}{2\mu} - \frac{p^2}{2\mu}} \right] \\ &\quad - i\pi\mu k_0 V(k', k_0)T(k_0, k), \quad (41) \end{aligned}$$

where μ is (still) the effective mass.

Explicit linear equations for the T-matrix's poles are obtained by replacing the integral in equation 23 by a discrete sum over grid points[14]. If we leave off the angular momentum and E subscripts (for clarity), the linear equations are

$$T(k_i, k_j) = V(k_i, k_j) + \frac{2}{\pi} \sum_{n=1}^N w_n p_n^2 \frac{V(k_i, p_n)T(p_n, k_j)}{E - E(p_n) + i\epsilon} \quad (42)$$

The weight function w_n is determined by the particular integration method used, in our case Gaussian quadrature.

Equation (42) can be rewritten in a convenient form by using subscripts to show the dependence on grid points, and by defining

$$M_{ij} = \frac{2}{\pi} w_j p_j^2 V_{ij} G_j. \quad (43)$$

Equation (42) then becomes

$$T_{ij} = V_{ij} + \sum_{n=1}^N M_{in} T_{nj}. \quad (44)$$

This can now be viewed as a matrix equation that we solve for T

$$T = V + MT \quad (45)$$

$$(1 - M)T = V \quad (46)$$

$$\Rightarrow T = (1 - M)^{-1}V. \quad (47)$$

The condition for a pole of the T-matrix then has the same form as the operator equation (29)

$$\det(1 - M) = 0. \quad (48)$$

We solve (48) numerically in the code.

3 The Code BS.f

The code `BS.f` is divided into two source files of fortran subroutines. `BSmain.f` contains the main program as well as most key subroutines. `BSlibe.f` contains the library routines to do the matrix manipulations and to search for the zero of the determinant. We recommend that you browse `BSmain.f` to get a feel for the program. Here's a list of the major subroutines:

program bsmain The main program (where execution begins).

detcnl Sets up the major parts of calculation needed to calculate the determinant.

gausbs, gauss Computes and scales the integration points and weights.

optpbs Sets up the matrix $1 - GV$.

snsq Nonlinear Search for zero.

vcoulb Coulomb potential in momentum space for bound states (calls `vcdiag` for diagonal terms).

3.1 Source Code Libraries

Some common tasks come up repeatedly in scientific programming. Solving a system of equations, evaluating elementary function, finding eigenvalues, interpolating and extrapolating are examples. It is a great idea to have a package of subroutines to accomplish such tasks and which can be used in all the programs you write. The key is to have experts write these subroutines so that they are optimized, reliable, and robust. It is not uncommon to have execution times dropped by an order or magnitude after taking advantage of a good scientific subroutine library. That can mean running a day instead of a month!

The program `BS.f` incorporates subroutines from the SLATEC (Sandia, Los Alamos, Air Force Weapons Laboratory Technical Exchange Committee) library [www.netlib.org]. These subroutines are identified in the comment fields. We use these routines in `BS.f` to evaluate the determinant of $(1 - GV)$ and then to search for the zeros of the determinant.

Now let's look through the code and see if we can make some sense of it.

