

Comitato Nazionale Energia Nucleare

KISS - A FORTRAN Code for Quadrupole Direct Radiative Capture Cross Section Calculation

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KISS - A FORTRAN CODE FOR QUADRUPOLE DIRECT RADIATIVE CAPTURE CROSS SECTION CALCULATION

F. Fabbri, G. Longo and F. Saporetti

1. INTRODUCTION

The main features of the FORTRAN programme KISS are described in this report. The code was written in order to calculate the cross section for quadrupole direct radiative capture of nucleons by nuclei. The dipole direct and collective capture cross section can be calculated by using the DIRCO programme [1], while the SPEC programme [2] is written for the calculation of the spectra of high energy photons following the capture of fast nucleons.

Here the particle is assumed to interact with a spinless target nucleus through a spherical optical potential including spin-orbit interaction. The details of the physical model and the theoretical formalism are described in paper [3].

The output data are the cross sections and the matrix element values (real part, imaginary and square) for individual transitions at a given nucleon energy; by option, the integrals and the wave functions can be printed versus the nuclear radius. The wave functions can also be plotted as functions of the nuclear radius. The plots of total and partial cross sections and of the radial integral squares versus the incident nucleon energy can be given, too.

The programme is particularly useful when the incident particle is a proton of relatively high energy (20-50 MeV). The code was used to investigate the ¹⁴²Ce(p, γ) reaction in the (10+50) MeV energy range [3].

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This report contains the mathematical formulation, a detailed description of the programme written in FORTRAN IV language for an IBM 360/75 computer, the input list and the output data of a calculation for a test run.

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2. MATHEMATICAL FORMALISM

2.1. Cross section

The direct mechanism describes the capture of a nucleon by a target nucleus as a transition from a continuum state to a single-particle bound state, with a simultaneous emission of a photon. According to the formalism of the mentioned paper [3], the cross section for quadrupole direct radiative capture of nucleons by nuclei can be written as

$$tot(E2) = \frac{2\pi}{75} \frac{\bar{e}^2 M}{\hbar^2 k'} \sum_{ljj'} k_{\gamma}^5 |Q_{ljj'}|^2 Z^2(l'j'lj; \frac{1}{2}2) , \qquad (1)$$

where $M = \frac{M_t M_i}{M_t + M_i}$ is the reduced mass and M_t and M_i are the mass of the target nucleus and incident nucleon, respectively; e is the effective nucleon charge given by

$$\bar{e} = \begin{cases} e(1 - \frac{2}{A} + \frac{Z}{A^2}) & (\text{for a proton}) \\ e \frac{Z}{A^2} & (\text{for a neutron}) , \end{cases}$$
(2)

with Z, N and A the proton, neutron and mass numbers of the target; l', j' and l, j are the quantum numbers of the initial and final states of the nucleon; k' and k are the incident and photon wave numbers; $Q_{l'j'}$ is the quadrupole radial integral

$$Q_{l'j'} = \int u_{lj}(r) \psi_{l'j'}(r) r^2 dr$$
, (3)

where $u_{lj}(r)$ and $\psi_{l'j'}(r)$ are the radial parts of the bound state and incident nucleon normalized wave functions, as defined in ref. [1]; the function Z is a combination of Racah and Clebsh-Gordan coefficients given by

$$Z(\ell'j'\ell_j;\frac{1}{2}) = -i^{\ell-\ell'} \left[(2\ell'+1)(2j'+1)(2\ell+1)(2j+1) \right]^{\frac{1}{2}} \cdot W(\ell'j'\ell_j;\frac{1}{2})(\ell'\ell_0) | 20 \right]$$
(4)

The E2 selection rules permit only those transitions with $\Delta j = 0$, ± 1 , ± 2 (no $0 \rightarrow 0$, no $\frac{1}{2} \rightarrow \frac{1}{2}$, no $0 \rightarrow 1$, no $1 \rightarrow 0$) and no change of parity.

