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EXOTIC: A Computer Code for Energy Levels
of Exotic Atoms

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Justus H. Koch*
Morton M. Sternheim**

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EXOTIC: A COMPUTER CODE FOR ENERGY LEVELS OF EXOTIC ATOMS

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ABSTRACT

EXOTIC is a FORTRAN code which finds the eigenfunctions and complex eigenvalues of the Klein-Gordon equation for K-mesic atoms. Provisions are made to allow for various models of the nuclear interaction. With some modifications this program can also be used for other exotic atoms.

I. INTRODUCTION

EXOTIC is a FORTRAN code which finds the eigenfunctions and complex eigenvalues of the Klein-Gordon equation for K-mesic atoms. It contains an optical potential, V_N , which is proportional to the nuclear density, and a finite charge distribution Coulomb potential, V_C :

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - (E - V_C)^2 + m^2 + 2EV_N \right] u = 0. \quad (1)$$

Here m is the kaon reduced mass.

This program can also be used for other exotic atoms. With some modification of V_N , the Krell-Ericson local form¹ of the Kisslinger potential² for pions could be incorporated. If one neglects fine structure effects, it can also be used for $\bar{p}$ and Σ^- atoms.

The nuclear potential, V_N , can be chosen to be of the form

$$V_N(r) = -(2\pi/m)(1 + m/m_N)b\rho(r) \quad (2a)$$

for

$$\rho_n(r)/N = \rho_p(r)/Z = \rho(r)/A,$$

or

$$V_N(r) = -(2\pi/m)(1 + m/m_N)[b_n\rho_n(r) + b_p\rho_p(r)]. \quad (2b)$$

Here m_N is the proton mass and the nuclear densities are normalized to

$$\int \rho_p d^3r = Z, \quad \int \rho_n d^3r = N, \quad \text{and} \quad \int \rho d^3r = A.$$

The complex b 's are the "effective scattering lengths" for the K-N systems.

The shifts ϵ and widths Γ resulting from the strong interaction are defined according to

$$\epsilon - i\Gamma/2 = E(\text{calculated}) - E(\text{point Coulomb}), \quad (3)$$

i.e., $\epsilon > 0$ corresponds to a repulsive shift. Note that Eq. (3) will also include the small effects due to a finite charge distribution if V_C does not correspond to a point charge. EXOTIC has been used to calculate energy levels of several K-mesic atoms.^{3,4}

II. NUMERICAL METHODS

The differential equation, Eq. (1), is integrated using standard techniques.⁴ A modified Noumerov⁵ method is used to integrate out from the origin and in from a radius, r_n , where the wave function is closely approximated by its asymptotic form. An iteration procedure discussed below reduces the discontinuity in u'/u at the matching point as the eigenvalue is approached.

A. Integration

To begin the outward integration for a state with quantum numbers n, ℓ , we use

$$u(0) = 0, u(r_1) = r_1^{\ell+1}.$$

To begin the inward integration, we use

$$u(r_n) = \text{const.},$$

$$u(r_{n-1}) = u(r_n) e^{-ik(r_n - r_{n-1})},$$

where k , the average wave number in the starting region, is

$$k = \frac{1}{2} \left\{ \left[E_0 - V_C(r_n) \right]^2 - m^2 \right\}^{1/2} + \frac{1}{2} \left\{ \left[E_0 - V_C(r_{n-1}) \right]^2 - m^2 \right\}^{1/2}, \quad \text{Im } k < 0. \quad (4)$$

The initial trial eigenvalue, E_0 , is either the point Coulomb value or one inferred from preceding calculations with slightly different optical potentials.

Except for s -states, the wave function has two classical turning points. The inward integration is started where $u(r_n)$ is a factor e^{-15} times its value at the outer turning point. (An optional input control permits this factor to be changed.) Normally, we take r_m , the point where we match the two wave functions, to be the inner turning point. (This can also be adjusted with an optional input.)

The numbers of mesh points in the two integrations are chosen independently. This allows the use of a finer mesh in the outward integration, thus producing a greater accuracy in calculating the nuclear shifts for a given total number of points.