3.2 Subroutine Listings (edited)

```
      program bsmain
c   1=output,tape4=64,tape8=64,tape7,debug=output)
c   bound states via det(1-gv)=0
c   ridge32 version july 85
c   implicit real*8 (a-h,o-z)
c   external detcal
c   real*8 xeri(2),w(31),drr(10),dri(10),detri(2)
c   common/det/ar11,alfanz
c   the open stmts are c'ed out so files spefied on run card
c   open(5,file='runbs3',status='unknown')
c   open(6,file='outbs',status='unknown')
c   open(7,status='scratch',access='sequential',
1      form='unformatted')
c   i=signal(119,dumsub,1)
c   write(6,879)
879  format(' BOUND STATE calculation via det(1-GV)=0, 8/86')
10  read(5,*,end=233)drr(1),eim,(drr(i),i=2,7)
c   read(5,*)tol,aitmax
880  format(8f10.6)
c   write(6,882)drr(1),eim,(drr(i),i=2,7)
c   write(6,882)tol,aitmax
882  format(' input Es, tol, max iterations',/8f15.6)
c   maxit = aitmax
c   nrei=2
c   if(eim.ge.0.d+00)nrei=1
c   l=0
c   calculate point coulomb b.e. for sch eqtn or kge
c   no dirac yet, i.e. no spin
c   fjl=1 +- 1/2...i.e.fjl=1 for these cases
c   fjl=1
c   ekge=0.
226  format(24h nbohr,e(se),e(kge1,2)= ,i3,3(1pe20.10),6h eta= ,
1  e20.8)
c-----do loop over energies
c   do 213 ix=1,7
c   if(drr(ix).eq.0.d+00) go to 213
c   xeri(1)=drr(ix)
c   xeri(2)=eim/ix
c   write(6,880)xeri(1),xeri(2)
c   call snsqe(detcal,jac,2,2,xeri,detri,tol,-1,info,w,31,maxit)
c   if (info .eq. 0)then
c   write(6,100)
100  format(1h0,'improper input parameters in search')
c   else if (info .eq. 1) then
c   write(6,101) tol
101  format(1h0,'normal termination, relative error is at most',
1  f13.10)
c   else if (info .eq. 2)then
c   write(6,102) maxit
102  format(1h0,'iterations exceed ',i4)
c   else if (info .eq. 3) then
c   write(6,103) tol
103  format(1h0,f13.10,'tol too small.no further
1improvement possible in xeri')
c   else if (info .eq. 4) then
c   write(6,104)
104  format(1h0,'iteration not making good pr
```

```

logress')
endif
nmin=l+1
if(ix.ne.1) go to 211
do 223 nbohr=nmin,4
esch=(-ar11/2.)*(alfanz/nbohr)**2
dri(nbohr)=esch
eta=nbohr-(fj+.5d+00)+sqrt((fj+.5d+00)**2-(alfanz)**2)
wron1=(alfanz/eta)**2
eta=sqrt(1.+wron1)
wron2=ar11*(-.5*wron1+wron1**2/8-.5*wron1**3/16.)
ekge=ar11*(1./eta-1.)
write(6,226) nbohr,esch,ekge,wron2,eta
223 continue
211 epsev=(dri(ix)-xeri(1))
gamev=-xeri(2)*2.
esch=-epsev
write(6,881) xeri(1),xeri(2),epsev,gamev,esch,xeri(2)
881 format('0E(MeV)=' ,2f16.14,' eps,gamma(eV)=' ,2(6pf10.1)/
1 ' Del E(ev)=' ,2(6pf10.1))
213 continue
go to 10
233 write(6,841)
841 format(' *****eof in main*****')
stop
end
C=====
subroutine detcal(nrei,xeri,detri,iflag)
c version modified sept85 for antiproton bs, 8/86 for reltv
implicit real*8 (a-h,o-y)
integer mypvt(192)
complex*16 detin(2),work(192)
complex*16 h, x1,x2,x3,x4,x5,x6,x7,x8,x9,x10,x11,x12,
1 x13,x14,x15,x16,x17
complex*16 zi,zw(10), za(192,192),zdet
1 ,den(192,3),sum1,sum2,sum3,zk22,zk33,zk11,zk2,zk1,zk3
2 ,ze,zs,ar11,ar22,ar33
real*8 kapg,mn,mn2,k0,ko,ko2,k,k2,kk,mpi,mpi2,mr,k02
1, imtij,bnuc,bn,retij,xbarc,xi,xpi,xn,xgam,zcm,zch,theta,
1dsig,bnucf,bnf,dflip,dnof,wsp, achp, acmp,ymin1,
2ymin2
c NB NEED MATCH DIMEN AND NO ENTRIES IN DATA STM FOR IBM
dimension ... intger(192),mm1(192),
4 mm2(192),xeri(2),detri(2)
dimension kk(130),u(36864,2),f(36864),gp(66),wt(66)
1,ptptw(66),wa(130)...
common, equivalence...
c revised constants and masses nov 81 for bound s problem
data alfa /7.29735d-3/,an,ap,akmn,ak0,asig,ndim/
1 939.5731d+00,938.2796d+00,493.699d+00,497.67d+00,1193.35d+00,
2 192/,ix/1/
data hbarc,api,pi/197.3289d+0,139.5669d+0,3.14159265d+0/,
...
if(ix.ne.1) go to 150
10 continue
C MN HERE REFERS TO NUCLEUS MASS,XN (IN COMMON) TO NUCLEON
C
READ MOMENTA IN CENTRE_OF_MASS C NR.LE.0 IS
NONRELATIVISTIC NR .GT. 0 > RELATIVISTIC CASe
read(5,*,end=650) nr,lxmax
write(6,740) nr,lxmax
read(5,*) ngp,kode,b,nang,ymin1,ymin2
if (nang.eq.0) nang = 3
write(6,760) ngp,kode,b,nang,ymin1,ymin2
if (ngp.le.0) go to 650
write(6,790) ngp
C ----READ IN DATA
read(5,*) nz,na,(nifty(n),n=1,20)
write(6,830) nz,na,(nifty(n),n=1,20)
nifty(15)=abs(nifty(15))
C PRINT OUT NIFTY
...
25 continue
read(5,*) nes,nwaves,b0r,b0i,c0r,c0i
write(6,910) nes,nwaves,b0r,b0i,c0r,c0i
...
write(6,910) nes,nwaves,b0r,b0i,c0r,c0i
if (nwaves.lt.0)write(6,884)nwaves
884 format(' Nwaves lt 0 for % partial absorption, Nwaves=' ,i4)
40 continue
mpi=api

```

```

        if ((nifty(1).eq.7).or.(nifty(1).eq.8).or.(nifty(1).eq.-1)) mpi =
        1 akmn
        if(nifty(1).eq.10.or.nifty(1).eq.11)mpi=akmn
if (nifty(1).eq.12)mpi=ap
        zcm = acmp
        amass=na
        zch = achp
        zws = wsp
        nifty1 = nifty(1)
c
c      DEFINE MASSES WHICH DONT CHANGE WITH ENERGY
c
c      ...
c-----come here directly on all but 1st call-----
150 continue
C      bs ENERGY IS ke IN com FOR BOTH rEL AND nR
c      need redefine for scatt where KE is lab KE
        e=xeri(1)
        eimin =xeri(2)
        zdet=zi*eimin
        ze=e+zdet
        e2=e+e12
        e3=e+e13
        if(nr.gt.0)goto 156
c      calc complex*16 e s and momenta for chan 2
        zk11= (e+zdet)*2.*mr
        zk22=(e2+zdet)*ar222
        zk33=(e3+zdet)*ar332
        go to 157
c      RELATIVISTIC ENERGY
c      take sqrt(s) = e + m1 +m2 as def of E, same in all channels
c      zk11 is now k2 in channel 1, NOT energy, ar is complex mr
156 ze = e + zdet +mn +mpi
        zs = ze**2
        zk11 = (zs-am12)*(zs-am1m)/4./zs
        zk22 = (zs-am22)*(zs-am2m)/4./zs
        zk33 = (zs-am32)*(zs-am3m)/4./zs
        ar11 = sqrt((zk11 + mn2)*(zk11+mpi2))/ze
        ar22 = sqrt((zk22 + a21)*(zk22+a22))/ze
        ar33 = sqrt((zk33 + a31)*(zk33+a32))/ze
        if(ix.eq.1)write(6,781) ar11,ar22,ar33
157 continue
c      place complex momentum in quadrant II for BS analytic continuation
c      place complex momentum in quadrant IV for Resonance (nif(3)=1)
        x = zk11
        yi = -zi*zk11
        th = atan2(yi,x) + 2.*pi
        if(nifty(3).eq.1) th = atan2(yi,x)
        zk1 = sqrt(sqrt(x**2 + yi**2))*(cos(th/2.) + zi*sin(th/2.))
        x = zk22
        yi = -zi*zk22
        th = atan2(yi,x) +2.*pi
        if(nifty(3).eq.1) th = atan2(yi,x)
        zk2 = sqrt(sqrt(x**2 + yi**2))*(cos(th/2.) + zi*sin(th/2.))
        x = zk33
        yi = -zi*zk33
        th = atan2(yi,x) +2.*pi
        if(nifty(3).eq.1) th = atan2(yi,x)
        zk3 = sqrt(sqrt(x**2 + yi**2))*(cos(th/2.) + zi*sin(th/2.))
        if(ix.eq.1)
1      write(6,108) e,eimin,e2,eimin,e3,eimin,zk1,zk2,zk3
c      theta(1),(2) used in call to optpbs if whant complex momentum
        theta(1)=zk2
        theta(2)=-zi*zk2
c
c-----SET UP GRID POINTS-----
c
c      n1 = ngp+1
c      n2 = n1+n1
c      a = zk2
c      a=abs(a)
c      special check if b=0,use different distrb of points
        if(ix.gt.1)go to 89
        if (b.eq.0.) a = 200.
        if(kode .lt. 0) go to 84
        if(ngp.gt.48) go to 82
        call gauss (ngp,kode,a,b,gp,wt)
        go to 83
c      ngp gt 48,redistrb pts, 0-ko ,k0-inf(half up to 10*ko)
82 npt1=24
        npt2=ngp-npt1