Using masses, energies and lengths in a.m.u., MeV and im respectively, the cross section (microbarns) for an individual single particle bound state (1,j) may be written in the final form ready for computer calculation

$$\sigma_{lj}(E2) = 882 \cdot 10^{-9} \left(\frac{\bar{e}}{e}\right)^2 k^{5} \left(\frac{\varepsilon_{lab}}{M_i}\right)^2 \left[\frac{\varepsilon_{lj}}{\varepsilon_{lab}} \frac{M_i + M_t}{M_t} + 1\right]^5 \sum_{j'} |Q_{j'}|^2 Z_{j'}^2, \quad (5)$$

where k' = 0.218739 $\sqrt{\epsilon_{ij}}$ M, with ϵ_{kj} the nucleon energy in the final bound state, ϵ_{lab} and $\epsilon_{j'}$ the incident energy in the laboratory and centre of mass systems, respectively. The Z^2 values of interest for quadrupole transitions can be calculated using the relations listed in Table I.

The code calculates expression (5) for all the possible final bound states and gives the total cross section as a sum of the contributions over all these states.

2.2. Interaction potentials

A detailed description of the optical and bound state potentials available in this programme is given in chapter 2 of ref. [1], which we assume is known to the reader. Here, only a small change has been introduced in the optical potential. This is assumed to have the more general form

U(r) = -

This addition is useful when the incident particle is a fast proton. Indeed, very good fits [4] are found in the elastic scattering of (20:60) MeV incident protons using the reformulated Greenlees optical model [5], which considers the real central part of the optical potential formed by two components.

Here, we report the parameters of a potential for 30.3 MeV incident protons, as a further example of the "assigned potential" case of ref. [1], namely the SINHA, EDWARDS and SATCHLER-potential [4,6].

V vol roR aR

V surf 8_R roR

$$\begin{bmatrix} V_{vol} \ f_{R}(r) + V_{surf} \ g_{R}(r) \end{bmatrix} - i \begin{bmatrix} W_{vol} \ f_{I}(r) + W_{surf} \ g_{I}(r) \end{bmatrix} - V_{s}h_{s}(r) \ \overline{\sigma} \ . \ \overline{\ell} + \begin{cases} V_{c}(r) & (for protons) \\ 0 & (for neutrons) \end{cases}, \qquad (6)$$

where the derivative Woods-Saxon term in the real part of the potential may be regarded as a symmetry potential arising from the excess neutrons in the target nucleus. The function $g_R(r)$ has the same form as $g_I(r)$ with the nuclear radius $R_R = \frac{r_o}{r_o} A^{1/3}$

=	^v ° ^{+v} 1 ^e j'	MeV ^(*)	∫ ^W vol	= 2.38	MeV	∫ ^V s	=	5.85	MeV
=	1.128	fm	^r _{oI}	= 1.287	fm ,	r	=	1.152	fm
=	0.85	fm	a _I	= 0.751	fm	a s	£	0.514	fm
3	8.037	MeV	{ W surf	= 7.85	MeV				
	derivativ	ve 🛛	g _I	= deriva	rtive				
E	0.865	fm	$\frac{1}{r_{oI}}$	= 1.287	fm	r	=	1.2	fm
8	0.80	fm	Ρ ^I	= 0.751	fm				

* $(V_0 = 52.52 ; V_1 = 0)$.

3. PROGRAMME

W. A.

3.1. General description

The programme consists of a total of 19 subroutines:

1	Main routine	KISS
2	Subroutine	STLEG
3	11	POTSL
4	**	ROM
5	**	UINT
6	**	UEXT
7	**	BETA
8	**	FUX
9	**	DUX
10	**	FUNZ
11	**	WITTAK
12	**	PSQUA
13	**	POTSM
14	**	DOX
15	**	FOX
16	11	FGET
17	**	PLOTSQ
18	**	PINSQ
19	Function	DER

The subroutine DUMP is also used.

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The programme assumes the presence of the following FORTRAN elementary function subroutines:

ALOG	(natural logarithm)	ATAN	(arc-tangent)
EXP	(exponential)	SQRT	(square-root)
SIN	(sine)	GAMMA	(gamma function)
COS	(cosine)		

and the standard routines for input/output.

The plots are made by CALCOMP; if this feature is not available, the programme could also be used without the PINSQ and PLOTSQ subroutines replacing them with two dummy subroutines.

The data are brought in from tape 5 and the whole output is on tape 6; all input data are read in by the main routine.

