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NRCC NATIONAL RESOURCE FOR COMPUTATION IN CHEMISTRY

ALGORITHMS AND COMPUTER CODES FOR ATOMIC AND MOLECULAR QUANTUM SCATTERING THEORY

Volume II

Proceedings
of the workshop reconvened at Lawrence Berkeley Laboratory
October 26-27, 1979

First meeting at Argonne National Laboratory
June 25-27, 1979

NRCC Proceedings No. 5
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PROCEEDINGS

of the workshop

ALGORITHMS AND COMPUTER CODES FOR ATOMIC AND MOLECULAR QUANTUM SCATTERING THEORY

Volume II

Sponsored by the

NATIONAL RESOURCE FOR COMPUTATION IN CHEMISTRY

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NRCC Proceedings No. 5

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FOREWORD

The National Resource for Computation in Chemistry (NRCC) was established to make information on existing and developing computational methodologies available to all segments of the chemistry community, to make state-of-the-art computational facilities (hardware and software) accessible to the chemistry community, and to foster research and development of new computational methods for application to chemical problems.

Workshops form an integral part of the NRCC's program. A workshop in the titled area was judged timely by researchers in the field and led to a planning meeting held February 23-24, 1979 at the University of Utah in Salt Lake City. The workshop was organized in two parts. The first meeting was held June 25-27, 1979 at Argonne National Laboratory under the chairmanship of Professor John Light, University of Chicago, and Dr. Lowell Thomas of the NRCC. Volume I of the present workshop proceedings contains the papers presented at the first meeting.

The workshop reconvened October 26-27, 1979 at the NRCC to compare the performance of algorithms on selected test problems that were solved in the interim since the first meeting. We are indebted to Dr. Lowell Thomas for his considerable effort in developing the test problems and in organizing the data and in summarizing the findings of these tests.

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Preface to Volume II

The goals of this workshop have been to identify which of the existing computer codes for solving the coupled equations of quantum molecular scattering theory perform best on a range of physical problems, and to make tested versions of those codes available to the chemistry community. Since the completion of Volume I of this workshop proceedings, these goals have been fully met and even exceeded. Eleven different programs have been tested on twenty-four different test problems and in this volume we report the results and conclusions from those tests.

A second meeting was held at Berkeley, October 26-27, 1979 at which the test results were discussed and analysed. One of the chief results from that meeting was the development of a new hybrid program which is roughly twice as fast as any other program tested. Although these tests were far from exhaustive, we believe that they are the most extensive test of the methods which has been done to date and that the new hybrid program is the current state of the art. We hope that these tested programs, now available from the NRCC, together with Volume I and this volume will serve the scientific community as useful research tools.

The delay in the completion of this volume has been due to a number of causes. Sifting through the enormous amount of data generated by the tests proved to be a much more difficult and lengthy task than anticipated. Also, the very success of the workshop has been due to a great deal of dedicated hard work by all of the participants - work which had to be done in addition to normal research and administrative duties. As a consequence, many of the individual tasks necessary to the completion of this volume simply had to await the completion of higher priority commitments.

June 1980
John C. Light
Lowell D. Thomas

SECTION I

INTRODUCTION

Approximately one and a half years ago the NRCC began organizing a workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory" with Lowell Thomas (NRCC) and John Light (University of Chicago) as co-chairmen. The workshop has proceeded through the five phases:

I. February 1970: Salt Lake City. Preliminary planning meeting.

Attendees: Johnson, Lester, Light, Parker, Thomas.

II. June 25-27, 1979: Argonne National Laboratory. First meeting - presentation of methods, final choice of tests, introduction to remote computing at LBL.

Attendees: Alexander, Allison, Askar, Gordon, Harvey, Johnson, Krogh, Lester, Light, Malik, Parker, Rabitz, Redmon, Schmalz, Secrest, Shin, Thomas, Truhlar, Walker, Yung.

III. July-October, 1979: Participants set up their programs and run tests remotely at LBL; preparation of Vol. I of Proceedings.

IV. October 26-27, 1979: Lawrence Berkeley Laboratory. *Second meeting of workshop for those who participated in tests* - presentation and evaluation of results, recommendations to NRCC. Attendees: Alexander, Johnson, McLenithan, Lester, Light, Parker, Redmon, Schmalz, Thomas, Walker.

V. November 1979-February 1980: Final activities - preparation of individual reports, construction and testing of hybrid code, some additions to test results, preparation of this final report.

The purpose of the workshop was to evaluate the algorithms and computer codes currently in use for atomic and molecular quantum scattering theory and to make the best of them available to the chemistry community through the NRCC software library. The codes were to be evaluated, in a common environment (CDC 7600) on a variety of test problems, qualitatively for their ease of use, portability, and reliability; and quantitatively for efficiency and accuracy.

The Proceedings of the first two phases of this workshop, containing detailed descriptions of the various methods and the test problems are available from the NRCC as Lawrence Berkeley Laboratory report LBL-9501 (1979), hereafter referred to as Vol. I. The present volume reports the developments of Phases III-V of the workshop.

Because of the considerable efforts of the participants there is an enormous amount of information to report. In the four-month interval between meetings eight individuals (or

groups), working remotely, brought their codes up on the LBL computer and solved the test problems - a total of 24, considering all basis sets and energies - to produce selected transition probabilities to a specified accuracy.

Altogether 11 different programs were used to solve the test problems. All of these programs are now available through the NRCC software library. Thus, the original objectives of the workshop have been fully met. Owing to the enthusiasm and dedication of the participants, however, the overall results of the workshop have far exceeded the initial expectations and several very important, unforeseen benefits to both the participants and the user community have resulted.

The first meeting appears to have been the first time experts in atomic and molecular quantum scattering theory were brought together to discuss computational algorithms and their computer code implementation. A great deal of information was exchanged and a number of new ideas were presented with the result that many of the participants improved their codes significantly before tackling the test problems. These software changes are described in Section IV of this volume. The comparison of the results from different codes, as discussed in Section III, revealed that further significant improvements could be made by producing a hybrid code which incorporated two or more algorithms for use in different scattering regions. This has been accomplished and the resulting hybrid code (VIVAS), now available at the NRCC, is approximately twice as fast as any of the codes previously tested and in some cases,

300 times faster. Thus the workshop not only served to test existing codes, but led directly to the creation of a significantly superior code. In addition, the workshop has developed a minimal set of test problems with a large "dynamic range" for testing scattering codes, a detailed comparative test for different codes within a given problem (timing histograms), and a set of recommendations to the NRCC to aid in future development and testing of scattering codes and to increase the accessibility of superior codes to both novices and experts in the field.

In Section II we present a brief description of the test problems, computer environment, methods and codes tested. In Section III we discuss and summarize the test results. In Section IV the individual participants discuss their changes to algorithms and programs made since the first report, specific details of how they ran the test problems, any difficulties they encountered, advantages and disadvantages of their methods and speculations on how their programs might be improved. In Section V we present a set of recommendations to the NRCC and conclude with a summary of the workshop in Section VI.

SECTION II

SUMMARY OF WORKSHOP CODES, METHODS AND TEST PROBLEMS

Although the test problems and most methods were described in some detail in Vol. I, we present here a very brief recapitulation for the convenience of the reader.

METHODS AND CODES

All of the algorithms presented in Vol. I were not tested. However, eleven computer codes were tested against at least some of the test problems. All codes were written entirely in FORTRAN (no machine language), were compiled with the same compiler (CDC extended, version 4.6), and were run on the CDC 7600 at LBL.

The codes can be divided into four groups:

1) General integration codes based on algorithms not developed originally for close coupling problems. These are a predictor-corrector method, the DeVogelare method, and the Numerov method. All may be classed as approximate wavefunction methods (see D. Secrest, Vol. I, pp. 1-12, for a more detailed classification);

2) Approximate wavefunction methods developed for close coupling problems. These are the log derivative method, the Sams-Kouri integral equation method, and an integral equation method with constant reference potentials;

3) Approximate potential methods in which analytic approximations to the solutions are generated by some means over relatively large intervals. These are the Airy function method developed originally by Gordon, the variable-interval variable-step method, the perturbatively corrected R-matrix propagation method, and the L^2 R-matrix propagation method:

4) A hybrid combination of the log derivative and variable-interval, variable-step method.

These are each described very briefly below, with the acronyms given which will be used henceforth and with the name of the person who solved the test problems.

Approximate Wavefunction Codes

PC: (L. D. Thomas). Predictor-corrector methods are common although an improved code due to Shampine and Gordon was used for these tests. See the articles by Krogh, Vol. I, and Thomas in Section IV below, for more details and references.

DEVOG: (L. D. Thomas). The DeVogelare algorithm was tested in a form coded by Thomas. It is described by Lester, Vol. I, and Thomas, below in Section IV of this volume.

MNN: (L. D. Thomas). Although the Numerov method is not new, the code tested (Minnesota Numerov, MNN) was the version provided by Brandt, Truhlar, Onda, and Thirumalai, and is described by Truhlar, Harvey, Onda, and Brandt in Vol. I. Discussions of other improved variations of the Numerov algorithm are given in Vol. I by Allison and by Johnson, although codes based on these algorithms were not tested at this workshop.

LOGD: (B. R. Johnson). The log derivative method was developed, coded, and applied to the test problems by Johnson. He described the algorithm in Vol. I. A variation using a multichannel WKB procedure for the long-range region was used on one test and is described later by Johnson in Section IV. It is a hybrid computer code.

SAMS: (K. McLenithan and D. Secrest). The Sams-Kouri integral equation method was coded for this workshop by McLenithan and Secrest. They describe the method in Vol. I and give a detailed description of its use for the test problems below in Section IV.

INSCAT: (M. J. Redmon). This is a constant potential integral equations method. The differential equations are converted to Volterra integral equations (as with SAMS), but a constant potential approximation is made (over a step) leading to analytical approximations to the quadratures for each step. Since the approximate potential is not diagonalized, however, this method is "intermediate" between the approximate wavefunction and potential methods. It is described by Redmon in Vol. I and below in Section IV.

Approximate Potential Codes

In these methods a basis in which the reference potential is diagonal is used in each region, and transformations between the different basis sets are required. Since this information is usually energy independent, it is stored during the first energy calculation and re-used at following energies. Thus for

these methods both 1st energy (E1) and subsequent energy (E2) times are given.

GORDON: (M. H. Alexander). The original approximate potential method based on piecewise linear potentials developed and coded by Gordon was modified by Alexander as described in Vol. I and below in Section IV.

VIVS: (G. A. Parker). This new variable-interval variable-step method uses piecewise constant potentials and a fixed basis within each interval. Analytic perturbation corrections to the solutions are summed over the steps in an interval and the solutions are carried in R-matrix form. The algorithm was developed by Parker, Schmalz, and Light, coded by Parker and Schmalz, run by Parker, and is described in Vol. I and below in Section IV.

RMAT: (T. G. Schmalz). The perturbatively corrected R-matrix propagation method is an outgrowth of the R-matrix propagation method of Walker and Light in which the analytic R-matrices are perturbatively corrected in each sector, but propagated as in the original method. It is described by Light, Schmalz, and Lill in Vol. I, and further modifications are described by Schmalz below in Section IV.

L2RMAT: (R. B. Walker). This new L^2 modification of the R-matrix propagation method, developed by Walker and Schneider, uses an L^2 expansion of the wavefunction in the region of rapidly changing potential followed by the standard R-matrix propagation. It is described in Vol. I and below in Section IV. This is essentially a hybrid method.