```

```

      b=a
      call gauss(npt1,011,0.d+00,b,gp,wt)
      if(npt2.gt.48)write(6,107)
      b=8.*a
      call gauss(npt2,041,b,a,dflip,dnof)
      ngp=npt1+npt2
      write(6,730)ngp,npt1,npt2
      do 81 i=1,npt2
        ii=i + npt1
        gp(ii)=dflip(i)
81    wt(ii)=dnof(i)
      go to 83
107  format(20h NPT2 GT 48 IN MAIN )
c    special bs point distb for kode lt 0-
84    cpmax=10.d+00**(-kode)
      catom=b
      write(6,883) kode,catom
883  format(' kode < 0, use bs points,cpmax=10**(-kode), '
1    ', 'catom <,>0 :gausbs-rhl mod of kt',
2    'gausbs-kt version ,kode,catom=',i4,e12.4)
      nnuc=nang
      if(nang.eq.3)nnuc=0
      cnucl=ymin2
      csize=ymin1
      write(6,104) ngp,nnuc,catom,csize,cnucl,cpmax
104  format(40h Ngp,Nnuc,Catom,Csize,Cnucl,Cpmax(MeV)= ,2i4,4e12.4/)
      if(catom.ge.0.)
1call gausb2(ngp,nnuc,catom,csize,cnucl,cpmax,gp,wt,ptptw)
      if(catom.lt.0.)
1call gausbs(ngp,nnuc,-catom,csize,cnucl,cpmax,gp,wt,ptptw)
83    continue
      write(6,105)(gp(i),i=1,ngp)
      write(6,106)(wt(i),i=1,ngp)
105  format(8h points= ,10e12.4)
106  format(8h weight= ,10e12.4)
89    continue
      sum1=0.
      sum2=0.
      sum3=0.
      if (nr.gt.0) go to 100
c    -----
c    NONRELATIVISTIC      DENOMINATOR
c    -----
      do 90 i1=1,ngp
      k = gp(i1)
      kk(i1) = k
      k2 = k*k
      ak2w=k2*wt(i1)
      den(i1,1)=ak2w/(k2-zk11)*rhl2
      if(nifty(15).eq.0) go to 90
      den(i1,2)=ak2w/(k2-zk22)*rhl22
      den(i1,3)=ak2w/(k2-zk33)*rhl23
c      2 closed channels, replace den2 with den3 and dont use channel 3
c      closed channels: (K-p,Kobar-n) or (p-pbar,n-nbar)
      if(nifty(15).eq.3)den(i1,2)=den(i1,3)
      if(nifty(15).eq.3)den(i1,3)=0.
c      include Prin Value sum in denom for open channel
      if(e .gt.0.)sum1 = sum1 +wt(i1)/(k2-zk11)
      if(e2.gt.0.)sum2 = sum2 +wt(i1)/(k2-zk22)
      if(e3.gt.0.)sum3 = sum3 +wt(i1)/(k2-zk33)
90    continue
c      SET DEN(N1) WITH DEN2 CONTAINING BOTH I EPS AND p SUBTRN
c      can use this procedure for any real/complex energy, here use reE>0 switch
      if(e .lt.0.)den(n1,1)=0.
      if(e2.lt.0.)den(n1,2)=0.
      if(e3.lt.0.)den(n1,3)=0.
      kk(n1)=zk1
      if(nifty(15).eq.0.and.e.lt.0.) go to 120
c      channel 2 (usually the only open one)
      if(e2.gt.0.)then
c      channel 2 open
      kk(n1)=zk2
      zw(1)= - sum2*rhl22*zk22
      zw(2)= + zi*ar222*zk2
      den(n1,2)= zw(1) +zw(2)
      endif
      if(e3.gt.0.)then
c      channel 3 open
      zw(1)= - sum3*rhl23*zk33
      zw(2)= + zi*ar332*zk3
      den(n1,3)= zw(1) +zw(2)