One tape is used as a temporary; the parameter N3, near the beginning of this programme, should be set to specify the temporary tape.

3.2. Detailed description of the specific routines

Main routine KISS controls the whole flow of the programme.

- 1) First the following input data are read in successively:
 - a) a card containing alphanumeric information;
 - b) control card: MPH, KPOT, KVV, KENER, KVS, KPLOT, KINT, KSTAMP;
 - c) if KPLOT = 0 are required: NSPER, AUTORE and XSPER(I), YSPER(I), DSPER(I), I=1, NSPER;
 - d) FMTB, FMB, FMZ, FNU;
 - e) RO, A, ROR, AR, RI, AI, RIS, BI, RSO, ASO, RC;
 - f) V_0 , V_1 , V_S , W, WS, VSO, ENER(I), I=1, KENER;
 - g) ROH, ABH, RCH, VSL;
 - h) NH(I), LH(I), JH(I), EPH(I), VL(I), I=1, MPH.
- 2) Sets up a loop for varying IENER from 1 to KENER.
- 3) Computes the values of the potential depths V, W, WS, if they are required by input; computes FKAY and ETA, then prints out input data.

4) If lENER is equal to 1, calls STLEG, otherwise proceeds.

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))	Ca	1	1	8

KENER.

6) Increases IENER by 1 and returns to step 3 until IENER is equal to 7) If KPLOT is not equal to 0, calls PLOTSQ, otherwise proceeds. 8) If KINT is not equal to 0, cills PINSQ, otherwise proceeds. 9) Then returns to step 1.

STLEG

computes the l- and ϵ -independent part of the potentials for POTSL the bound-state wave function in each mesh point to be used.

computes the matching radius RM for the bound state. ROM

UINT integrates the internal wave function from 0 to RM; calls subroutines DUX, FUX, DER.

UEXT integrates the external wave function from RMAX to RM. Calls subroutines WITTAK, DUX, FUX, DER.

BETA

FUNZ

DUX

FUX

Ψ**i**+

where h is the integration step.

PSQUA

PSQUA.

calculates the bound-state wave function u_{li}(r) using the following subroutines: POTSL, FUNZ, ROM, UINT, UEXT, BETA. The function u_{li}(r) is stored on tape N3.

computes the normalization factor β .

computes the form FVC of optical potential in bound state.

computes differential equations.

are two subroutines FUX1 and FUX2 that perform the numerical integration of a differential equation of the form $\Psi = F\psi$, using the following expression

$$H = \frac{(2 + \frac{5}{6}h^2 F_i)\psi_i - (1 - \frac{1}{12}h^2 F_{i-1})\psi_{i-1}}{1 - \frac{1}{12}h^2 F_{i+1}}$$

WITTAK computes the Wittaker function and its derivative.

This subroutine controls the second part of the programme. 1) Computes the incident wave function $\psi_{\ell'i'}(r)$; 2) Computes the integrals Q_{lii};;

