Faddeev Bound State program EFADDY

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Version 1.71: with coupled occupied & transfer states

Introduction

This program calculates the bound states of two nucleons with a third core. Interactions are by local potentials, with the nucleon wave function orthogonal to set of occupied states in the core. The core may have a set of states of arbitrary energies, spins & parities, and these states may be coupled together by a collective model using a multipole-deformed potential.

Input Specifications

HEADER: A80
Card for text describing run.

FPOT (String in quotes)
Name of file stem: to create FPOT.mout with additional output, and (if NMAX=0) FPOT.spec, FPOT.mel and FPOT.occ with files for STURM.

AC,ZC,RCORE

AC mass of core nucleus

ZC charge of core nucleus

RCORE r.m.s. matter radius of target nucleus

NTARG,KTARG,(DEF(I),I=2,5)

NTARG abs(NTARG) = number of target states
If NTARG < 0, then the VOLCON logical variable is set TRUE for use by the potential function routines UC(L,R) etc. and read:

(DEFH(I),I=2,5) Deformation lengths for 3-body Hamiltonian, as DEF only used for occupied states.

KTARG K projection for coupling states by the rotational model (real)

DEF(2:5) deformation lengths δ_2, δ_3, δ_4, and δ_5. These deformation lengths are found from the fractional deformations β_K by $\delta_K = \beta_K R$ for nuclear radius R.

JTARG(i),PTARG(i),ETARG(i) Card repeated for i=1,NTARG: specification of each target state

JTARG spin J_c (real)

PTARG parity π_c (integer +1 or -1)

ETARG energy E_c

Q0CORE Card read only if maxval(JTARG(:))>0

Q0CORE Intrinsic quadrupole moment of core, used for E2 transitions.

AN,ZN,RN,SN,TT,(ZN2,RSCR)

AN mass of valence particle

ZN charge of valence particle

RN r.m.s. matter radius of valence particle (0 for nucleons!)

SN spin s of valence particle, 0 or 0.5 (real)

TT isospin of valence particle, 0 or 1 (integer)

ZN2 charge of second valence particle (read in if ZN>0)

RSCR screening radius for Coulomb potentials (RSCR=0 is no screening) (read in if ZN>0)

H2M

H2M $\hbar^2/2m$ for unit mass m. Use 20.900795 for AC, AN in amu, and 20.721 for masses in units of neutron mass. With neutron mass units, use 20.748 for the old HH programs and 20.735 for the old CSF programs.

KMAX,LNCMAX,LNNMAX,SMAX,LLMAX,L2MX,EQN,JNNMX(1:-L2MX)

KMAX Max. hyperharmonic K

LNCMAX Max. angular momentum L_{cn} (between core and neutron) with non-zero potential

LNNMAX Max. angular momentum L_{nn} (between two neutrons) with non-zero potential

SMAX Max. spin S of the two neutrons (integer 0 or 1)

LLMAX Max. angular momentum $L = L_{cn} + L_{nn}$

L2MX Absolute value is max. angular momentum λ between the interacting pairand the spectator.

EQN (character in quotes) Type of equation to solve: `'F'`=Faddeev, `'T'`=T-Schrodinger:HH, `'Y'`=Y-Schrodinger.
If 'a' lle EQN lle 'z', then set FESH=true for Feshbach reduction.

JNNMX(1:-L2MX) Max. angular momentum J_{nn} of valence pair, for each L (i.e. read only if L2MX< -1).

If KMAX < -1**: K3MAX(L,IC),L=0,MAXLR+1**
Max. hyperharmonic K for each particular L=L_{nn} and IC, followed by max. K for both $L_{nn} \geq 2$ and $L_{(nn)c} \geq 2$, where MAXLR=min(MAXL,3) with MAXL = max(LNNMAX,LNCMAX,L2MX). This card is repeated for each IC=1 to NTARG.

If K3MAX(0,1) < -1**: K2MAX(L,IC),L=0,MAXLR+1**
Max. hyperharmonic K for each particular L=L_{cn} and IC, followed by max. K for both $L_{cn} \geq 2$ and $L_{(cn)c} \geq 2$.
This card is repeated for each IC=1 to NTARG.