Hybrid Methods

VIVAS: (G. A. Parker). This is a hybrid code consisting of LOGD over the rapidly varying portion of the potential followed by an improved version of VIVS. It was constructed by Parker following the Berkeley meeting, and is described below in Section IV.

For easy reference, the abbreviations for the different methods and the participants that tested each method are listed in Table 1. (Tables 1-11 begin on Page 22.)

TEST PROBLEMS

Table 2 provides a summary of the 24 test problems. Table 2 gives the number of channels, the S-matrix element for which two significant figures of accuracy were required, the correct magnitude squared of that S-matrix element and the values of r_{min} and r_{max} for the integration range used to calculate the S-matrix. The naming conventions for the tests follow.

Test 1. This is the problem of rotational and vibrational excitation of H_2 by He impact. The total angular momentum was fixed at J = 4 and four different basis sets were chosen to yield 2, 8, 18 and 28 channel problems. These four basis sets are designated as J4B1, J4B2, J4B3, and J4B4 respectively. All calculations were done at a relative collision energy of .0224 Hartree atomic units (27.21 eV.)

Test 2. This problem was chosen to test the codes on a long range potential. The problem is rotational excitataion of CO by Li^+ impact. Basis sets were chosen for two different collision energies, 0.0000779 and 0.00195 Hartrees. The total

angular momentum was chosen to keep the impact parameter low (b = 4 Bohr). These choices were J = 5 and J = 25 for the lower and higher energies, respectively. Four different basis sets were chosen for each J. These are designated J5B1, J5B2, J5B3, and J5B4 for the low-energy case and J25B1, J25B2, J25B3, and J25B4 for the high-energy case.

Test 3. This problem is identical to Test 2 in every respect except that the integration was stopped at exactly r = 7.0 Bohr and and the S-matrix computed by matching to spherical Bessel functions.

Test 4. This problem is rotational excitation of N_2 by electron impact. A local approximation to the exchange potential is used which is valid only for a collision energy of 1.1025 Hartree. Four different basis sets were chosen for total angular momentum J = 5. These are designated J5B1, J5B2, J5B3, and J5B4.

SECTION III

PRESENTATION AND DISCUSSION OF THE TEST RESULTS

PRELIMINARY COMMENTS

Before presenting detailed comparisons of the methods some preliminary comments are necessary. The test problems were chosen to be representative of research problems of current interest. It was not possible with these tests to cover all of the important physical situations which arise in atom-molecule collision studies. For example, there were no problems with long range Coulomb potentials, no reactive scattering problems, none with very high energy, none with multiple electronic surface crossings and none with very large numbers of channels. However, the numbers of channels did vary from 2 to 32, the integration ranges needed for convergence varied from 16 to 1000 Bohr, the collision energies varied from 0.0000779 to 1.1025 Hartrees and the magnitudes of the transition probabilities, for which two significant figures of accuracy was requested, varied over ten orders of magnitude. Hence, the tests, though far from exhaustive, were demanding.

Except for Test 4/J5B2, none of the participants had prior knowledge of the correct answers or of the numerical difficulties that might be encountered. Hence, each participant did things slightly differently in setting up the calculations. For example, a wide range of r_{min} amd r_{max}, the beginning

and ending of the integration range, were chosen. If everyone were to start over again, with hindsight we could make our calculations much more uniform, providing a more precise comparison of the individual algorithms and computer programs. However, as it is, another important comparison is possible. The test problems were approached and solved as new and unsolved research problems. The timings and accuracies and the individual comments in Section IV therefore provide a comparison of the methods in an actual research situation - the mode in which they will normally be used.

Also, it should be pointed out that Test 3 was designed to compare the methods on the inner integration range. During discussions at the second workshop meeting, however, we developed an histogramic approximation to dt/dr, the computer time necessary for the method to integrate a unit distance, as a function of r. This considerably lessens the need for Test 3.

ACCURACY

Considering all the basis sets, a total of 24 test problems were solved and a total of 5494 S-matrix elements were generated by each code. Obviously, not every one of them can be examined in detail. Therefore, we decided to look at one inelastic S-matrix element for each case, and to try to achieve two significant figures of accuracy in the transition probability, $|S_{ij}|^2$. Table 2 gives a list of the elements considered for each case. Two significant figures of accuracy were not always obtained, but the level of accuracy for all methods is close enough for a meaningful comparison.

Many of us in fact solved most of the test problems at varying degrees of accuracy and these results are interesting because they show how the computer time varies with the accuracy on a given problem and how the accuracy varies with the number of integration steps. Appendix A contains the numbers of steps, computer times and values of the selected S-matrix elements for all of the runs saved on tape of all tests by all participants. Complete S-matices for all of these runs are available on microfiche.

Appendix B contains a complete listing of all the S-matrix elements of all the tests. Only two significant figures of accuracy for the specified r_{min} and r_{max} in the matrix elements of Table 2 are claimed. However, most elements are very likely accurate to more than two figures. For Tests 1, 3, and 4 the elements in Appendix B are from the predictor-corrector program of L. D. Thomas, determined with a tolerance parameter much smaller (overkill in many instances) than that used for the results which are compared with the other methods. For Test 2, they are from the log derivative program of B. R. Johnson, and again, often with a smaller stepsize than that used for the timing comparisons.

COMPARISON OF THE METHODS

Before comparing times, it is necessary to consider the widely varying r_{min} and r_{max} used for the different programs. The actual values used in each case are given in Table 3. An extreme example is the comparison of the PC and MNN programs. Because $r_{max} = 150.0$ was used for PC and

r_{max} = 1000.0 for MNN, the large difference in times (122 vs 706 sec) is meaningless. Also, one must realize that due to the idiosyncracies of the computer's operating system, there are 2 - 5% differences in the CPU times of exactly the same computer job run at different times of the day. Nonetheless, for the most part, the comparison of computer times for the different methods is meaningful and these are shown in Table 4. The hybrid method, VIVAS, is discussed later and should for the moment be left out of the comparisons.

One interesting feature is that no single method performs best on all of the problems. It seems clear that the best method is different for different physical problems. A striking example of this finding is the comparison between the LOGD and SAMS programs. LOGD outperforms SAMS by a wide margin on all tests except test 4 where SAMS is a factor of 2 faster. One should note, however, that for Test 2 which required a very large integration range, the LOGD method was combined with Johnson's multichannel WKB method and the latter was used for the bulk of the integration range.

If one considers only the first energy calculations the LOGD program seems to be the best all-round performer. However, if calculations are to be done at many energies the VIVS program seems to be the one to recommend. Again, one must be cautioned to consider the physical problem before selecting a method. On Test 4 SAMS is faster than VIVS even at a second energy.

Also of interest is the number of potential evaluations (usually also the number of integration steps taken) used by each method. These are show in Table 5. The SAMS, PC, DEVOG, and MNN methods, which fit the wavefunction or its derivatives to a polynomial, take many more steps than the others. Since the potential evaluation was a small part of the over-all computation time (3 - 10%), this did not hurt them much. However, if a problem had a potential which was very expensive to evaluate, these methods would suffer relative to the others.

Finally, we compare in Table 6 the squared magnitudes of the selected S-matrix elements for all the methods and for all the tests. Comparisons with other methods and other levels of accuracy indicate, with a high degree of confidence, that all of the values for the LOGD program meet the requested accuracy when rounded to two significant figures. It is quickly apparent that not all methods achieved this accuracy on all tests. The accuracy is however, good enough to permit a valid over-all comparison.

It is also necessary to comment on some apparent discrepancies in Test 3. When one computes an S-matrix in the presence of closed channels, strictly speaking, the asymptotic values of the closed channels must be taken into account. However, for large r, closed channel wavefunctions die out exponentially and can be ignored. For Test 3 the S-matrix was computed at r = 7.0 where the closed channels are not negligible. Therefore different results are obtained when the closed channels are ignored. For Test 3 J25B4, J5B3, and J5B4, the answers of GORDON, VIVS,

RMAT, and L2RMAT which ignore closed channels, are different from those of LOGD, SAMS, PC and DEVOG which include closed channels.

The results contained in Tables 3-6 allow a reasonable overall comparison of the methods. Each is organized with the different methods across the top and the different tests in each row. The integration ranges, times (sec), numbers of potential evaluations, and values of the selected transition probabilities are given in Tables 3-6, respectively. As we have tried to emphasize, although the quantitative comparisons available from these tables are, in general, meaningful, the optimal choice for a given problem will depend on the accuracy desired, the difficulty of potential evaluation, the range of the potential, the energy range, the numbers of energies, etc. Thus, we feel it is very important that the individual comments in Section IV be taken into account in making the choice.

TIMING HISTOGRAMS

Discussions at the second workshop meeting led to a means of comparing the methods in a much more detailed way than had previously been developed. By dividing the total time by the total number of integration steps taken, we can determine the average computer time per step. Then, by dividing the entire integration range into smaller intervals and counting the number of steps taken in each interval, we can get an histogramic approximation to dt/dr, the computer time to integrate a unit of distance i.e.,

$$dt/dr = \frac{T_{tot}}{N_{tot}} \frac{N(r+\Delta) - N(r)}{\Delta}$$

where N(r) is the number of steps required to integrate from r_{min} to r. Note that the inverse of this, dr/dt, is the "velocity" with which the computer integrates over r.

After the second meeting, each participant either resolved the problems or reexamined his output for the basis B3 of Tests 1,2, and 4 and compiled the histogram information. For each method, the midpoints of the histogram bars were connected with straight lines. These straight lines were then used to interpolate and find dt/dr for a common set of grid points for all methods. This procedure also enables an integrated total time to be determined for all methods with common values of r_{min} and r_{max}. The comparison of dt/dr among all the methods for Tests 1,2, and 4 is shown in Tables 7-10 and Figs. 1-4.

With fourteen columns to compare, it is not possible to scrutinize Tables 7-10 at a glance. Figures 1-4 give a complete graphical representation of the same data, but because of the large number of lines, these figures also require some effort to study. For an easier, though incomplete, comparison, Figs. 5-8 show the same data for the LOGD and VIVS methods along with the best other first-energy method for each test.

Figures 1-4 are log-log plots and are broken into two r-ranges with different scales for each range. The computer-generated, spline curves are sometimes abnormal at discontinuities in the data, but these abnormalities are few and not misleading and in general the smooth curves are much easier to follow than

straight line segments. Discontinuities occur in the SAMS and LOGD data because step sizes are not continuously and automatically chosen. They also occur in the PC data at points where stabilizing transformations were made.

Figure 1 shows the comparison for Test 1/J4B3. Note dt/dr is on a log scale, thus the times are dominated by the ranges of r for which dt/dr (sec/Bohr) looks largest. It should be noted that because high absolute accuracy was required on this test, SAMS, a lower order method, is at a great disadvantage compared with LOGD. It is also interesting to note that the potential following methods (GORDON, RMAT, INSCAT, L2RMAT, and VIVS) all follow a similar general shape, although with as much as an eight-fold spread in dt/dr. LOGD is clearly the best program in the inner r-range and VIVS, at the second energy is clearly, the best in the outer r-range.

Figure 2 shows the comparison for Test 2/J25B3. This is a very long range problem and the total times are dominated by dt/dr at large values of r. GORDON, at the second energy, performs best for small r and VIVS, at the second energy, performs best for large r. The approximate wavefunction, methods--PC, DEVOG, MNN, and SAMS--are impractical for this type of problem. Note that the LOGD program switches to a multichannel WKB method at r = 20. Although this method was not discussed in Vol. I, it is clearly competitive with the approximate potential methods.