POTSM	 Computes the quadrupole direct cross section; Outputs all these data. Calls the subroutines POTSM, FGET, DOX, FOX, DER. computes the <i>l</i>-independent part of the potentials in each mesh point 	<pre>KVS = 0, if in = 1, if in DIRCO KINT = 0, if the</pre>	the bound state the bound state programme [1]. he plot of Q _{0;;} ,	V _S is in input. V _S is computed by formula (34) of the ² is not required.
	used for $\psi_{k'j}$, functions.	= 1, if t	ne plot of Q _{ljj} ,	² is required.
DOX	computes differential equations for $\psi_{\ell'j'}$.			
FOX	are two subroutines FOX1 and FOX2 that numerically integrate a	3.4. Basic data		
	system of differential equations.	KISS code Symbol	Mathematical Symbol	Description
FGET	computes the regular and irregular Coulomb functions and their	-,		
DED	derivatives.	A	a _R	Diffuseness parameter in optical po- tential (real, volume)
DEK	$v_{1}^{\prime} = \frac{1}{100} \left[v_{1} - v_{2} + 9 (v_{1} - v_{2}) + 45 (v_{1} - v_{2}) \right]$	ABH	a	Diffuseness parameter in bound state potential
PLOTS) plots the experimental and calculated cross sections.	AI	a _I	Diffuseness parameter in optical po- tential (imaginary, volume)
PINSQ	plots the integral squares $ Q_{ij} ^2$ at each energy.	AR	^b R	Width parameter in optical potential
		ASO	as	Diffuseness parameter in optical po-
3.3.	Description of input data	AUTORE		Name of authors of experimental val-
	The control data are:	IN IOAD		ues
MPH	= number of bound states (\leq 20).	BI	pI	Width parameter in optical potential (imaginary, surface)
КРОТ	= 0, if the incident particle is a neutron. = 1, if the incident particle is a proton.	DSPER	^{Δσ} ex	Error in experimental value of total cross section
		DR	Δr	Integration step
KVV	= -2 the real potential V is calculated by $V = V + V \epsilon_j$, and 0 1 j	ECM	۶ _i ,	Incident nucleon energy in C.M.S.
	= -1 the real potential V is calculated by $V = V_1 \varepsilon_1$, and	ELAB	εlab	Incident nucleon energy in laboratory system
	used with volume + surface absorption.	ELEM		Alphanumeric description
	= 0 Rosen et al. potential. = 1 Perev and Buck potential.	ENER(I) I=1 to KENER	^ɛ lab	Location for incident energy in in- put
	= 2 Becchetti and Greenlees potential.	EPH	ε _{li}	Single particle bound state energy
	= 3 Engelbrecht and Fiedeldev potential.	FMB	A	Mass number of target nucleus
	= 4 Sinha Edwards and Satchler potential.	FMIB	Mi	Mass of incident particle
KENER	= number of energies of the incident particles (≤ 60).	FMTB	M _t	Muss of target particle

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= 0,	if in the bound	state V _S	is in input.
= 1,	if in the bound	state V _S	is computed by formula (34) of the
	DIRCO programme	[1].	
= 0,	if the plot of	$ Q_{ii} ^2$	is not required.
= 1.	if the plot of	$ 0, ^2$	is required.

KISS code Symbol	Mathematical Symbol	Description	KISS code Symbol	Mathematical Symbol	Description
FMU	M	Reduced mass	W	W _{vol}	Depth of imaginary part of optical potential
FMZ	Z	Proton number of target nucleus	WS	W	Depth of imaginary part of anti-1
FNU	N	Neutron number of target nucleus		"surf	potential (derivative or gaussian)
FKAY	k'	Wave number of incident nucleon	XXX	X	Frehange force factor
NH,LH,JH	n l j	Bound state quantum numbers	XSPER	**	Experimental excitation operan
NPASSI		Numbe: of mesh points	YSPER	n	Experimental excitation energy
NSPER		Number of experimental values		~ехр	Experimental closs section
RC	r _{oc}	Coulomb radius parameter in optical potential	3.5. Input	rards	
RCH	r _c	Coulomb radius parameter in bound state potential	For	computations referring	to a single target nucleus, the follow
RI	r _{oI}	Nuclea: radius parameter in imaginary part of optical potential (volume)	ing cards are	e required:	
RO	r _{oR}	Nuclear radius parameter in real part of optical potential (volume)	1) FORMAT (2 2) FORMAT (2	l2A6) Alphanumeric data l013) MPH, KPOT, KVV, H	a KENER, KVS, KPLOT, KINT, KSTAMP
ROH	ro	Nuclear radius parameter in bound state potential	3) FORMAT () 4) FORMAT ()	I3,3A4) NSPER, AUTORE BE12.6) XSPER(I), YSPER	R(I), DSPER (I) , $I=1$, NSPER
RS	r _{oI}	Nuclear radius parameter in imaginary	5) FORMAT (5E12.6) FMTB, FMB, FMZ,	, FNU
		or gaussian)	6) FORMAT (1	12E6.6) RO, A, ROR, AR,	, RI, AI, RIS, BI, RSO, ASO, RC
RSO	ros	Spin orbit radius parameter in op- tical potential	7) FORMAT (6 8) FORMAT (6	5E12.6) VO, V1, VS, W, 5E12.6) ROH, ABH, RCH.	WS, VSO, (ENER(I), I=1, KENER) VSL
ROR	roR	Nuclear radius parameter in real part of optical potential (surface)	9) FORMAT (3	3F6.3, 2E12.6) NH, LH,	JH, EPH, VL (are MPH cards)
V	V	Depth of real part of central poten- tial	3.6. Output		
VO, V1	V_{0} and V_{1}	See expression (28) of DIRCO code [1]	m -		
VI	v ₁	Strength of symmetry term of optical potential	1) The alpha	numerical information	of card 1.
VL	V _R	Depth of bound state potential	2) 411 5		· · · · · · · · · · · · · · · · · · ·
VS	V surf	Depth of real part of central poten- tial (surface)	2) All input 3) For each	single particle lovely), 7.
VSO	v _s	Depth of spin orbit term in optical potential	o, ror each potential	and energy of γ -ray e	maune, binding energy, corresponding
VSL	V_{BS} or λ	Depth of spin orbit term in bound state potential or parameter λ (see expression (34) of DIRCO code [1])	quantum r parts and state: qu	umpers <i>L</i> ' and j' o l squares of the integr adrupole direct cross	ot initial state, real and imaginary cals Q _{ljj} , . For capture to each fina sections.