```

```

endif
if(e.gt.0.)then
c   channel 1 open
zw(1)= - sum1*rh12*zk11
zw(2)= + zi*ar2*zk1
den(n1,1)= zw(1) +zw(2)
endif
c   for closed channels set den(n1,channel)=0
c   for 2 channel case (nbar-n or kobar-n) switch channel 3 to 2
if(nifty(15).eq.3)then
    den(n1,2)=den(n1,3)
    den(n1,3)=0.
endif
go to 120
c   -----
c   RELATIVISTIC DENOMINATOR
c   -----
100 ...
c-----end relativistic denom-----
120 if(ix.eq.1.or.e.gt.0..or.e2.gt.0..or.e3.gt.0.)
1   write(6,91) (den(n1,i),i=1,3)
   if(ix.ne.1)go to 203
   ii=3
   if(nifty(15).eq.0)ii=1
   do 202 i=1,ii
202 write(6,102) (den(ii,i),i=1,n1)
102 format(' Zden(3/1,i)=' ,10e12.4)
c
C----- DO LOOP OVER L FOR THIS E AND STATE
c
203     l = ldmax-1
   if(ix.eq.1)write (6,1070) l
c
C   BOUND STATE OR EIGENENERGY CALCULATION ( A* RESONANCES )
c   calc bound state e's only for ldmax
c
   theta(3)=10.
   call optpbs(kk,n1,wt,ldmax,ldmax,lborn,theta,e,eimin)
c   for three coupled channels possible, need 3*maxngp as dimen
c   nunit=ngp or n1 is size of block matrix
nunit=ngp
if(nifty(15).eq.1.or.nifty(15).eq.2)nunit=ngp+1
nn=nunit
ng2=nunit*2
if(nifty(15).eq.2)nn=3*nunit
if(nifty(15).eq.1.or.nifty(15).eq.3)nn=ng2
c   WRITE OUT MATRICES
if(ix.ne.1)go to 208
write(6,229)
i=nn-1
if (nn .lt.6) then
do 9995 ii = 1,nn
9995   write(6,227) ii,(za(ii,ij),ij=1,nn)
   else
do 217 ii=1,nn,i
217   write(6,227) ii,(za(ii,ij),ij=1,nn)
endif
ii=nn
228 format(1h0,' 1-G(complex*16)*V matrix before determinant'
1 , ' found')
229 format(1h0,' complex*16 potential matrix before 1-GV formed')
227 format(1h0,i3,8e15.6/200(3x,8e15.6/))
208 continue
C   Determine Channel For Den + Row Of Submatrx
irow=1
do 219 ii=1,nn
if(ii.gt.nunit)irow=2
if(ii.gt.ng2)irow=3
do 216 ij=1,nn
jjj=ij
if(ij.gt.nunit)jjj=ij-nunit
if(ij.gt.ng2)jjj=ij-ng2
icol=1
c   revised version with g1 and g2 switched
if(ij.gt.nunit)icol=2
if(ij.gt.ng2)icol=3
za(ii,ij)=za(ii,ij)*den(jjj,icol)
2140 continue
if(ii.eq.ij)za(ii,ii)=za(ii,ii)+1.
216 continue
219 continue

```

```

C-----DO LOOP OVER II,IJ ENDS
c   write out matrices
   if(ix.gt.1)go to 298
   write(6,228)
   i=nn-1
   if (nn .lt. 6)then
     do 9996 ii=1,nn
9996   write(6,227) ii,(za(ii,ij),ij=1,nn)
     else
       do 297 ii=1,nn,i
297   write(6,227) ii,(za(ii,ij),ij=1,nn)
     endif
   if(nifty(6).eq.6.or.nifty(6).eq.7)go to 298
298   continue
212   continue
C   SEARCH FOR det=0 WITH LANDE SUBRTN IN VCOUL
   call cgefa(za,192,nn,mypvt,info)
   call cgedi(za,192,nn,mypvt,detin,work,10)
c   calculate deter
   zdet=(1.,0.)
   do 223 i=1,nn
     ipvt=wa(i)
     if(ipvt.ne.i)zdet=-zdet
     zdet=zdet*za(i,i)
223   continue
   if(ix.eq.1)ix=2
   rpow = detin(2)
   zdet = detin(1)*(10.d00**rpow)
   detri(1)=zdet
   detri(2)=-zi*zdet
   write(6,224)zk1,e,eimin,zdet
224   format(' zk1=',2(1pE11.3),' Er,Ei=',
1 2(1pe18.8),' zdet=',2(e15.3)/)
   return
C   ----- FORMATS
650   write(6,841)
   stop
c...
   end

```

As is often the case with working research codes, `BS.f` reads like a work in progress. In fact, this code was originally one that calculated scattering and was then merged with a bunch of scientific library subroutines to compute bound states by searching for the poles of the scattering matrix. Some of this history is evident in the different styles of `BS.f`.

Recall that the purpose of this code is to find the complex energies that solve $\det(1 - G_E V) = 0$. The main program, `bsmain.f` starts by reading in (and writing out) the initial guess for the energies, `dr(i)`, $i=2,7$, the tolerance required for convergence of the search `tol`, and the maximum number of iterations permitted before aborting the search `aitmax`. Given the initial guesses (usually the analytic Bohr energies), the search for the solution of $\det(1 - GV) = 0$ is initiated by the call to the `snsqe`. The subroutine `snsqe`, and the myriad of other subroutines that it spawns, is in `BSlib.f`.

Go look at `snsqe` now to see how this type of library program is set up. Notice how all the documentation for the program is given as comments, and the use of many, simple subroutines. Now if you go back to `bsmain` you will notice that the first argument in the call to `snsqe` is `detcal`. Actually `detcal` is not a variable, but rather the name of a subroutine that computes $\det(1 - GV)$ as a function of energy. `snsqe` calls `detcal` as many times as needed as it searches for a zero of the determinant.

If you look at the subroutine `detcal` in `BSmain.f`, you will notice that it is the largest subroutine in the program. In fact, it was once the main program for the scattering computation. `detcal` reads in the data needed to control the calculation, calls the `gauss` subroutines to compute the integration points and weights, and then sets up the integral equations to solve. `detcal` also calls the subroutine `optpbs` (optical potential for bound states) that computes the coupled-channels potential matrix, and then sets up the matrix $1 - GV$. It then calls the library routines `cgefa` and `cgedi` to compute the complex determinant, and these are returned to `snsqe`.