Figure 3 shows the comparison for Test 2/J5B3. This is the same physical problem as that in Fig. 2, but with a lower collision energy. The asymptotic wavelength in the first channel is 5 Bohr compared to 1 Bohr for Test 2/J25B3. Hence, the approximate wavefunction methods do comparatively better on this test. The LOGD program is best at small r and the WKB method of the LOGD program is best at very large r. VIVS at the second energy is best at intermediate r.

Figure 4 shows the comparison for Test 4/J5B3. Although the collision energy is much higher for this problem than for the others, the asymptotic wavelength is still quite long – 4.2 Bohr – because of the small mass of the electron. Consequently, the approximate wavefunction methods do much better than one might at first glance expect. Also, in contrast to the atom-molecule problems, the potential energy function is finite at the origin. Therefore, in the non-classical region, $r \lesssim 7$ Bohr, the interaction is dominated by the centrifugal terms. The SAMS program excels on this problem because the centrifugal terms are included exactly in the Green function. LOGD and SAMS perform equally well for small r and are best in that region. VIVS at the second energy is best for large r and SAMS is best at intermediate r.

Overall, one is struck by the widely varying performances of individual programs on the different physical problems. For example, INSCAT is the best long range (and overall) performer at first energies on Test 1 and a factor of 6 faster than SAMS. On Test 4, nearly the opposite is true. It is also quite clear

that the best program would be a hybrid which followed the lowest dt/dr curve. Although no single method is best for all tests in any r-range, the LOGD program is nearly always best for small r and VIVS is nearly always best for large r. LOGD and VIVS, therefore, seem the best choice of partners for a hybrid program. This is not the ideal hybrid for all problems, but such a hybrid is always better than any individual method. This is indicated in Table 11.

Table 11 summarizes the integrated total times from Tables 7 – 10, with the methods arranged in ascending order on the times. The entry labled HYBRID is not from an actual program. It was hand calculated by integrating dt/dr from r_{min} to r_0 for LOGD and from r_0 to r_{max} for VIVS. It can be seen that the second energy HYBRID time is always smallest. For the short range problems the HYBRID result is a factor of 1.5-2.0 times faster than either of the two methods individually. For the long range problems of Test 2 the improvement is minimal because the total time is dominated by the long-range region.

Following the second workshop meeting, a hybrid program, VIVAS, was developed by G. Parker. This program includes significant improvements to the original VIVS program as well as the log derivative method. It can be seen in Table 4 that the new VIVAS program is significantly better than any of the individual programs and as much as a factor of 300 faster in some cases (compare VIVAS and MNN for Test 2/J25B3.)

One final comment on Table 11 should be made. For any of the individual programs it is fair to say that improvements in speed by factors of 2 or 3 can often be made and probably could be made by fine tuning the input parameters on each problem. This means that the ordering of the methods in Table 11 should not be taken too seriously. However, factors of 20-30 are seen between the best and worst for each problem and this is significant. These differences could probably not be eliminated by fine tuning the calculations.

SPECULATIONS ON FURTHER DEVELOPMENT

In quantum scattering theory there are computational aspects of close coupling calculations which have not really been addressed here and which are important to the speed, accuracy, and ease of the calculations. Among these are the choice of basis sets (fixed or quasi-adiabatic), evaluation of potential matrices, variation of the dimensionality of the equations by dropping or picking up channels as needed, use of totally different algorithms (e.g., finite element methods), etc. By and large, these problems need significant analysis and algorithms development before overall scattering codes can be optimized. These factors were excluded from the tests run by this workshop so that we could focus on what has been the most time-consuming portion of scattering calculations - the numerical integration of coupled equations. We do not, however, want to leave the impression that the entire field is now mature.

TABLE 1. Definitions of the abbreviations used for the different programs.

Name	Method	Participant Using the Method	Vol.I[a]	Vol.II[a]
PC	Variable-order, variable-step, predictor-corrector	L. D. Thomas	312	41
DEVOG	DeVogelaere's method	L. D. Thomas	105	41
MNN	Numerov's method	L. D. Thomas	86,111	41
LOGD	Log derivative method	B. R. Johnson	86	47
SAMS	Sams-Kouri method	K. McLenithan and D. Secrest	199	53
INSCAT	Integral equations with reference potentials	M. J. Redmon	290	67
GORDON	Gordon's method	M. H. Alexander	13,75	71
VIVS	Variable-interval, variable-step method	G. A. Parker	172	81
RMAT	R-matrix propagation	T. G. Schmalz	116	93
L2RMAT	L^2 approach to R-matrix propagation	R. B. Walker	376	97
VIVAS	Combination of LOGD and an improved version of VIVS	G. A. Parker	____	107

[a]Page numbers where methods are described.

TABLE 2. List of the transitions for which two significant figures of accuracy were requested.[a]

	i	f	n	j	ℓ	n'	j'	ℓ'	No. chan.	No. open chan.	$\lvert S_{if} \rvert^2$	r_{min}	r_{max}
TEST 1													
J4B1	1	2	0	0	4	1	0	4	2	2	.9167E-10	2.5	45.0
J4B2	1	5	0	0	4	1	0	4	8	8	.1681E-8	2.5	45.0
J4B3	1	15	0	0	4	1	0	4	18	18	.1184E-8	2.5	45.0
J4B4	1	20	0	0	4	1	0	4	28	23	.1112E-8	2.5	45.0
TEST 2													
J25B1	1	3		0	25		1	26	3	3	.3956	3.0	800.0
J25B2	1	4		0	25		2	23	10	10	.5523E-2	3.0	800.0
J25B3	1	4		0	25		2	23	22	22	.1715E-1	3.0	800.0
J25B4	1	4		0	25		2	23	32	31	.3446E-1	3.0	800.0
TEST 2													
J5B1	1	3		0	5		1	6	3	3	.2308	3.0	1500.0
J5B2	1	4		0	5		2	3	6	6	.1415E-1	3.0	1500.0
J5B3	1	4		0	5		2	3	15	6	.7770E-2	3.0	1500.0
J5B4	1	4		0	5		2	3	27	6	.1608E-1	3.0	1500.0
TEST 3													
J25B1	1	3		0	25		1	26	3	3	.4727	3.0	7.0
J25B2	1	4		0	25		2	23	10	10	.1710	3.0	7.0
J25B3	1	4		0	25		2	23	22	22	.6569E-1	3.0	7.0
J25B4	1	4		0	25		2	23	32	31	.6266E-2	3.0	7.0
TEST 3													
J5B1	1	3		0	5		1	6	3	3	.4185E-1	3.0	7.0
J5B2	1	4		0	5		2	3	6	6	.2056	3.0	7.0
J5B3	1	4		0	5		2	3	15	6	.1039E-2	3.0	7.0
J5B4	1	4		0	5		2	3	27	6	.6097E-2	3.0	7.0
TEST 4													
J5B1	1	2		0	5		2	3	4	4	.4330E-2	.01	120.0
J5B2	1	2		0	5		2	3	15	15	.2912E-2	.01	120.0
J5B3	1	2		0	5		2	3	21	21	.2873E-2	.01	120.0
J5B4	1	2		0	5		2	3	27	27	.2882E-2	.01	120.0

[a] i is the initial channel number and f is the final channel number. n, and j, and ℓ are the initial quantum numbers and n', j' and ℓ' are the final quantum numbers. These are followed by the number of total and open channels and the correct transition probability. The last two columns give the integration range used to calculate the transition probability.

TABLE 3. Starting and ending values of r (Bohr) used by each method.

	PC	DEVOG	MNN	LOGD	SAMS	INSCAT	GORDON	VIVS	RMAT	L2RMAT	VIVAS
TEST1	2.50	2.50	2.50	1.50	2.25	2.25	2.10	2.30	1.70	1.70	2.30
J4	45.0	45.0	45.0	30.0	40.0	16.5	19.0	40.0	45.0	35.0	40.0
TEST2	3.00	3.00	3.00	3.00	3.50	3.00	3.04	3.30	3.00	3.30	3.30
J25	150.	1000	1000	800.	900.	500.	1000	.500E+04	.200E+04	700.	.500E+04
TEST2	3.00	3.00	3.00	3.00	3.50	3.00	2.80	3.30	3.00	3.30	----
J5	150.	1000	1000	.150E+04	1000	500.	1000	700.	.200E+04	700.	----
TEST3	3.00	3.00	----	3.00	3.50	----	3.00	3.30	3.00	3.30	----
J25	7.00	7.00	----	7.00	7.00	----	7.00	7.00	7.00	7.00	----
TEST3	3.00	3.00	----	3.00	3.50	----	2.78	3.30	3.00	3.30	----
J5	7.00	7.00	----	7.00	7.00	----	7.00	7.00	7.00	7.00	----
TEST4	.100E-01	.100E-01	.100E-05	.100E-03	.500E-01	.200E-01	.300E-01	.150	.100	.500E-05	.150
J5	120.	120.	120.	50.0	50.0	75.0	70.0	160.	250.	50.0	160.

TABLE 4. CPU seconds used for each test by each of the methods.[a]

TIME	PC	CEVOG	MNN	LOGD	SAMS	INSCAT	GORDON E1	VIVS E1	RMAT E1	LRMAT E1	VIVAS E1	GORDON E2	VIVS E2	RMAT E2	LRMAT E2	VIVAS E2
TEST1																
J4B1	1.34	.80	.39	.10	.39	.18	1.38	.50	.73	.53	.08	.47	.09	.29	.13	.03
J4B2	15.31	7.14	2.99	.89	3.17	.84	7.13	1.29	4.04	6.96	.33	1.53	.30	1.61	1.08	.16
J4B3	75.64	45.35	18.92	5.75	20.21	3.73	43.40	9.45	28.21	22.52	1.80	8.54	3.29	10.79	3.69	1.03
J4B4	256.45	151.74	67.86	18.79	56.64	11.71	104.18	31.67	71.64	---	8.96	24.06	7.87	26.59	---	4.56
TEST2																
J25B1	2.83	18.11	17.87	.54	2.63	---	---	.59	.87	.67	.30	---	.09	.29	.18	.08
J25B2	22.21	82.17	101.96	2.61	12.13	5.74	27.81	2.30	4.57	9.67	1.27	5.08	.53	1.70	2.37	.47
J25B3	121.63	541.30	705.55	18.08	77.04	31.62	43.16	14.82	36.51	63.33	7.34	7.49	3.88	13.95	21.85	2.28
J25B4	603.10	---	---	47.29	---	---	278.73	---	108.38	---	34.75	46.83	---	37.99	---	11.47
TEST2																
J5B1	.98	3.89	2.56	.47	1.[illegible]	---	5.07	.73	.83	1.51	---	1.31	.10	.28	.58	---
J5B2	3.34	7.37	5.49	1.03	[illegible].09	1.94	11.21	1.51	1.85	4.51	---	2.39	.29	.66	1.59	---
J5B3	31.95	45.09	74.45	6.96	54.17	---	64.05	6.02	13.17	41.42	---	13.47	1.55	4.86	14.14	---
J5B4	132.27	203.49	---	29.87	214.36	---	298.65	27.75	59.47	---	---	65.83	7.32	22.13	---	---
TEST3																
J25B1	.28	.19	---	.15	1.86	---	.89	.30	.22	.32	---	.24	.04	.08	.02	---
J25B2	3.11	.92	---	.68	8.74	---	5.01	1.37	1.24	4.70	---	1.04	.32	.46	.37	---
J25B3	19.48	6.08	---	4.31	54.82	---	14.24	7.33	9.27	23.55	---	2.90	1.97	3.50	5.88	---
J25B4	79.40	21.20	---	11.70	147.73	---	50.08	19.85	34.62	---	---	11.32	5.70	12.14	---	---
TEST3																
J5B1	.29	.19	---	.15	1.30	---	1.11	.32	.20	.40	---	.29	.04	.07	.12	---
J5B2	.77	.36	---	.28	2.48	---	2.67	.55	.35	1.41	---	.59	.11	.20	.30	---
J5B3	8.79	2.09	---	1.62	24.81	---	11.67	3.13	4.46	14.04	---	2.32	.79	1.63	3.15	---
J5B4	37.53	9.56	---	7.21	105.33	---	26.60	12.93	18.34	---	---	5.66	3.37	6.83	---	---
TEST4																
J5B1	.79	.44	.38	.25	.07	.36	1.67	.34	.29	.82	.16	.45	.08	.11	.19	.05
J5B2	14.48	6.77	6.85	2.16	.92	4.42	11.50	3.96	3.95	6.60	1.49	7.29	1.00	1.55	1.23	.63
J5B3	26.01	16.50	15.34	5.35	2.16	10.74	24.85	9.20	9.98	11.49	3.70	4.83	2.24	3.82	2.29	1.50
J5B4	51.51	33.27	30.46	10.58	4.26	22.66	58.36	19.84	23.46	---	6.90	11.06	4.73	8.86	---	2.73

[a]E1 designates a first-energy calculation and E2 a second-energy calculation.