If KMAX = -1**: PWFILE, THRESH**

PWFILE (string in quotes) name of file of partial wave weights from previous calculation.

THRESH real positive threshold for including partial waves in this calculation.

At present, the KMAX=–1 option only works for EQN='F'

If FESH**: Kmaxf(1:NTARG),EFesh,RLOC,NDROP**

Kmaxf(1:NTARG) Perform Feshbach reduction to $K_{\max}$ for each target state.

EFesh Feshbach target eigenenergy

RLOC Radius for local Pauli blocking

NDROP Number of adiabatic energy surfaces to drop for Pauli Blocking.

RR,NLAG,NJAC,RINNER

RR Scaling factor for hyperradius grid

NLAG Number of hyperradial grid points.
If NMAX $\neq$ 0, use NLAG Gauss-Laguerre quadrature points, and perform diagonalisation for eigen-energies
If NMAX = 0, use NLAG *regularly spaced* hyperradial points from RR to RR*NLAG, and write the output files FPOT.spec, FPOT.mel and FPOT.occ with files for STURM

NJAC Number of Gauss-Jacobi hyperangular quadrature points.

RINNER Radius for orthonormalisation of Pauli Projection operators

If NDROP>0**: NJT,JTOTS(i),PARITIES(i),i=1,NJT**

NJT Number of angular momentum/parity sets (integer)

JTOTS(i) Total angular momentum (real)

PARITIES(i) (character in quotes) Parity ('+' or '-')

If NDROP<0**: NJT,(JTOTS(i),PARITIES(i),DROPS(i),i=1,NJT**

NJT,JTOTS,PARITIES As above

DROPS Number of adiabatic energy surfaces to drop for Pauli Blocking for each spin/parity combination given.

NMAX,EMIN,DE,EMAX,MEIGS,MOMDIS

NMAX Number of Legendre-polynomial basis functions for diagonalisation.
If NMAX $\neq$ 0, use NLAG Gauss-Laguerre quadrature points, and perform diagonalisation for eigen-energies
If NMAX = 0, use NLAG *regularly spaced* hyperradial points from RR to RR*NLAG, and write the output files FPOT.spec, FPOT.mel and FPOT.occ with files for STURMXX

EMIN If NMAX > 0, energy for inverse iteration: find eigenstates nearest to EMIN. Find MEIGS states.
If NMAX < 0, find all eigensolutions. MEIGS must be large enough.

DE (Read if NMAX<0) Energy step for discrete response functions.

EMAX (Read if NMAX<0) Maximum energy for discrete response functions.

MEIGS Number of eigensolutions to find.

MOMDIS For each solution calculate the spherical & projected momentum momentum distributions, using momentum up to $k_{max} = 2$ fm^{-1}.

DX,XMAX,DY,YMAX,RNODE,ITRBS,LBSMAX,KAPP, {EPS2,N3BLOCK}

DX step size for bound states

XMAX max. radius for bound state wave functions.

DY spacing of splines for y dimension of each blocked state

YMAX maximum y of each spline set.

RNODE max. radius for counting nodes in bound state wave functions.

ITRBS Non-zero to print bound state details (e.g. odd for wave functions).

LBSMAX Maximum l for bound-state wave functions.

KAPP Non-linearity parameter for spline functions in Pauli blocking (if zero, use 1d-3)

EPS2 {read if KAPP<0}: threshold norm of Pauli projection operators, (default value is 0.1)

N3BLOCK {read if KAPP<0}: number of 3-body bound states to read in 51, to give blocking projection operators (default value is zero).

BKIND,NV,LV,JV,BE,START,NOM

Occupied Y states $\sum_{ljc} \; |(sl)j, I;\; J\rangle$ for s = SN and core state I = JTARG(c):
or occupied T states $\sum_{l,S} \; |(ss)S, l;\; J\rangle$ for s = SN:
card repeated until the following line of zeros is read.