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4) If KSTAMP \neq 0 prints also: the bound state wave function $u_{lj}(r)$; the real and imaginary parts of the continuum wave functions $\operatorname{Rey}_{l'j'}(r)$, $\operatorname{Imy}_{l'j'}(r)$; the radial integrals $\operatorname{ReQ}_{ljj}(r)$, $\operatorname{ImQ}_{ljj'}(r)$, $|Q_{ljj'}(r)|^2$.

KPOT = 1

 $\mathbf{KPLOT} = \mathbf{1}$

The parameters used are: FMZ = 58.FMB = 142.RO = 1.25A = 0.65RI = 1.25AR = 0.65RIS = 1.25BI = 0.7 RC = 1.25ASO = 0.65VS = 0. V1 = 0.WS = 7.5 VSO = 5.5ENER(I) = 20.; 24.; 28.; 32.; 36.; 40.; 44.; 48.; 52.RCH = 1.27**ABH = 0.67** LH(1) = 2.JH(1) = 2.5EPH(1) = 5.488VL(1) = 56.JH(2) = 5.5LH(2) = 5.EPH(2) = 3.872VL(2) = 56.NH(3) = 2. LH(3) = 0. JH(3) = 0.5 EPH(3) = 3.075 VL(3) = 56. NH(4) = 1. LH(4) = 2. JH(4) = 1.5 EPH(4) = 2.950 VL(4) = 56.

As an example, the quadrupole direct radiative capture cross section of protons by the target nucleus ¹⁴²Ce is calculated at 32 MeV proton

 $\mathbf{K}\mathbf{V}\mathbf{V} = \mathbf{0}$

KINT = 1

KENER = 8

KSTAMP = 0

The list of input cards and the output are given in Appendices 1 and 2.

The following plots are also given:

- 1) The quadrupole direct cross section versus the incident energy in the (20:50) MeV energy range.
- 2) The partial cross section for capture leading to the $lh_{11/2}$ final bound state from all the initial states allowed by selection rules, as a function of energy in the (10+50) MeV range.
- 3) The square of radial integral Q_{ljj} , versus the incident proton energy in the (10-50) MeV energy range for the $j_{15/2} \neq h_{11/2}$ transition.

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5. TYPICAL RUNNING TIME

The time required to carry out the test case was 8" for each energy.

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TABLE I

Z² values for quadrupole transitions

j '	$\frac{4}{15} z^{2}(x'j''j; \frac{1}{2} 2)$
j + 2	$\frac{(j + \frac{5}{2})(j + \frac{3}{2})(j + \frac{1}{2})}{(j + 2)(j + 1)}$
j + 1	$\frac{(j + \frac{3}{2})(j + \frac{1}{2})}{(j + 2)(j + 1)j}$
j	$\frac{2}{3} \frac{(j + \frac{3}{2})(j + \frac{1}{2})(j - \frac{1}{2})}{(j + 1)j}$
j - 1	$\frac{(j + \frac{1}{2})(j - \frac{1}{2})}{(j + 1)j(j - 1)}$
j - 2	$\frac{(j + \frac{1}{2}) (j - \frac{1}{2}) (j - \frac{3}{2})}{j (j - 1)}$

APPENDIX 1

LIST OF INPUT CARDS

SAMPLE PROBLEM ** KISS ** INPUT DATA CE-142 (P,GAM) SIGMA(E) 4 1 0 8 0 1 0 . 0 0.
 141.9091
 142.
 58.
 84.