TABLE 5. Number of potential evaluations used.

STEPS	PC	DEVOG	MNN	LOGD	SAMS	INSCAT	GORDON	VIVS	RMAT	L2RMAT	VIVAS
TEST1											
J4B1	2699	6791	1343	879	3051	318	493	1746	217	450	217
J4B2	2771	6791	1347	879	3051	248	519	950	241	466	217
J4B3	2996	6791	1347	879	3051	198	680	1000	277	217	217
J4B4	3181	6791	1349	879	3051	197	570	1425	221	---	301
TEST2											
J25B1	3329	50171	31351	1347	7101	---	---	1025	185	359	339
J25B2	3497	50171	31370	1143	7101	999	1369	1125	209	593	367
J25B3	3388	50171	31373	1143	7101	1008	424	1275	216	754	381
J25B4	5881	---	---	1143	---	---	1102	---	217	---	661
TEST2											
J5B1	1168	10595	4353	1171	2901	---	1207	1300	175	995	---
J5B2	1489	10595	4364	1171	2901	850	1221	1550	189	1064	---
J5B3	2298	10595	8171	1753	11576	---	1395	1300	206	1338	---
J5B4	2406	---	---	1753	11576	---	1767	1475	202	---	---
TEST3											
J25B1	355	497	---	401	5001	---	198	525	45	82	---
J25B2	564	497	---	401	5001	---	230	650	50	102	---
J25B3	595	497	---	401	5001	---	139	625	52	204	---
J25B4	835	497	---	401	5001	---	186	650	---	---	---
TEST3											
J5B1	357	477	---	401	3501	---	273	550	41	215	---
J5B2	382	477	---	401	3501	---	292	550	45	203	---
J5B3	641	477	---	401	5001	---	253	675	68	313	---
J5B4	717	477	---	401	5001	---	158	675	---	---	---
TEST4											
J5B1	646	1591	557	1003	190	328	299	600	44	280	185
J5B2	1022	1591	721	527	190	347	255	825	55	139	199
J5B3	857	1591	672	527	190	382	266	825	59	102	213
J5B4	933	1591	703	527	190	415	356	925	76	---	213

TABLE 6. Values of the selected transition probabilities, $|S_{if}|^{2a}$

	PC	DEVOG	HNN	LOGD	SAMS	INSCAT	GORDON	VIVS	RMAT	L2RMAT	VIVAS
TEST1											
J4B1	.9167E-10	.9203E-10	.9640E-10	.9144E-10	.9201E-10	.9094E-10	.9443E-10	.9393E-10	.9041E-10	.9071E-10	.1016E-09
J4B2	.1601E-08	.1681E-08	.1683E-08	.1681E-08	.1679E-08	.1699E-08	.1695E-08	.1607E-08	.1682E-08	.1683E-08	.1676E-08
J4B3	.1184E-08	.1183E-08	.1181E-08	.1185E-08	.1181E-08	.1149E-08	.1278E-08	.1213E-08	.1193E-08	.1170E-08	.1164E-08
J4B4	.1112E-08	.1111E-08	.1112E-08	.1112E-08	.1110E-08	.3264E-06	.1177E-08	.1120E-08	.1158E-08	----	.1102E-08
TEST2											
J25B1	.4073	.3948	.4026	.3954	.4003	----	----	.3953	.3959	.3959	.3964E-02
J25B2	.5899E-02	.5991E-02	.4931E-02	.5571E-02	.4372E-02	.5645E-02	.4960E-02	.5583E-02	.5541E-02	.5437E-02	.5377E-01
J25B3	.2036E-01	.1722E-01	.1666E-01	.1715E-01	.1752E-01	.2154E-01	.1702E-01	.1732E-01	.1709E-01	.1718E-01	.1710E-01
J25B4	.3755E-01	----	----	.3446E-01	----	----	.3485E-01	----	.3450E-01	----	.3446E-01
TEST2											
J5B1	.2253	.2285	.2294	.2308	.2269	----	.2279	.2291	.2287	.2301	----
J5B2	.1768E-01	.1394E-01	.1397E-01	.1385E-01	.1412E-01	.1755E-01	.1439E-01	.1423E-01	.1513E-01	.1410E-01	----
J5B3	.1025E-01	.7885E-02	.7375E-02	.7720E-02	.7574E-02	----	.7349E-02	.4139E-01	.7844E-02	.7975E-02	----
J5B4	.1460E-01	.1593E-01	----	.1608E-01	.1618E-01	----	.1492E-01	.6035E-01	.1564E-01	----	----
TEST3											
J25B1	.4761	.4728	----	.4727	.4735	----	.4677	.4725	.4717	.4726	----
J25B2	.1708	.1700	----	.1710	.1715	----	.1707	.1711	.1708	.1707	----
J25B3	.6562E-01	.6594E-01	----	.6568E-01	.6572E-01	----	.6350E-01	.6565E-01	.6586E-05	.6571E-01	----
J25B4	.6269E-02	.5973E-02	----	.6277E-02	.6434E-02	----	.7148E-02	.6871E-02	----	----	----
TEST3											
J5B1	.4205E-01	.4141E-01	----	.4186E-01	.4237E-01	----	.4378E-01	.4179E-01	.4191E-01	.4164E-01	----
J5B2	.2036	.2066	----	.2056	.2062	----	.2086	.2052	.2043	.2062	----
J5B3	.1039E-02	.9381E-03	----	.1041E-02	.1099E-02	----	.8706E-03	.8596E-03	.8556E-03	.8604E-01	----
J5B4	.6092E-02	.6124E-02	----	.6097E-02	.6344E-02	----	.3014E-01	.2903E-01	----	----	----
TEST4											
J5B1	.4326E-02	.4334E-02	.4338E-02	.4329E-02	.4387E-02	.4305E-02	.4403E-02	.4319E-02	.4325E-02	.4303E-02	.4304E-02
J5B2	.2913E-02	.2914E-02	.2913E-02	.2907E-02	.2914E-02	.2928E-02	.2900E-02	.2904E-01	.2911E-02	.2892E-02	.2905E-02
J5B3	.2864E-02	.2874E-02	.2874E-02	.2868E-02	.2876E-02	.2887E-02	.2860E-02	.2867E-02	.2885E-02	.2865E-02	.2861E-02
J5B4	.2883E-02	.2883E-02	.2884E-02	.2877E-02	.2870E-02	.2872E-02	.2871E-02	.2886E-02	.2890E-02	----	.2873E-02

[a]For each test the values of i and f are defined in Table 1.

TABLE 7. Test 1/J4B3. dt/dr (sec/Bohr), computer time for integrating a unit distance vs r.[a]

r	PC	DEVOG	MNN	LOGD	SAMS	INSCAT	GORDON E1	VIVS E1	RMAT E1	L2RMAT E1	GORDON E2	VIVS E2	RMAT E2	L2RMAT E2
2.8	4.241	1.020	.810	.202	2.208	1.500	10.396	2.130	5.019	7.607	2.043	.542	1.920	.520
2.9	3.540	.912	.719	.202	2.211	1.196	12.184	2.354	4.988	6.966	2.394	.600	1.908	.580
3.0	2.839	.805	.628	.202	2.213	1.105	13.330	2.579	4.957	6.325	2.620	.657	1.896	.640
3.1	2.138	.698	.537	.202	2.213	1.040	14.202	3.000	4.927	5.684	2.792	.764	1.884	.700
3.2	1.438	.591	.446	.202	2.213	.979	15.074	3.532	4.896	5.043	2.964	.899	1.873	.760
3.3	1.013	.560	.391	.202	2.213	.932	14.943	4.064	4.865	4.403	2.938	1.033	1.861	.820
3.4	1.583	.635	.412	.202	2.213	.882	13.810	4.515	4.835	3.762	2.714	1.147	1.849	.880
3.5	2.154	.710	.434	.202	2.213	.820	12.677	4.945	4.804	3.121	2.489	1.256	1.837	.940
3.6	2.725	.786	.455	.202	2.211	.758	11.647	4.845	4.589	2.480	2.286	1.231	1.755	1.000
3.7	3.295	.861	.477	.202	2.208	.725	11.029	4.595	4.375	2.354	2.166	1.169	1.673	.950
3.8	3.787	.919	.492	.202	2.205	.694	10.412	3.900	4.160	2.229	2.046	.993	1.591	.900
3.9	3.382	.940	.481	.202	2.203	.661	9.794	3.133	3.945	2.103	1.926	.798	1.509	.850
4.0	2.978	.961	.470	.202	2.200	.623	9.201	2.366	3.731	1.978	1.811	.603	1.427	.800
5.0	1.663	1.076	.439	.202	2.213	.341	5.057	1.151	2.095	1.035	.999	.293	.801	.420
6.0	1.751	1.076	.439	.202	1.776	.186	2.980	.795	1.278	.580	.590	.202	.489	.233
7.0	1.751	1.076	.439	.202	1.325	.117	1.760	.582	.869	.300	.350	.148	.332	.120
8.0	1.751	1.076	.439	.202	1.325	.090	1.580	.368	.715	.255	.314	.094	.274	.105
9.0	1.817	1.076	.439	.202	1.325	.079	1.400	.155	.715	.210	.278	.039	.274	.090
10.0	2.531	1.076	.439	.202	.994	.072	1.265	.123	.673	.197	.251	.031	.258	.083
11.0	1.821	1.076	.439	.202	.663	.067	1.174	.117	.589	.183	.233	.030	.225	.077
12.0	1.552	1.076	.439	.202	.663	.063	1.083	.111	.517	.170	.215	.028	.198	.070
13.0	1.628	1.076	.439	.202	.663	.059	1.006	.105	.482	.162	.195	.027	.184	.066
14.0	1.754	1.076	.439	.202	.663	.055	.934	.099	.447	.154	.175	.025	.171	.062
15.0	1.754	1.076	.439	.202	.398	.052	.868	.094	.412	.146	.159	.024	.158	.058
16.0	1.764	1.076	.439	.202	.133	.051	.821	.088	.382	.138	.155	.022	.146	.054
TIME	25.494	13.799	5.894	2.668	15.825	2.602	39.007	9.298	16.421	9.376	7.667	2.366	6.281	2.772

[a]E1 and E2 refer to first and second energy calculations, respectively. Time (at the bottom) is the integrated, total time for integrating between the first and last values of r in column 1.