3.3 File Read Parameters (runbs)

The parameters needed to run BS are read in from a text file `runbs` in the same directory as the program (the output from the program is placed in the file `outbs` also in this same directory). This

allows the user to make changes between consecutive runs without altering and recompiling the code. A typical example of `runbs` is:

```
-0.008715 -0.00080 -0. -0. -0. -0. -0. -0.
0.0001 64.0
0 1
40 -8 -2.4 08 100. 2400.
1 1 10 +0 0 1 7 0 0 0 0 5 0 0 0 0 +2 0 0 0 0 0
002 +14 0. 0. 0. 0.
```

representing the coded variables:

```
drr(1) eim drr(2) drr(3) drr(4) drr(5) drr(6) drr(7)
tol aitmax
nr lxmax
ngp kode catom nnuc csize cnuc
achp acmp wsp achn acmn wsn rcoul rcut
nz na nifty(1) nifty(2) nifty(3) ... nifty(20)
nes nwaves b0r b0i c0r c0i
```

Decimal points in the input data help ensure that the number is interpreted as floating point. Some of the entries above are:

- `drr(1)`: The initial guess for the real part of the energy at which the search starts. `drr(2-7)` are further guesses.
- `eim`: The initial guess for the imaginary part of the energy at which the search starts.
- `tol`: The energy for which $\det 1 - GV = 0$ is searched for until the changes in energy are less than `tol`.
- `aitmax`: The maximum number of iterations permitted in search.
- `ngp`: Number of grid points used in the solution of the integral equation. You need to try values up to 66.
- `catom`, `csize`, `cnuc`: Integration points are distributed over the nuclear and Coulomb regions in momentum space using these values (in fermis) to set the scale.
- `achp`, `acmp`, `wsp`: Not used.
- `achn`, `acmn`, `wsn`: Not used.
- `rcoul`: Not used.
- `rcut`: A large radius, beyond which the Coulomb potential is assumed to vanish.
- `nz=1`: For a proton as the nucleus
- `na=1`: For a proton as the nucleus.
- `nifty(1)=10`: An incident K^- .
- `nifty(2)=0`: Not used.
- `nifty(3)=0`: Specifies quadrant in which to search for poles; determines whether solution is bound state or resonance. `nifty(3)=0` for bound state, = 1 for resonance.
- `nifty(4,5)=0`: Not used.
- `nifty(6)=0`: include strong force.
- `nifty(6)=6`: turn off strong force (leave Coulomb if requested).
- `nifty(7,8,9)`: Not used.
- `nifty(10)=5`: Bound state calculation with point Coulomb (use this).
- `nifty(10)=6`: Bound state calculation with Coulomb sphere.
- `nifty(10)=8`: Bound state calculation with no Coulomb force.
- `nifty(11,12,13,14)=0`: Not used.
- `nifty(15)`: Specifies the number of open channels:
 - 0 one channel, $K^- p$
 - 1 three channels, $K^- p, \Sigma\pi, \overline{K}^0 n$
- `nifty(16,17)=0`: Not used
- `nes=2` Sets potential parameters. Negative values used for pure $K^- p$ in `vkbarp`, i.e., to look for strong bound state.
- `nwaves=14` Negative values used to scale channel coupling.

3.4 Execution

Compile and link BS.f to form the executable BS:

```
f77 BSmain.f BSlibe.f -o BS
```

The `-o` flag places the executable in the file name that follows (BS). The program is run by entering the BS at the prompt.

3.5 Interpretation of Output

Output is placed in the file `outbs` in the same directory as the executable. The beginning of the output is mostly an echo of input parameters, some of which were discussed above. Echoing is a valuable technique that shows that these data were read in correctly, as well as showing that the program has executed up to that point (or beyond it if there is an abnormal ending since some output gets left in a buffer). It is also useful for later reference.

The program next prints out some of the masses that it uses in the various channels. These are all in MeV/c^2 and start with the line `Mproj, At, MA =` (we use the variable `M` and `a` for masses). There is the projectile mass `Mproj`, the target mass number `At`, the target mass `MA`, and the reduced masses in channels 1, 2, and 3. This is followed by the real and imaginary parts of the energy and the momentum in each channel.

Next, there is a table headed by the line `Ngp,Nnuc,Catom,Csize,Cnucl ...` that gives all the integration points and weights. This is followed by lines with `Zden(3/1,i)=` which give the denominator (Green's function) in channel 3. Since it is easy to make errors in setting up large matrices, it is good to check that the end values look reasonable.

The next major section of output begins with the heading `opt poten for k =k0(k1-bs)= 0.78480E-03 and 1=0(1-bs)`. This tabulates the actual potential computed by `BS.f` and its various components. In the units we are using (energies in MeV, lengths in inverse MeV), most of the values for the potential will be less than 1, with values of 1000 or so occurring when we get the Coulomb singularity, $k' \simeq k$.

The indication that the program is actually searching through a complex energy space is given by lines of the form

```
zk1= -1.089E-01 2.377E+00 Er,Ei= -8.715E-03 -8.0E-04 zdet= 4.382E-05 -1.987E-05
```

We see here the values for the complex momentum, energy, and determinant. Of particular importance is how the value of the determinant decreases from 10^{-5} to 10^{-12} , and passes through zero. The latter value is what we accept as zero. We clearly have started with a pretty good guess of the energy to get $\det(1 - GV) = 10^{-5}$, but since we are looking for a small perturbation to a very large number, high precision is required.

The output terminates by giving all pure Coulomb atomic energies for both nonrelativistic and relativistic cases, as well as the level shift from the Bohr value, and its width.