 1.25 0.65
 1.25 0.65
 1.25 0.65
 1.25 0.7
 1.25 0.65
 1.25

 0.
 0.
 7.5
 5.5

 29.
 32.
 36.
 40.
 0. 0. 20. 24. 48. 52. 44. 1.27 0.67 1.27 2.5 5.488 56. 1.27 33. 1. 2. 5.53.8720.53.0751.52.950 0. 5. 56. 2. 56. Q • 1. 2. 56. CE-142 SIG(1H 11/2) 1 1 0 10 0 1 0 0 0.
 141.9091
 142.
 58.
 84.

 1.25
 0.65
 1.25
 0.65
 1.25
 0.65
 1.25
 7.5 0. 0. 18. 22. 42. 46. 0. 0. 5.5

 10.
 14.
 18.

 34.
 38.
 42.

 1.27
 0.67
 1.27

 0.
 5.
 5.5
 3.872
 56.

 22. 26. 30. 46. 50. 33. CE-142 Q2(H 11/2) 1 1 0 10 0 0 1 141.9091 142. 58. 84. **1.25** 0.65 **1.25** 0.65 **1.25** 0.65 1.25 0.7 1.25 0.65 1.25 0. 7.5 0. 0. 0. 5.5 14. 38. 0.67 18. 22. 10. 26. 30. 10. 34. 42. 46. 50. 0.67 1.27 1.27 33. 0. 5. 5.5 3.872 56.

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APPENDIX 2

TEST RUN OUTPUT

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) Z= 58.0 \= 84.0 \T= 141.9091 \T= 1.0073 12.79 FCM= 31.77 A= 0.670 RD= 1.270 RC= 1.270	<pre>* R= 1.250 4= 0.650</pre>		24 VB= 56.00 0.594F 01 02= 0.595E 02 22= 14.2957 0.634F 01 02= 0.137E 03 22= 1.1429 0.637F 01 02= 0.548E 02 22= 6.8571 0.873F 01 02= 0.422E 02 22= 1.7143 0.873F 01 02= 0.495E 02 22= 6.0000		4 V(1= 54,00 -0.4000 10= 0.1135 03 22= 25.9461 -0.4000 10= 0.5545 03 72= 0.5874 -0.2335 02 12= 0.5545 03 72= 0.5874 -0.2345 01 12= 0.5545 03 72= 14.6853 -0.5445 01 12= 0.5405 02 72= 14.6853 -0.5315 01 12= 0.9055 01 22= 18.1819	04 - V3= 53.00 0.3235 01 - 22= 2.8125 02 - 72= - 6.03.00 0.1355 02 - 22= 7.1215 03 - 72= - 4.03.00		
SET + INCTORNT PARTICLE 1= 142.0 ELAB= 3 VO STATE PARAMETERS LAM= 33.	FIJUUM STATE PARAMETENS V= 43.314 W= 0.0 VSN= 5.	ICAL POTENTIAL ADSEN TYPE	5/2 ER= 5.48P0 FGAM= 37.262 4. Jl= 4.5 RQ= 0.494F 01 10= 4. Jl= 3.5 RQ= 0.944F 01 10= 2. Jl= 2.5 RQ= 0.244F 01 10= 7. Jl= 1.5 RQ= 0.244F 01 10= 7. Jl= 0.5 RQ= 0.244F 01 10= 0. Jl= 0.5 RQ=-0.570F 01 10=	544(2*, 2.5)= 0.091F 2	<pre>11.2 En= 1.8720</pre>	644[5.,5.5]=],[245] 1/2 [9= 4,0750 - 2442 440 2. J1= 2.5 -23=-0,472-01 [1= 1.5 33=-0,472-01 [1= 1.5 33=-0,472-01 [1=	10 JAR 0** J*2)= 0* 1342 JI	

APPENDIX 3

TEST RUN PLOTS

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