TABLE 8. Test 2/J25B3. dt/dr (sec/Bohr), computer time for integrating a unit distance vs r.[a]

r	PC	DEVOG	MNN	LOGD	SAMS	INSCAT	GORDON E1	VIVS E1	RMAT E1	L2RMAT E1	GORDON E2	VIVS E2	RMAT E2	L2RMAT E2
3.5	14.089	2.521	3.710	.979	2.136	5.592	4.470	3.209	3.396	16.800	.610	.840	1.298	.790
3.6	12.262	2.157	3.143	.979	2.136	5.209	4.522	3.322	3.396	16.800	.633	.870	1.298	.790
3.7	10.435	1.793	2.576	.979	2.136	4.844	4.588	3.434	3.396	15.619	.661	.900	1.298	1.029
3.8	8.867	1.496	2.160	.979	2.136	4.494	4.653	6.519	3.396	14.499	.690	1.709	1.298	1.268
3.9	7.614	1.325	1.940	.979	2.136	4.160	4.718	9.033	3.396	13.348	.719	2.368	1.298	1.506
4.0	6.360	1.154	1.719	.979	2.136	3.840	4.783	8.812	3.396	12.198	.747	2.309	1.298	1.745
4.1	5.107	.983	1.499	.979	2.136	3.532	4.849	8.590	3.396	11.047	.776	2.251	1.298	1.984
4.2	3.853	.812	1.279	.979	2.136	3.235	4.914	4.727	3.396	9.896	.804	1.237	1.298	2.223
4.3	3.054	.708	1.147	.979	2.136	2.949	4.979	4.480	3.260	8.746	.833	1.173	1.246	2.462
4.4	2.940	.786	1.209	.979	2.136	2.669	5.045	4.660	2.989	7.595	.861	1.221	1.142	2.701
4.5	2.826	.865	1.271	.979	2.136	2.393	5.110	4.757	2.717	6.876	.890	1.248	1.038	2.762
4.6	2.712	.944	1.333	.979	2.136	2.113	4.895	3.835	2.445	6.588	.852	1.006	.934	2.647
4.7	2.598	1.023	1.394	.979	2.136	1.829	4.680	2.914	2.174	6.301	.814	.763	.831	2.531
4.8	2.508	1.089	1.444	.979	2.136	1.506	4.465	2.015	1.970	6.013	.776	.527	.753	2.416
4.9	2.463	1.091	1.444	.979	2.136	1.179	4.250	1.858	1.834	5.725	.738	.486	.701	2.300
5.0	2.418	1.093	1.444	.979	2.136	1.069	4.035	1.702	1.698	5.437	.700	.445	.649	2.184
6.0	2.248	.976	1.444	.979	2.136	1.565	2.960	.629	1.189	3.172	.510	.165	.454	1.276
7.0	1.667	.804	1.082	.979	1.897	1.314	2.620	.461	1.456	1.897	.454	.121	.556	.765
8.0	1.401	.691	.722	.979	1.658	1.046	2.020	.372	1.844	1.615	.354	.098	.704	.651
9.0	1.107	.624	.722	.538	1.418	.830	1.660	.328	1.916	1.411	.289	.086	.732	.568
10.0	.954	.587	.722	.538	1.179	.665	1.357	.285	1.673	1.515	.234	.075	.639	.610
11.0	.937	.565	.722	.538	.940	.537	1.223	.254	1.430	1.619	.212	.067	.547	.652
12.0	.756	.553	.722	.538	.837	.435	1.090	.223	1.187	1.615	.190	.058	.454	.649
13.0	.784	.545	.722	.538	.735	.351	.957	.192	.944	1.584	.168	.050	.361	.636
14.0	.639	.541	.722	.538	.632	.280	.823	.162	.701	1.540	.146	.042	.268	.619
15.0	.847	.538	.722	.430	.530	.213	.754	.142	.458	1.486	.133	.037	.175	.598
16.0	.550	.537	.722	.430	.427	.170	.705	.134	.440	1.414	.124	.035	.168	.570
17.0	.612	.535	.722	.430	.427	.130	.657	.125	.421	1.241	.115	.033	.161	.501
18.0	.651	.535	.722	.430	.427	.141	.608	.117	.402	1.068	.105	.031	.153	.432
19.0	.788	.535	.722	.430	.427	.164	.560	.109	.383	.895	.096	.028	.146	.364
20.0	.707	.535	.722	.430	.427	.174	.512	.100	.364	.807	.087	.026	.139	.328
25.0	.871	.535	.722	.074	.427	.168	.318	.065	.269	.476	.050	.017	.103	.194
30.0	.649	.535	.722	.061	.427	.149	.272	.056	.174	.257	.043	.015	.067	.105
35.0	.555	.535	.722	.052	.427	.131	.226	.048	.079	.224	.036	.012	.030	.091
40.0	.716	.535	.722	.046	.248	.117	.179	.039	.075	.191	.029	.010	.029	.078
45.0	.658	.537	.722	.041	.126	.105	.133	.030	.071	.158	.021	.008	.027	.064
50.0	.658	.537	.722	.036	.107	.095	.086	.025	.067	.125	.014	.007	.026	.050
100.	.658	.537	.722	.018	.107	.048	.020	.013	.040	.059	.003	.003	.015	.023
150.	.658	.537	.722	.012	.107	.032	.013	.007	.025	.046	.003	.002	.010	.019
TIME	110.176	81.001	108.733	15.137	38.449	22.754	37.945	14.529	28.598	56.514	6.407	3.805	10.927	19.634

[a]E1 and E2 refer to first and second energy calculations, respectively. Time (at the bottom) is the integrated, total time for integrating between the first and last values of r in column 1.

TABLE 9. Test 2/J5B3. dt/dr (sec/Bohr), computer time for integrating a unit distance vs r.[a]

r	PC	DEVOG	MNN	LOGD	SAMS	GORDON E1	VIVS E1	RMAT E1	L2RMAT E1	GORDON E2	VIVS E2	RMAT E2	L2RMAT E2
3.5	7.212	.987	1.496	.269	.936	2.818	1.620	2.998	7.450	.596	.410	1.106	.280
3.6	6.344	.844	1.267	.269	.936	2.946	1.620	2.570	7.450	.623	.410	.948	.280
3.7	5.476	.701	1.037	.269	.936	3.075	1.620	2.141	7.450	.649	.410	.790	.280
3.8	4.743	.587	.872	.269	.936	3.203	1.603	1.876	7.155	.675	.406	.692	.321
3.9	4.149	.519	.776	.269	.936	3.331	1.548	1.773	6.566	.702	.392	.654	.404
4.0	3.555	.451	.681	.269	.936	3.459	1.493	1.670	5.976	.726	.378	.616	.486
4.1	2.962	.383	.586	.269	.936	3.587	1.438	1.568	5.387	.755	.364	.578	.568
4.2	2.368	.316	.491	.269	.936	3.715	1.384	1.465	4.798	.781	.350	.541	.651
4.3	1.963	.272	.444	.269	.936	3.844	1.329	1.362	4.208	.807	.336	.503	.733
4.4	1.767	.302	.473	.269	.936	3.972	1.274	1.259	3.619	.834	.322	.465	.815
4.5	1.572	.331	.501	.269	.936	4.100	1.219	1.156	3.029	.860	.308	.427	.898
4.6	1.377	.360	.529	.269	.936	3.935	1.164	1.054	2.440	.826	.294	.389	.980
4.7	1.181	.390	.557	.269	.936	3.770	1.109	.951	2.458	.792	.280	.351	.987
4.8	1.078	.415	.578	.269	.936	3.605	1.055	.861	2.476	.758	.266	.318	.993
4.9	1.112	.415	.578	.269	.936	3.440	1.000	.784	2.494	.724	.252	.289	1.000
5.0	1.147	.414	.578	.269	.936	3.275	.945	.707	2.512	.690	.238	.261	1.007
6.0	1.094	.352	.564	.269	.936	2.495	.455	.578	2.642	.525	.113	.213	1.056
7.0	.882	.268	.289	.269	.936	2.352	.407	.499	2.624	.494	.101	.184	1.051
8.0	.746	.204	.289	.269	.936	1.981	.360	.437	2.368	.421	.090	.161	.946
9.0	.555	.161	.263	.269	.936	1.626	.313	.389	1.952	.346	.078	.144	.786
10.0	.444	.130	.144	.090	.936	1.319	.266	.354	1.637	.281	.066	.131	.655
11.0	.437	.109	.144	.090	.936	1.153	.219	.320	1.368	.247	.055	.118	.543
12.0	.328	.094	.144	.090	.936	.988	.172	.285	.199	.212	.043	.105	.477
13.0	.463	.083	.144	.090	.936	.823	.160	.250	1.030	.177	.040	.092	.410
14.0	.288	.074	.074	.090	.936	.715	.155	.215	.925	.154	.039	.079	.367
15.0	.163	.067	.072	.090	.936	.665	.150	.180	.821	.143	.038	.066	.324
16.0	.191	.062	.072	.090	.936	.615	.145	.174	.716	.132	.037	.064	.281
17.0	.757	.059	.072	.090	.936	.565	.139	.167	.647	.121	.035	.062	.253
18.0	.199	.055	.072	.090	.936	.515	.134	.161	.590	.110	.034	.059	.231
19.0	.122	.053	.072	.090	.936	.465	.129	.155	.534	.099	.033	.057	.209
20.0	.124	.051	.072	.090	.936	.415	.124	.148	.477	.088	.031	.055	.187
25.0	.095	.046	.072	.090	.936	.326	.101	.117	.325	.067	.026	.043	.128
30.0	.065	.044	.072	.040	.936	.255	.089	.085	.241	.050	.023	.031	.095
35.0	.065	.043	.072	.040	.936	.208	.078	.054	.157	.040	.020	.020	.062
40.0	.065	.043	.072	.040	.936	.183	.066	.049	.098	.036	.017	.018	.039
45.0	.065	.043	.072	.040	.936	.159	.055	.044	.092	.031	.014	.016	.037
50.0	.065	.043	.072	.040	.425	.134	.050	.040	.086	.027	.013	.015	.034
100.	.065	.043	.072	.002	.023	.060	.032	.014	.030	.012	.008	.005	.010
150.	.065	.043	.072	.001	.023	.049	.026	.008	.026	.010	.006	.003	.009
TIME	20.469	8.309	13.168	5.251	54.625	38.048	11.631	10.936	37.851	7.925	2.932	4.035	13.116

[a]E1 and E2 refer to first and second energy calculations, respectively. Time (at the bottom) is the integrated, total time for integrating between the first and last values of r in column 1.