B. Iteration Procedure

Blatt⁶ has given a very efficient method of determining the correct eigenvalue from a reasonably good trial eigenvalue based on the variational principle. Let E_0 be the trial eigenvalue, and u_1^0 and u_2^0 be the corresponding solutions of Eq. (1) for $r < r_m$ and $r > r_m$, respectively. The normalization of u_2^0 is adjusted so that $u_1^0(r_m) = u_2^0(r_m)$. Define E_1 by

$$E_1^2 = N^{-1} \int u^{0*} \left[-\frac{d^2}{dr^2} + G(r) \right] u^0 dr, \quad (5)$$

where

$$N = \int u^{0*} u^0 dr,$$

and

$$G(r) = \ell(\ell+1)/r^2 + 2E_0 V_C - V_C^2 + 2E_0 V_N + m^2. \quad (6)$$

E_1 is an improved trial eigenvalue. Since u^0 satisfies

$$\left[-\frac{d^2}{dr^2} + G(r) \right] u^0(r) = E_0^2 u^0(r), \quad (7)$$

except at $r = r_m$, we obtain

$$E_1^2 = E_0^2 + \Delta, \quad (8)$$

where Δ is a term arising from the discontinuity in u_1^0 . Explicitly,

$$\Delta = (u_1^{0*} u_1^{0'} - u_2^{0*} u_2^{0'}) / N. \quad (9)$$

Usually, we have found that this procedure converges extremely rapidly. If E_0 is not a sufficiently good starting value for this method to converge, the code will automatically find a better trial value, E_1 , with a gradient search and eventually return to the Blatt iteration method.

C. Accuracy and Speed

Using 500 mesh points in each region, i.e., $NPTS(1) = NPTS(2) = 500$, the maximum provided for in EXOTIC, we have reproduced the point Coulomb binding energies to a part in 10^9 , e.g., to 10^{-3} eV or better for sulfur. Normally, with the optical potential, V_N , turned on, the eigenvalue iteration procedure requires only 1 to 4 iterations to yield a binding energy stable to a part in 10^8 or 10^9 , i.e., a shift and width stable to better than 1 eV.

With $NPTS(1) = NPTS(2) = 250$, a sequence of eigenvalue calculations for closely spaced complex well depth parameter values can be done at the rate of 5 per second on a CDC 6600.

As noted above, various optional inputs are available. They make it possible to change the mesh sizes, the matching point, the starting point for the inward integration, and the convergence criterion. Thus, one can determine empirically the

optimum choices for these parameters and verify the accuracy for particular situations.

III. ORGANIZATION OF PROGRAM

The program is organized in the conventional way with a main program and several subroutines. Each of these will be discussed briefly below.

A. EXOTIC (Main program)

This reads the input data, makes suitable unit conversions, calls the major subroutines, and prints the inputs and some intermediate quantities.

B. WELLS

Called by EXOTIC. At start of run it calls the subroutines which tabulate VR, VI, and VC, the real, imaginary, and Coulomb well shapes, respectively. For each set of (Keh, Imb) values, it multiplies VR and VI by the appropriate factor.

C. WREAL, WIMAC, WCOUL

Called by WELLS. These tabulate VR, VI, and VC for uniform spheres or Saxon-Woods densities.

D. EIGEN

Called by EXOTIC. Controls integration and iteration procedures, prints principal results.

E. SMOOTH, SMOOTH4

Called by EIGEN. Extrapolate results of preceding 3 or 4 calculations to provide starting E_0 for current value of b.

F. INT

Called by EIGEN. Integrates differential equation and obtains new trial eigenvalue E_1 using iteration procedure. (See Sec. II above.)

G. FARRAY

Called by INT. Tabulates F, where

$$F = d^2[m^2 - E^2 + 2E(V_C + V_N)] + F3, \quad (10)$$

and

$$F3 = d^2[L(L+1)/R^2 - V_C^2]. \quad (11)$$

Here d is the step size, which is different in the two regions.

H. GRADIN

Called by EIGEN. Used to obtain an E only if iteration procedure of INT fails to converge.

I. PRINT

Called by EIGEN. Prints wave functions.

J. PERT

Called by EXOTIC. Calculates strong interaction shifts at widths in first order perturbation theory using Klein-Gordon Coulomb wave functions.

K. CHANGE

Called by EXOTIC. Changes specified parameters and restarts same series of calculations. Avoids need to read complete new input deck.

IV. PROGRAM INPUT

All integer inputs must be right justified.