BKIND Component kind: 1 for β (nucleon-core=Y), 2 for α (NN=T) occupied states.
BKIND=3 or 4 (resp.) for transfer states.
BKIND=5 or 6 (resp.) for continuum bin states (unoccupied!).
If BKIND < 0, use |BKIND| as a test wavefunction only (not occupied).
If BKIND > 10, then use BKIND–10 (and BKIND+10 if BKIND< -10) and also, if searching for potential scaling factor, save this factor in array VSCALE(mod(l,2)) for use by potential function UC(L,R) for e.g. rescaling the central potential to depend on the parity of the ground state. Also read in DE,NK,ISC

NV Number n of nodes (including origin) in first component with l = LV (except if NOM < 0).
If NV < 0, force unbound state search.
For continuum bins, the incoming channel is number NV.

LV An l value in the bound state: $(-1)^l \times \pi_1$ gives overall parity

JV BKIND=1,3: Total angular momentum J in state $\sum_{ljc} \; |(sl)j, I;\; J\rangle$ (real)
BKIND=2,4: Total angular momentum J in state $\sum_{l,S} \; |(ss)S, l;\; J\rangle$ (real)

BE If positive, use this binding energy, and rescale the potential;
if zero, find binding energy for fixed potential;
if negative, search for unbound state giving phase shift $\delta = 90°$.

START Initial value for binding energy or potential multiplier

NOM If NOM < 0, make NV the number of nodes in channel number |NOM|, and ensure that this channel is non-zero.
If NOM > 0, read in list of omitted partial waves:
one per new card in format (integer, real, integer): l, j, c (c = core state index).

If BKIND=5 or 6 Also read a card with:

DE Width of bin in MeV: from |BE|-DE/2 to |BE|+DE/2

NK Number of k values in quadrature for bin.

ISC Scaling weight factor before quadrature:
2: $\exp(-i\delta(k))$ 4: $\sin(\delta(k))\exp(-i\delta(k))$ 12: $k\exp(-i\delta(k))$ 14: $k\sin(\delta(k))\exp(-i\delta(k))$

(repeated until BKIND=0)

0 0 0 0 0 0 0

NN and NC potentials

These are specified by including FORTRAN functions for:

NN interaction: VC(L,R), VLS(L,R), VT(L,R), VLL(L,R) where VLS is the $(\mathbf{s_{n1}} + \mathbf{s_{n2}}) \cdot \mathbf{L}$ interaction;

NC interaction: UC(L,R), ULS(L,R), ULSC(L,R), ULL(L,R), UT(L,R) where ULS is the neutron spin-orbit $\mathbf{s_n} \cdot \mathbf{L}$ and ULSC the core spin-orbit $\mathbf{J_c} \cdot \mathbf{L}$ potential.

VT and UT are tensor potentials using spins $(\mathbf{s_{n1}} + \mathbf{s_{n2}})$ and $(\mathbf{s_n} + \mathbf{J_c})$ respectively, and do not change the core state $\mathbf{J_c}$.

When any $\delta_K \neq 0$, the central interaction UC(L,R) is deformed by all the non-zero δ_K according to

$$V_{\mathtt{L}}(r,\theta) = \mathtt{uc}(\mathtt{L}, r - \sum_{K=2}^{5} \delta_K P_K(\cos\theta)\sqrt{\frac{2K+1}{4\pi}})$$

and projected by 9-point Gaussian quadrature onto $K = 0$ and those multipoles $K \geq 2$ for which $\delta_K \neq 0$. The resulting $V_{\mathtt{L}}^K(r)$ are used to to couple core states J_c, J_c' for which $\Delta(J_c, J_c', K)$ holds, according to a collective model. The value of L is given by the angular momentum between the particle and the core in the partial wave being fed by the interaction.

If all the **JTARG** values are zero, then the quadropole deformation length is used to construct a form factor for monopole excitation couplings.

NC interaction outside RINNER: UUC(L,R), UULS(L,R) replace UC and ULS.

Three-body interaction: V3B(RHO,...), U3B(RHO,...) for NN and NC partitions respectively.