TABLE 10. Test 4/J5B3. dt/dr (sec/Bohr), computer time for integrating a unit distance vs r.[a]

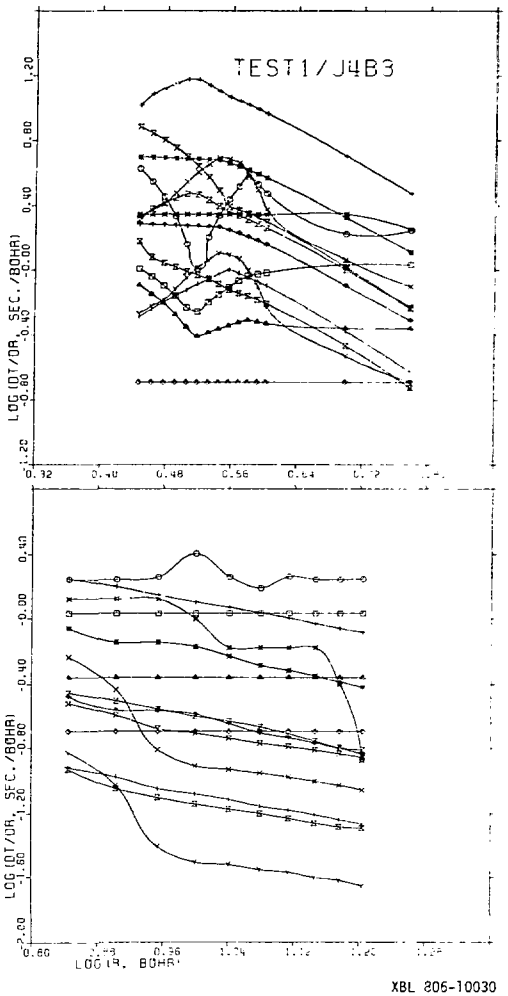
r	PC	DEVOG	MNN	LOGD	SAMS	INSCAT	GORDON E1	VIVS E1	RMAT E1	L2RMAT E1	GORDON E2	VIVS E2	RMAT E2	L2RMAT E2
.2	13.599	3.601	7.160	.216	.229	4.254	14.943	1.560	2.677	5.910	2.900	.380	1.025	.326
.4	10.695	2.809	5.371	.216	.229	4.316	7.043	1.560	2.677	5.910	1.364	.380	1.025	.358
.6	6.313	1.662	2.921	.216	.229	2.868	6.088	2.086	2.590	5.910	1.179	.508	.991	.390
.8	2.222	.555	.800	.216	.229	2.213	5.132	2.663	2.244	4.952	.994	.649	.859	.408
1.0	1.641	.453	.650	.216	.229	1.776	4.443	3.373	1.898	3.994	.860	.822	.726	.426
1.2	1.060	.351	.500	.215	.229	1.401	3.931	3.240	1.552	3.036	.761	.789	.594	.444
1.4	.852	.275	.409	.213	.229	1.224	3.419	2.262	1.205	2.078	.662	.550	.461	.462
1.6	1.174	.240	.385	.212	.229	1.073	2.907	1.855	981	1.120	.563	.452	.375	.480
1.8	1.497	.205	.361	.210	.229	.951	2.395	1.449	.878	1.013	.464	.353	.336	.431
2.0	1.281	.181	.321	.208	.229	.868	1.883	1.144	.774	.907	.364	.280	.296	.382
3.0	.199	.089	.178	.102	.229	.582	1.267	.764	.430	.552	.245	.186	.165	.222
4.0	.103	.048	.169	.102	.223	.442	.942	.509	.344	.397	.182	.124	.132	.156
5.0	.103	.081	.089	.102	.130	.352	.739	.387	.258	.334	.142	.094	.099	.135
6.0	.875	.095	.089	.102	.023	.293	.657	.316	.258	.279	.127	.077	.099	.128
7.0	.330	.104	.089	.102	.023	.250	.574	.251	.258	.243	.111	.061	.099	.153
8.0	.120	.108	.089	.102	.023	.221	.492	.224	.172	.206	.096	.055	.066	.179
9.0	.273	.111	.089	.102	.023	.193	.410	.198	.172	.182	.080	.048	.066	.171
10.0	.244	.114	.089	.102	.023	.177	.390	.171	.166	.167	.076	.042	.064	.138
11.0	.163	.115	.089	.102	.023	.162	.370	.144	.155	.153	.071	.035	.059	.104
12.0	.123	.116	.089	.102	.023	.146	.350	.118	.143	.138	.067	.029	.055	.071
13.0	.123	.117	.089	.102	.023	.135	.330	.101	.131	.127	.063	.025	.050	.051
14.0	.104	.118	.089	.102	.023	.127	.310	.098	.117	.120	.058	.024	.045	.048
15.0	.078	.119	.089	.102	.023	.119	.290	.094	.103	.113	.054	.023	.040	.045
16.0	.087	.119	.089	.102	.023	.110	.270	.090	.089	.106	.050	.022	.034	.042
17.0	.089	.119	.089	.102	.023	.102	.250	.087	.076	.099	.045	.021	.029	.039
18.0	.097	.120	.089	.102	.023	.097	.230	.083	.069	.092	.041	.020	.026	.037
19.0	.212	.120	.089	.102	.023	.093	.217	.079	.069	.087	.039	.019	.026	.035
20.0	.096	.120	.089	.102	.023	.089	.211	.076	.069	.084	.038	.018	.026	.033
25.0	.112	.121	.089	.102	.023	.070	.182	.057	.063	.068	.033	.014	.024	.027
30.0	.151	.122	.089	.102	.023	.059	.153	.039	.052	.057	.028	.009	.020	.023
35.0	.120	.122	.089	.102	.023	.050	.124	.024	.040	.050	.023	.006	.015	.020
40.0	.134	.122	.089	.102	.023	.044	.110	.023	.034	.043	.021	.005	.013	.017
45.0	.134	.122	.089	.102	.023	.038	.110	.021	.032	.041	.021	.005	.012	.016
50.0	.134	.122	.089	.102	.024	.035	.110	.020	.031	.041	.021	.005	.012	.016
TIME	14.422	7.298	7.592	5.321	2.128	9.375	22.095	9.352	7.937	11.778	4.222	2.280	3.038	3.345

[a]E1 and E2 refer to first and second energy calculations, respectively. Time (at the bottom) is the integrated, total time for integrating between the first and last values of r in column 1.

TABLE 11. Integrated total times from Tables 7-10 arranged in ascended order on the time.[a]

TEST 1/J4B3			TEST 2/J25B3			TEST 2/J5B3			TEST 4/J5B3		
Method	Energy	Time (sec)	Method	Energy	Time (sec)	Method	Energy	Time (sec)	Method	Energy	Time (sec)
HYBRID	2nd	1.31	HYBRID	2nd	3.3	HYBRID	2nd	2.82	HYBRID	2nd	1.56
HYBRID	1st	2.08	VIVS	2nd	3.8	VIVS	2nd	2.93	SAMS		2.13
VIVS	2nd	2.37	GORDON	2nd	6.4	RMAT	2nd	4.03	VIVS	2nd	2.28
INSCAT		2.60	HYBRID	1st	9.5	LOGD		5.25	RMAT	2nd	3.04
LOGD		2.67	RMAT	2nd	10.9	GORDON	2nd	7.92	L2RMAT	2nd	3.34
L2RMAT	2nd	2.78	VIVS	1st	14.5	DEVOG		8.31	GORDON	2nd	4.22
MNN		5.87	LOGD		15.1	HYBRID	1st	10.17	HYBRID	1st	4.43
RMAT	2nd	6.28	L2RMAT	2nd	19.6	RMAT	1st	10.94	LOGD		5.32
GORDON	2nd	7.67	INSCAT		22.8	VIVS	1st	11.63	DEVOG		7.30
VIVS	1st	9.30	RMAT	1st	28.6	L2RMAT	2nd	13.12	MNN		7.59
L2RMAT	1st	9.38	GORDON	1st	37.9	MNN		13.16	RMAT	1st	7.94
DEVOG		13.80	SAMS		38.4	PC		20.47	VIVS	1st	9.35
SAMS		15.82	L2RMAT	1st	56.5	L2RMAT	1st	37.85	INSCAT		9.37
RMAT	1st	16.42	DEVOG		81.0	GORDON	1st	38.05	L2RMAT	1st	11.78
PC		25.49	MNN		108.7	SAMS		54.62	PC		14.42
GORDON	1st	39.01	PC		110.2				GORDON	1st	22.09

[a]The HYBRID times are the sum of the times for LOGD integrated from r_{min} to r_0 and for VIVS integrated from r_0 to r_{max}. r_0 is 8.0, 6.0, 4.8 and 4.0 for Test 1/J5B3, Test 2/J25B3, Test 2/J5B3 and Test 4/J5B3, respectively.



Notation for Figs. 1-8

- L2RMAT E2
- RMAT E2
- VIVS E2
- GORDON E2
- L2RMAT E1
- RMAT E1
- VIVS E1
- GORDON E1
- INSCAT
- SAMS
- LOGD
- MNN
- DEVOG
- PC

Fig. 1. Comparison of dt/dr for all methods for Test 1/J4B3.

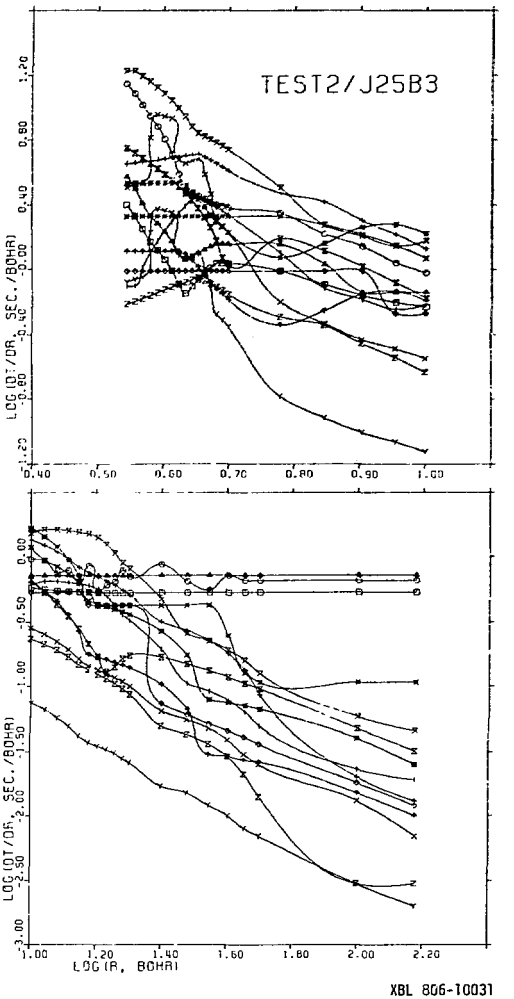


Fig. 2. Comparison of dt/dr for all methods for Test 2/J25B3.

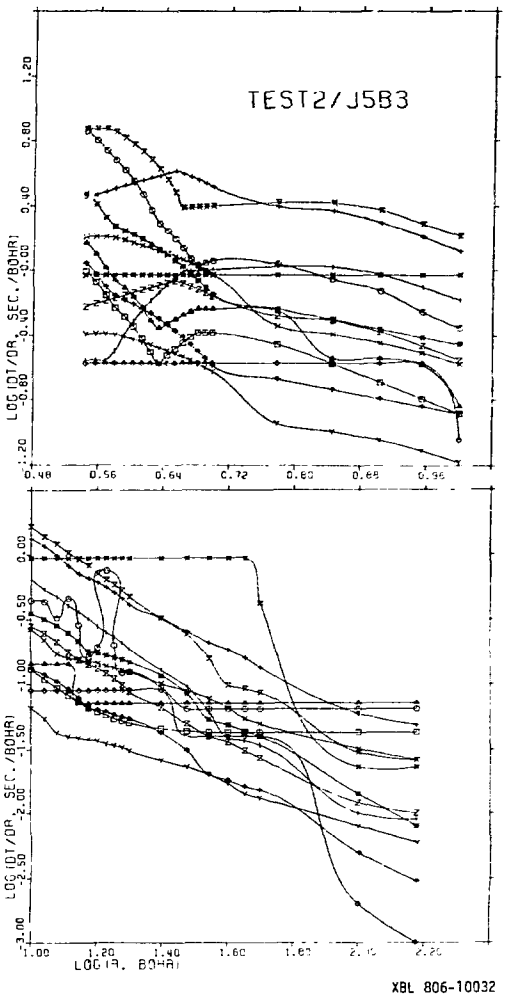


Fig. 3. Comparison of dt/dr for all methods for Test 2/J5B3.