3.6 Sample outbs

```
BOUND STATE calculation via det(1-GV)=0, ridge32, 8/86, program bsdetr, detcal
-0.008715      -0.000800      0.000000      0.000000      0.000000
0.000000
      0.000100      64.000000
-0.008715 -0.000800
Nr Lmax = 1 1
66 -8 2.40 3 100. 2400.
No of grid points= 66
1.550 1.550 0.000 1.5500 1.550 0.000 3.000 7.00
1 1 10 001700005 0 0 0 0 2 0 0 0 0 0
Nifty( 1)= 10 k-
Nifty( 2)= 0 *5=be shift
Nifty( 3)= 0 bs not res
Nifty( 4)= 1 nlsp-g(p)
Nifty( 5)= 7 e3b, aay
```



```

Nifty( 6)= 0      no spin ms
Nifty( 7)= 0      no abs/s-f
Nifty( 8)= 0      no del/fld
Nifty( 9)= 0      no pauli
Nifty(10)= 5      bs,pt coul
Nifty(11)= 0      pi0,pi-,k+ shift
Nifty(12)= 0      pi+,ko,k0b shift
Nifty(13)= 0      pi-channel shift
Nifty(14)= 0      pi+channelshift
Nifty(15)= 2      3 chn=ppin
Nifty(16)= 0      rhog,rho2g
Nifty(17)= 0      kmt
Nes,Nwaves,b0r,b0i,c0r,c0i= 2 14 0.00000 0.00000 0.00000 0.00000
Nes,Nwaves,b0r,b0i,c0r,c0i= 2 14 -0.04000 0.04000 0.00000 0.08000
RELATIVISTIC CALCULATION
1 1 10 001700005 0 0 0 2 0 1 0 0 0
Mproj, At, MA = 493.699 1.000 938.280
ar11, ar22, ar33= 323.488 0.00 158.450 0.0 325.343 0.0
ar11, ar22, ar33= 323.485 0.00 190.017 0.0 323.648 0.0

zE1, zE2, zE3 = -0.8715E-02 -0.8E-03 0.9905E+02 -0.8E-03 -0.5273E+01 -0.80E-03
zk1, zk2, zk3 = -0.1089E+00 0.2377E+01 -0.1772E+03 0.8580E-03 -0.4426E-02 0.5850E+02
kode < 0, use bs points,cpmax=10**kode, catom <, >0, kode,catom= -8 0.2400E+01
Ngp,Nnuc,Catom,Csize,Cnucl,Cpmax(MeV)= 66 0 0.2400E+01 0.1000E+03 0.2400E+04 0.1000E+09

points= 0.7848E-03 0.4139E-02 0.1019E-01 0.1896E-01 0.3050E-01 0.4486E-01 0.6209E-01 0.8229E-01
points= 0.1617E+00 0.1948E+00 0.2316E+00 0.2721E+00 0.3167E+00 0.3654E+00 0.4187E+00 0.4768E+00
...
weight= 0.2199E+01 0.2678E+01 0.3306E+01 0.4147E+01 0.5299E+01 0.6920E+01 0.9275E+01 0.1283E+02
weight= 0.4518E+02 0.8009E+02 0.1626E+03 0.4109E+03 0.1580E+04 0.1884E+05

den(n1,1-3) (P, Del parts) = 0.0000E+00 0.0000E+00 -0.1294E+06 -0.6732E+05 0.0000E+00
Zden(3/1,i)= 0.8988E-07 -0.8251E-08 0.5830E-05 -0.5352E-06 0.5570E-04 -0.5113E-05 0.2644E-03

----- Angular Momentum = 0-----
opt poten for k =k0(k1-bs)= 0.78480E-03and l=0(1-bs)
kp rev vc rabs(n0 flip) rabs(flip) -imv imvabs(noflip),imabs(flip)

ibag,iset,b0= 0 3 0.55600D+01 0.00000D+00acoup,iichanl= 1.000 1
10/b0(1,2,3 )= -0.32600D+03 0.00000D+00 -0.11200D+03 0.000D+00 -0.41200D+03 0.00D+00
b1,l1(iset)= 0.20000D+01 0.00000D+00 -0.30800D+02 -0.22400D+02

now in mev units,b=b*b,l=4pi*l--for lpt pot
ibag,iset,b0= 0 3 0.12037D+07 0.00000D+00acoup,iichanl= 1.000 1
10/b0(1,2,3 )= -0.44946D+07 0.00000D+00 -0.15442D+07 0.000D+00 -0.56803D+07 0.0D+00
b1,l1(iset)= 0.15575D+06 0.00000D+00 -0.76375D+05 -0.55545D+05

Oopt poten for k =k0(k1-bs)= 0.78480E-03and l=0(1-bs)
kp rev vc rabs(n0 flip) rabs(flip) -imv imvabs(noflip),imabs(flip)

0.7848E-03 -0.9875E+04 -0.9875E+04 0.000E+00 0.000E+00
2 -0.3920E-05 0.0000E+00
4 -0.7536E-06 0.0000E+00
3 -0.3125E-05 -0.1145E-05
5 -0.2316E-07 -0.1145E-05
6 0.7536E-06 0.0000E+00
0.4139E-02 -0.4312E+03 -0.4312E+03 0.000E+00 0.000E+00 -0.1145E-05
0.1019E-01 -0.7043E+02 -0.7043E+02 0.000E+00 0.000E+00 -0.1145E-05
0.3050E-01 -0.7845E+01 -0.7845E+01 0.000E+00 0.000E+00 -0.1145E-05
0.4486E-01 -0.3627E+01 -0.3627E+01 0.000E+00 0.000E+00 -0.1145E-05
0.6209E-01 -0.1893E+01 -0.1893E+01 0.000E+00 0.000E+00 -0.1145E-05
0.8229E-01 -0.1078E+01 -0.1078E+01 0.000E+00 0.000E+00 -0.1145E-05
...

0 complex*16 potential matrix before 1-GV formed
0 1 -0.987532E+04 -0.114482E-05 -0.431196E+03 -0.114482E-05 -0.704304E+02 -0.114482E-05 -0.203036E+02
-0.784506E+01 -0.114482E-05 -0.362693E+01 -0.114482E-05 -0.189268E+01 -0.114482E-05 -0.107756E+01
-0.222670E-05 -0.598368E-06 -0.162372E-05 -0.312208E-06 -0.676893E-06 -0.709222E-07 -0.368166E-07

1-G(complex*16)*V matrix before determinant found

1 0.999112E+00 0.814766E-04 -0.251387E-02 0.230762E-03 -0.392295E-02 0.360104E-03 -0.536756E-02
-0.683909E-02 0.627695E-03 -0.834162E-02 0.765449E-03 -0.988091E-02 0.906399E-03 -0.114631E-01
zk1= -1.089E-01 2.377E+00 Er,Ei= -8.71500000E-03 -8.00000000E-04 zdet= 4.382E-05 -1.987E-05

den(n1,1-3) (P, Del parts) = 0.0000E+00 0.0000E+00 -0.1294E+06 -0.6732E+05 0.0000E+00 0.0000E+00
zk1= -1.089E-01 2.377E+00 Er,Ei= -8.71499987E-03 -8.00000000E-04 zdet= 4.382E-05 -1.987E-05

den(n1,1-3) (P, Del parts) = 0.0000E+00 0.0000E+00 -0.1294E+06 -0.6732E+05 0.0000E+00 0.0000E+00
zk1= -1.089E-01 2.377E+00 Er,Ei= -8.71500000E-03 -7.99999988E-04 zdet= 4.382E-05 -1.987E-05