A. Basic Input Deck

Card 1: Title Card

- Col. 2: A "1" indicates the start of a new problem.
A "2" indicates the end of the job.
Negative entries in Col. 1-2 activate the change card procedure. (See Sec. IV.C below.)
- Col. 3-80: Title - to be printed as output heading.

Card 2: Control Card

- †Col. 1-10*: Z - nuclear charge number.
- †Col. 11-20: ANUM - nuclear mass number. Need not be rounded to an integer. (If blank or zero, 2Z is used.)
- †Col. 21-30: PMASS - meson mass in MeV. (If blank or zero, the K^- mass 493.84 MeV is used.)
- Col. 35*: N - principal quantum number of atomic state.
- Col. 40*: L - angular momentum quantum number of atomic state.
- Col. 43-45: NPTS(1) - number of mesh points in inner region, ≤ 500 . (If < 50 , 250 is used.)
- Col. 48-50: NPTS(2) - number of mesh points in outer region, ≤ 500 . (If < 50 , 250 is used.)
- Col. 55: IEXP - eigenvalue search or iteration procedure stops when fractional change in the energy-eigenvalue $< 10^{-IEXP}$. (If blank or zero, 6 is used.)

†Floating point quantity; must have a decimal point.

*This input must always be specified.

Col. 58-60: IPR - potential array print control.
 IPR = +n: Causes arrays to be printed at every nth point for each eigenvalue.
 IPR = -n: Causes arrays to be printed at every nth point for first eigenvalue only.
 $|n| \leq 50$.
 Arrays printed (in notation of Section III):
 $F1 = 2d^2 V_C$
 $F2 = 2d^2 (V_C + V_N)$
 VR, real potential normalized to ANUM.
 VI, imaginary.
 F, F3. See Eqs. (10) and (11).

Col. 65: INNER - if equal to 1 or 2 this will cause an extra card, number 6, to be read. See below.

Col. 70: IQ - iteration print control.
 IQ = 1: All trial eigenvalues and the corresponding discontinuity in the logarithmic derivative will be printed.
 IQ $\neq$ 1: Only the first and last step will be printed.
 In all cases, the output contains: input data, point Coulomb energy, Bohr radius, inner and outer turning points (RTURN), maximum radii of the inner and outer integration (RMAX), two mesh sizes (DR), "effective scattering length," calculated shift and width, and complex wave number $k = (E^2 - m^2)^{1/2}$.

Col. 73-75: IW - wave function print control.
 IW = +n: Real, imaginary parts for every nth point.
 IW = -n: Magnitude, phase.
 $|n| \leq 50$.

Col. 80: IPT = 0 or blank: Calculates exact eigenvalues and prints them.
 IPT = -1: Same as above, but also writes nuclear charge Z, shift EPS and width GAM on tape 93 (FORMAT 1X, F5.1, 2E15.6).
 IPT = +1: Calculates nuclear shift and width in perturbation theory.

IPT = +2: As above, but also writes perturbation theory shifts and widths on tape 92; same FORMAT as for IPT = -1.

Card 3: Coulomb Card

All radii on cards 3, 4, and 5 are in fermis.

Col. 10*: IC - Coulomb well type.
 1 - uniform sphere charge distribution.
 2 - Saxon-Wood:
 $\rho = \rho_0 \left(1 + \exp[(R - RC)/AC] \right)^{-1}$.

†Col. 11-20*: RC - Coulomb radius.
 If IC = 1, RC = radius of sphere.
 If IC = 2, RC = half density radius.

†Col. 21-30: AC - thickness parameter, required for IC = 2.

†Col. 31-40: XN(1). Controls location of matching inner and outer wave functions. Matching is at the inner classical turning point + $XN(1)/Im(2mW_0)^{1/2}$, where W_0 is the point Coulomb energy, and m is the meson mass, both in f^{-1} . Should normally be left blank or zero.

†Col. 41-50: XN(2). Controls location where outer wave function integration begins. This is at the outer classical turning point + $XN(2)/Im(2mW_0)^{1/2}$. If blank or zero, 15 is used. Should normally be left blank or zero.

†Col. 51-60: RTYPE - type of radial parameters.
 0.0 - all radii are used as given.
 1.0 - RC, RRE, RIM (see below) multiplied by $(ANUM)^{1/3}$.