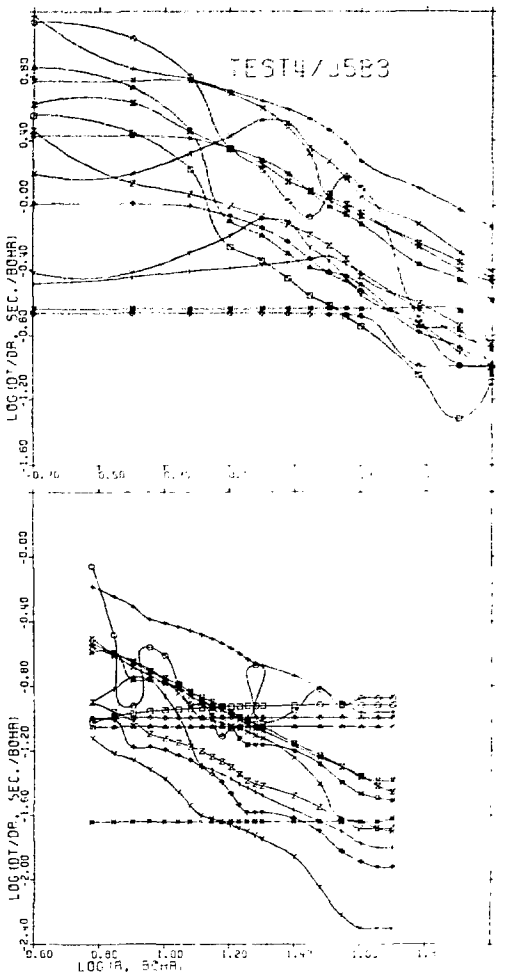


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Fig. 4. Comparison of dt/dr for all methods for Test 4/J5B3.

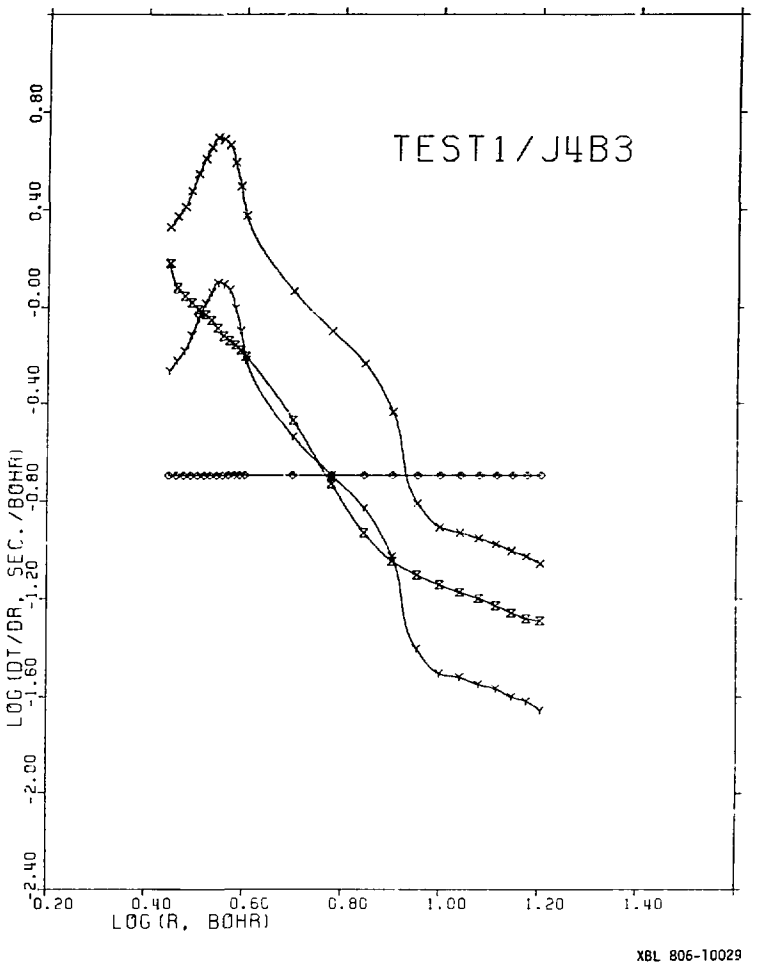

Fig. 5. Comparison of dt/dr for LOGD, VIVS, and INSCAT for Test 1/J4B3.

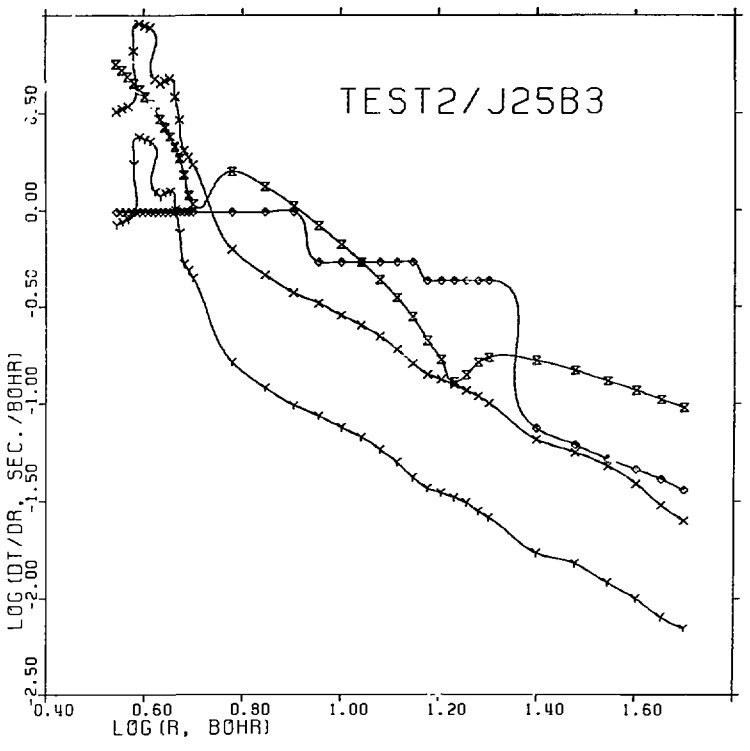

Fig. 6. Comparison of dt/dr for LOGD, VIVS, and INSCAT for Test 2/J25B3.

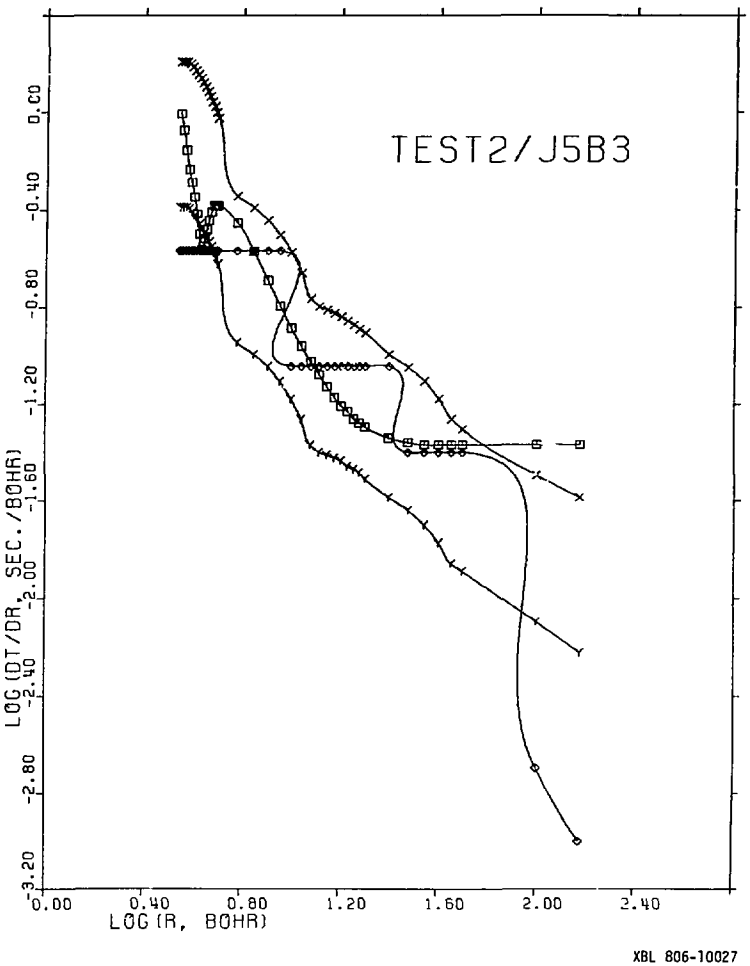

Fig. 7. Comparison of dt/dr for LOGD, VIVS, and DEVOG for Test 2/J5B3.

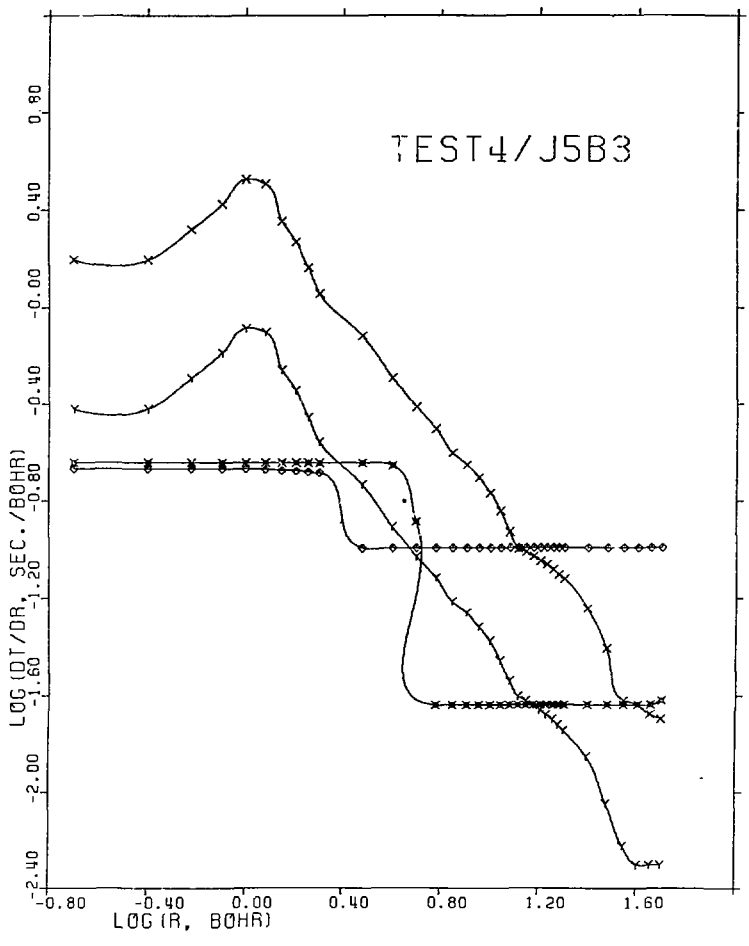

Fig. 8. Comparison of dt/dr for LOGD, VIVS, and SAMS for Test 4/J5B3.

SECTION IV

INDIVIDUAL COMMENTS ON METHODS AND TEST RESULTS

Solution of the Test Problems Using the Predictor-Corrector (PC), DeVogelaere (DEVOG), and Numerov (MNN) Algorithms

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Predictor-Corrector

Predictor-corrector methods for numerically solving differential equations are among the first ever developed and date back nearly 100 years.[1] Recent advances in the application of these methods have, however, improved them considerably.[2,3] These improved methods have been widely applied to the calculation of classical trajectories, but have not, to my knowledge, been given serious consideration for quantum mechanical calculations. It therefore seems of interest to solve the test problems of this workshop with a predictor-corrector method to see if the new methods which have been developed, in the past 10 years or so, are in fact improvements over their predecessors.