```

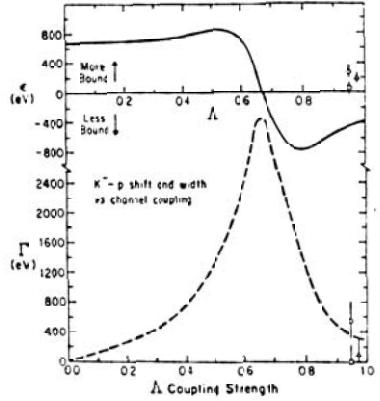


Figure 3: The level shift and width for the 1S level in kaonic hydrogen as a function of the strength of coupling to the $\Sigma\pi$ channel (as published by Landau). At $\Lambda \simeq 0.65$ a nuclear bound state is first formed.

```

den(n1,1-3) (P, Del parts) = 0.0000E+00 0.0000E+00 -0.1294E+06 -0.6733E+05 0.0000E+00 0.0000E+00
zk1= -1.923E-02 -2.318E+00 Er,Ei= -8.30331482E-03 1.37798748E-04 zdet= 7.762E-06 2.900E-06

den(n1,1-3) (P, Del parts) = 0.0000E+00 0.0000E+00 -0.1294E+06 -0.6734E+05 0.0000E+00 0.0000E+00
zk1= -4.517E-02 -2.328E+00 Er,Ei= -8.37590845E-03 3.25078934E-04 zdet= 1.232E-07 2.860E-06

den(n1,1-3) (P, Del parts) = 0.0000E+00 0.0000E+00 -0.1294E+06 -0.6734E+05 0.0000E+00 0.0000E+00
zk1= -4.464E-02 -2.337E+00 Er,Ei= -8.44150430E-03 3.22558220E-04 zdet= -7.893E-07 4.548E-07

den(n1,1-3) (P, Del parts) = 0.0000E+00 0.0000E+00 -0.1294E+06 -0.6734E+05 0.0000E+00 0.0000E+00
zk1= -4.167E-02 -2.338E+00 Er,Ei= -8.44451178E-03 3.01134572E-04 zdet= -5.031E-08 1.686E-08

den(n1,1-3) (P, Del parts) = 0.0000E+00 0.0000E+00 -0.1294E+06 -0.6734E+05 0.0000E+00 0.0000E+00
zk1= -4.149E-02 -2.338E+00 Er,Ei= -8.44441201E-03 2.99806773E-04 zdet= -3.288E-11 4.268E-10

den(n1,1-3) (P, Del parts) = 0.0000E+00 0.0000E+00 -0.1294E+06 -0.6734E+05 0.0000E+00 0.0000E+00
zk1= -4.149E-02 -2.338E+00 Er,Ei= -8.44442175E-03 2.99801698E-04 zdet= 6.129E-12 -7.789E-12

Onormal termination, relative error is at most 0.0001000000
nbohr,e(se),e(kge1,2)= 1 -8.6130774298E-03 -8.6136508160E-03 -8.6138801937E-03 eta= 1.00002663E+00
nbohr,e(se),e(kge1,2)= 2 -2.1532693574E-03 -2.1533625309E-03 -2.1533768655E-03 eta= 1.00000666E+00
nbohr,e(se),e(kge1,2)= 3 -9.5700860331E-04 -9.5703833353E-04 -9.5704116498E-04 eta= 1.00000296E+00
nbohr,e(se),e(kge1,2)= 4 -5.3831733936E-04 -5.3833032970E-04 -5.3833122553E-04 eta= 81.00000166E+00
OE(MeV)=-.008444421752510.00029980169841 eps,gamma(eV)= -168.7 -599.6
Del E(ev)= 168.7 299.8
*****eof in main*****

```

4 Exploration

4.1 Electronic Hydrogen

While `BS.f` can clearly do some fancy computations, we need to believe its results before we can use it to study new physics. As a way of both tuning up and checking the code, we first try to calculate ordinary electronic hydrogen. We know that for a nonrelativistic computation, the bound state energies should be the Bohr values (2) with μ the ep reduced mass.

To have `BF.f` compute electronic hydrogen with no nuclear forces acting (not something it was written for), make the following changes (after saving the original in a different file):

1. `drr(n)th` should be near, but not too near, to the electronic values for hydrogen.
2. `eim=0.0` since there is no decay and the levels have no width.
3. `catom=0.01` for a smaller scale factor for integration grid.