†Col. 61-70: STEPO - fractional step size for start of gradient search. (If blank or 0, 0.01 is used. Should normally be left blank.)

Col. 71-80: DENS = 1: Will cause the code to use a two-density potential, Eq. (2b). The format of cards 4' and 5', to be used in this case in place of cards 4 and 5, is given below in Sec. IV.B.

†Floating point quantity; must have a decimal point.

*This input must always be specified.

Card 4: Real Well Card

Col. 10: IR - real well type.
-1 - same well type and parameters as Coulomb.
0 - no real well.
1 - uniform sphere.
2 - Saxon-Wood.

†Col. 11-20: RRE - real well radius.
Required for IR = 1,2.
If IR = 1, RRE = radius of sphere.
If IR = 2, RRE = half density radius.

†Col. 21-30: ARE - real well thickness parameter, required for IR = 2.

†Col. 31-40: BRO - initial value of real part of scattering length (in fermis).

†Col. 41-50: DBR - increments in real part of scattering length (in fermis).

Col. 51-60: NBR - number of real well depth values to be computed.

Card 5: Imaginary Well Card

Col. 10: II - imaginary well type.
-1 - same well type and parameters as real well.
0 - no imaginary well.
1 - uniform sphere.
2 - Saxon-Wood.

†Col. 11-20: RIM - imaginary well radius.
Required for II = 1,2.
If II = 1, RIM = radius of sphere.
If II = 2, RIM = half density radius.

†Col. 21-30: AIM - imaginary well thickness parameter, required for II = 2.

†Col. 31-40: BIO - initial value of imaginary part of scattering length.

†Col. 41-50: DBI - increments in imaginary part of scattering length.

Col. 51-60: NBI - number of imaginary well depth values to be computed.

Card 6: Starting Values (Required only if INNER = 1 or 2 on card 2)

If INNER = 1:

†Col. 1-10: WRL - starting value for real part of energy for eigenvalue search (in f^{-1}).

†Col. 11-20: WIG - starting value of imaginary part of energy (in f^{-1}).

If INNER = 2: The program prints χ^2 , experimental values for shift and

width (including the errors) and puts the χ^2 (CHISQ) on tape 91 [FORMAT (E15.6)]. The user can then in a separate run use the information stored on that tape to construct χ^2 - maps, etc.

†Col. 1-10: Experimental shift (in keV).
†Col. 11-20: Experimental error in shift (in keV).
†Col. 21-30: Experimental width (in keV).
†Col. 31-40: Experimental error in width (in keV).

B. Two Densities, ρ_n and ρ_p

If DENS = 1 on card 3, the program will use separate densities for neutrons and protons. There are no provisions made to execute DO-loops for the effective scattering lengths in this optional mode.

Card 4':

Col. 1-10: Well type, proton. Code for different types as above for card 4.

†Col. 11-20: Well radius for protons.

†Col. 21-30: Thickness parameter for proton well.

†Col. 31-40: Re b_p , see Eq. (2b).

†Col. 41-50: Im b_p , see Eq. (2b).

†Col. 51-60: Leave blank.

Card 5': Same as card 4', but for neutrons.

C. Change Cards

It is possible to change parameters between problems without making a complete new input deck by using the procedure below.

Card 7:

Col. 1-2: -J, where J is the number of parameters to be changed ($J \leq 8$).

Col. 3-80: Title, to be printed as a heading for the output.

Card 8:

Col. 1-2: 1st parameter number (see Table I).
†Col. 3-10: 1st parameter value.
Col. 11-12: 2nd parameter number.
†Col. 13-20: 2nd parameter value.
etc.: With up to 8 parameter numbers and values on the card.

†Floating point quantity; must have a decimal point.
*This input must always be specified.

TABLE I

Parameter Name	Parameter Number
Z	1
ANUM	2
PMASS	3
RC ^a	4
AC	5
RRE ^{a,b}	6
ARE	7
RIM ^{a,c}	8
AIM	9
XN(1)	12
XN(2)	13
N	14
L	15
NPTS(1)	16
NPTS(2)	17

^a If RTYPE = 1, ANUM^{1/3} scaling will be used.

^b If IR = -1, RRE will be set equal to RC, and ARE to AC.

^c If II = -1, RIM will be set equal to RRE, and AIM to ARE.

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