4. `nifty(1)=10` sets K^- as orbiting particle.
 5. `nifty(6)=6` turnf on only the Coulomb force.
 6. `nifty(15)=0` uses only channel 1, the incident channel.
 7. Replace the numerical value 493.699 for the kaon mass (in MeV/c^2) by the electron's value, 0.51072075.
1. Vary the number of grid points from 8 to 66 to see the effect upon the accuracy.
 2. Notice that if the initial guesses that start the search are not close the energy for a particular nS level, the program may end its search at a neighboring level instead.
 3. Based on the known properties of the hydrogen spectrum, what would you expect to happen as you search for large nS levels?

4.2 Pure Coulomb Kaonic Hydrogen

Now change the rest mass of the electron back up to that of a K^- , 493.699 MeV, and run through the series of integration point again. Check that you obtain energies that agree with the Bohr values using the appropriate reduced mass. If needed, adjust `catom` for a better distribution of integration points.

4.3 Kaonic Hydrogen with Strong Interaction

Because of the much smaller Bohr radius for the more massive K^- , the strong, but short-ranged nuclear force significantly affects the 1S state of kaonic hydrogen. The higher orbits are affected to a much smaller degree. Although not yet the full calculation, let's turn on the nuclear force, still with just one channel open.

Set `nifty(6) = 0` to turn on the strong force. This should be the attractive strong force, but without the open channel in (11) that causes absorption. Accordingly, the level should become more bound. Is it more bound, and if so, by how much?

4.4 Include Additional Channels

We now make the problem realistic by including the open channel 2 and the charge exchange channel 3. Set `nifty(15) = 2` for three channels. This should the absorption that gives the level a finite width.

1. Take note of the change in the 1S level width and whether its shift is to the more or less bound. Explain.
2. Take note of the effect of including the open channel 2 on the 2S and 3S levels. Is the shift inversely proportional to the distance from the nucleus, $\epsilon \propto R^{-1}$?

4.5 Importance of Relativity

The equations in `BS.f` are written so that the relativistic or nonrelativistic definitions of energy can be used:

$$E_{nonrel}(p) = \frac{p^2}{2m_1} + \frac{p^2}{2m_2} \equiv \frac{p^2}{2\mu}, \quad (49)$$

$$E_{rel}(p) = \sqrt{p^2 + m_1^2} + \sqrt{p^2 + m_2^2}. \quad (50)$$

The input variable `Nr =0, 1` controls whether a nonrelativistic or relativistic computation is performed. It may well be that the effect of relativity is more important in kaonic hydrogen than in electronic hydrogen. Let's see.

1. Explore the effect of relativity on the 1S energy level in electronic hydrogen. You will need to run the calculation for a single channel with the kaon mass set equal to the electronic mass, and with no nuclear forces.
2. Compare the size of the relativistic effect that you found with your computation for electronic hydrogen to that which is predicted by the Klein-Gordon equation (a relativistic generalization of the Schrödinger equation)[14]. The energy for the hydrogen levels in the Klein-Gordon equation has the form

$$E = \frac{mc^2}{\sqrt{1 + \frac{\gamma^2}{[n - (l + \frac{1}{2}) + \sqrt{(l + \frac{1}{2})^2 - \gamma^2}]^2}}} \simeq mc^2 - \frac{\text{Ry}}{n^2} - \frac{\text{Ry}\gamma^2}{n^3} \left(\frac{1}{l + \frac{1}{2}} - \frac{3}{4n} \right), \quad (51)$$

$$\gamma = \frac{Ze^2}{\hbar c}, \quad \text{Ry} = 13.605692 \text{ eV}. \quad (52)$$

3. Now look at the full kaonic hydrogen computation with the strong interaction present in three channels. Does the relative importance of relativity increase or decrease as compared to electronic hydrogen?

4.6 Map the Energy Space Search

The search that `BS.f` uses is nonlinear (in contrast to the bisection algorithm, that is linear). Typically it will start with large steps, and then switch its technique when it gets closer to a zero. The aim is to make the search fast and flexible. In our case the search is also complicated by its need to make a 2D search for the best values for *both* the real and imaginary parts of the energy.

In this section we want you to map the convergence of the search routine. Draw up the path taken through complex energy space for several searches that succeed, as well as for ones that fail. Label each energy point by the corresponding value of `zdet`. Note that you may need to employ logarithmic scales to visualize the search best. Describe in words what is happening for a successful and unsuccessful search.

4.7 Complex Energy Shift vs Coupling Strength

In Fig. 3 we show the shift and width of the 1S level in kaonic hydrogen as a function of the strength Λ of coupling between the incident channel 1 and the open channel 2. As expected for an attractive interaction, for small values of Λ the shift is towards the more bound, but for $\Lambda \simeq 0.65\%$ something happens and the shift changes sign. That “something” is that the nuclear interaction has become strong enough to form a K^-p nuclear bound state (a new elementary particle) deep within the 1S atomic bound state. In this part of the lab you should try to reproduce Fig. 3 and to find the energy of the nuclear bound state.

1. The subroutine `vkbarp` computes the coupled channels, strong interaction potential for the K^-p system. Browse through that subroutine and take note of the use of the coupling strength variable `acoup`. This is the value of Λ . As indicated there, negative values of the input variable `nwaves` change `acoup` according to

$$\text{acoup} = - \text{nwaves}/100.$$

This means that a value of `nwaves` = -60 corresponds to $\Lambda = 0.6$. Vary the value read in for `nwaves` to generate your own version of Fig. 3.

2. If you obtain a sign change in ϵ , this means there is a nuclear bound state being formed. Search for that state. You will need to change the sign of `nes`, say from 2 to `nes` = -2. You then need to try initial energy guesses in the Million eV range.

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