The program of Shampine and Gordon[3] was recently tested by me in the calculation of classical trajectories on the Li^+ - CO potential energy surface used in Test 2, and found to be not only superior to the Gear and fixed-order predictor-corrector methods previously used, but much easier and more fool-proof to use. The classical trajectory program ABCRR[4] was therefore modified to solve the quantum mechanical differential equations of the test problems.

The program of Shampine and Gordon solves arbitrary sets of first-order differential equations. Krogh[2] also has programs for higher order methods and has found that use of them is usually faster than the use of first-order methods when the equations to be solved are of higher order. However, since my intention was to make a simple modification to the existing ABCRR program, no attempt was made to use a second-order method.

Instead the second-order quantum mechanical equations were simply written as twice as many first-order equations, i.e.,

$$u' = v \tag{1}$$

$$v' = W u \tag{2}$$

where

$$u'' = W u \tag{3}$$

is the original second-order equation to be solved.

Secrest has pointed out[5] that stabilizing transformations are in many cases necessary much less often than previously supposed. The following criterion was used to automatically decide when to do a stabilizing transformation. Since the transformation is only necessary to maintain numerical linear independence of the solutions, it suffices to check that the absolute values of different channel wavefunctions within a given column of wavefunctions are not too widely separated. At each step a check was made on the first column of the wavefunction matrix. If the absolute value of,

$$u_1/u_i \qquad i = 2, \ldots, \text{NCHAN}$$

was larger than 100 for any i, a stabilizing transformation was done. In addition, if

$$| u_1 |$$

became larger than 100, a transformation was also done. This criterion indeed resulted in only 5-10 transformations over the entire integration range, for most of the test problems.

The resulting program is quite simple (not counting the Shampine-Gordon program, treated here as a black box) and quite simple to use. The only user input to the program is the energy, r_{min} and r_{max} which define the integration range, and one tolerance parameter which governs the accuracy of the solution. Some experimentation with the tolerance parameter is necessary

but this can be done on the smaller basis sets and a safe, if not optimum value, is easy to find.

To the credit of those people who have developed new methods in recent years, the predictor-corrector method never performed best for any test. However, it was often not the worst. The method does best, as might be expected, at low energy where the wavelength is long. The method has to work very hard in the non-classical region and the number of steps necessary seems to be dependent not only on the problem and energy but on the number of channels as well.

The values of r_{min} and r_{max} actually used are given in Table 3. One comment is, however, in order. The value of r_{max} = 150.0 for Test 2 and much to small. Based on the B1 basis sets, this value was judged sufficient for one significant figure of accuracy, not two. For some of the larger basis sets not even one was achieved.

The program has been run only on LBL's CDC 7600, but conversion to other machines should not involve more than changing from single to double precision.

DeVogelaere's Method

The predictor-corrector program described above is quite modular, and modifying it to integrate with DeVogelaere's method was a simple task. The equations used were taken from Lester's paper.[6] These were programmed so that the formula for changing the stepsize is used at every step, even if the old and new stepsizes are the same. This can be done with negligible loss of efficiency. The stepsize is chosen so that the number of steps per local wavelength [computed from the (1,1) element of the interaction matrix] is within a certain range, given by the user. At each step the local wavelength is computed and the number of steps within that wavelength is checked to see if it is within the specified range. If not, a new stepsize is computed such

that the number of steps is in the middle of the range.

The DeVogelaere method consistently outperforms the predictor-corrector method by a wide margin. The program is even simpler than the predictor-corrector program and equally simple to use. The user need only supply the energy, r_{min} and r_{max} and the range for the number of steps per local wavelength. The wavelength is considered to be the full period of 2π. Some experimentation is necessary to find a suitable number but this can be done on the smaller basis sets. Twenty-five steps per local wavelength was chosen as optimum for all tests except Test 1. Fifty steps were necessary for Test 1. No difficulties were encountered with any of the tests. The program has been run only on LBL's CDC 7600, but it is expected that only a change of precision is necessary to run it on most other computers.

Numerov's Method

A Numerov program written by M. A. Brandt, D. G. Truhlar, K. Onda and D. Thirumalai[7] (version 79-6 of this program, MNN) was donated to the workshop and I have used it to solve the test problems 1, 2 and 4. The program is a completely general and modular close-coupling program and like all the other programs used in this report, is now available from the NRCC software library.

This program has automatic stepsize selection and performed without numerical difficulty on all of the test problems. The only difficulty encountered in using the program was that it does not stop the integration at exactly the specified r_{max}. The necessary changes to do this are probably not difficult but no attempt to modify the program was made. Since the S-matrices of Test 3 must be computed at exactly r = 7.0 in order to make a meaningful comparison, Test 3 was not done.

The negative δ option was used and a value of δ = - .1E-6 was found to be the largest value which resulted in two significant figures of accuracy. This value was used for all of the problems. Some further refinement is possible through variation of the parameter HSTART, the initial stepsize. This however, was not done and a value of .125E-3 was used on all of the problems.

An assembly language linear equation solver is available for this program which does improve its performance. This however, was not used for the test problems. The comparison is nonetheless a fair one since none of the other programs used any specialized assembly language programs either. This program has been run only on CDC computers and its portability to other machines has not been tested.

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The Log Derivative Test Calculations

The log derivative and renormalized Numerov algorithms were presented in volume 1 of this report. Because of time limitations, only one of these methods could be evaluated on the NRCC test problems. The log derivative method was chosen because of two convenient features. The grid spacing can be easily changed with no restrictions on the change, whereas with the renormalized Numerov the spacing can only be conveniently doubled or halved. In addition, the potential matrix function of test problem 4 has a discontinous first derivative at R = 1.034. The log derivative method can handle this easily, whereas special programming would be required with the renormalized Numerov method to compensate for the increased trunction error that is produced when integrating over this point.

A fortran program which utilizes the log derivative formulas given in volume 1 of this report was written to solve the special test problems. The program was designed to allow the integration range to be divided into a maximum of three partitions, with a different grid spacing in each partition. The number of partitions, the boundaries of the partitions and the grid spacings are parameters that are set by the user.

Since test problem 2 has an extremely long range potential, an additional option was added to the program which allows the user to switch over to a very efficient WKB calculation in the far asymptotic region. This WKB method was developed several years ago and is fully described as "Method B" in the reference; B. R. Johnson, "A Generalized JWKB Approximation for Multichannel Scattering," Chem. Phys. 2, 381 (1973). The WKB option was only used on problem 2. It could have also been used to decrease the computation time of problems 1 and 4, but was not, since we were primarily interested in evaluating the log derivative algorithm.

Following are the parameters that were used in each of the test problems employing the basis sets B3. (In most cases these same parameters were also used with the other basis sets.)

Test 1 (J4B3). The integration range was from 1.5 to 30 with a grid spacing h = 0.0325. This grid spacing is a nominal value set by the user. The program then re-adjusts it so that an even number of spacings will fit into the integration range.

Test 2 (J5B3). The integration range was 3 to 1500. The log derivative method was used from 3 to 100 and the WKB method from 100 to 1500. The log derivative range was divided into 3 partitions; 3-10, 10-30 and 30-100 with grid spacings h = 0.015, 0.045, 0.1. The log derivative part of the calculation required 6.49 sec. While the WKB part took 0.47 sec.

Test 2 (J25B3). The integration range was 3 to 800. The log derivative method was used from 3 to 20 and the WKB method from 20 to 800. The log derivative range was divided into 3 partitions; 3-9, 9-15 and 15-20 with grid spacings h = 0.011, 0.02, 0.025. The log derivative calculation required 11.25 sec. while the WKB calculation took 6.83 sec.

Test 3 (J5B3 and J25B3). The integration range was 3 to 7 with a grid spacing h = 0.01.

Test 4. The integration range was 0.0001 to 50. This wes divided into 3 partitions; 0.0001-1.034, 1.034-2.4 and 2.4-50 with grid spacings h = 0.05, 0.05, 0.1. The potential matrix in this problem has a discontinous first derivative at R = 1.034. Setting one of the partition boundaries at this point is the easiest way to insure that the cusp in the potential will not have an adverse effect on the truncation error.

No major difficulties were encountered in solving any of these test cases. It was easy to obtain any desired accuracy by adjusting the grid spacing and range of integration. The truncation error of the log derivative method varies as the fourth power of the grid spacing. We believe that the basic strengths of the log derivative method are its complete reliability and trouble free operation on any type of problem and its great simplicity combined with a reasonable efficiency.

A significant improvement that could be made in the existing program would be the incorporation of a reliable algorithm to optimally and automatically adjust the grid spacing as the calculation proceeds so that the user only has to supply a single truncation error tolerance parameter.

The most time consuming calculation in the log derivative algorithm is the symmetric matrix inversions. Therefore any improvements in the matrix inversion subroutine would be very useful. The second most time consuming part of the calculation is the evaluation of the potential matrix. In fact, for a one or two channel problem it is possible for this calculation to dominate. Therefore, one should try to make this calculation as efficient as reasonably possible.

The program is easily portable. The entire, self contained, fortran program to compute the S-matrix (without the WKB option and excluding the user supplied potential subroutine) is a deck of cards less than 3½ inches thick.

Erratum

The Log Derivative and Renormalized Numerov Algorithms.

The third formula in Eq. (7) which appears on page 88 of Vol. I is in error. The plus and minus signs should be interchanged. The correct formula is

$$8I - 8[I + (h^2/6)\, Q(x_n)]^{-1}, \quad n = 1, 3, \ldots N-1.$$

Integral Equation Methods for Inelastic Scattering. II. Calculations (SAMS)

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Integral Equation Methods for Inelastic Scattering. II. Calculations.

A. Introduction

This article will deal with the computational features of the integral equation method widely known as the Sams and Kouri method. For a discussion of the mathematical details of this method the reader is referred to Part I of this series. A detailed practical description is given of how one performs close coupling calculations by this method in general and the test calculations of the Workshop in particular. Since it is important to have a clear conception beforehand of the accuracy desired in quantum mechanical scattering calculations, a brief treatment of accuracy criteria has been included. A number of changes have been made in the computer program since Part I was written six months ago. These modifications are described in detail. Advantages and limitations of the method are discussed in the conclusion. A few comments are made for the benefit of the inexperienced user which will aid in the effective use of this method.

B. Philosophy and Practice of Close Coupling Calculations

The computer program in its present form requires the choice of a number of parameters by experimentation. For a given energy (E), total angular momentum (J) and basis set, these parameters (in the order in which they are experimentally adjusted) are:

1. integration starting point (x_0),
2. integration stopping point (x_N),
3. trapezoid rule interval (step size, h),
4. (optional) new step sizes (h_i) and at which points (x_{n_i}) in the integration they are used,

5. number and location of stabilizing transformations,
6. the point after which energetically inaccessible closed channels are to be eliminated.

Generally one chooses some starting h, x_0 and x_N, and then adjusts x_0 by moving more and more deeply into the nonclassical region. In this manner x_0 is rapidly found in just a few runs. Next, one extends the integration farther out into the asymptotic region in order to fix x_N. This is somewhat more difficult than choosing x_0 (particularly for slowly-but-surely changing long range potentials). Choice of x_N can usually be accomplished in about five runs. Next, one varies h until the desired accuracy is obtained (cf. Section 3), and a few runs are sufficient. For a multichannel problem it may be necessary to tentatively select a few stabilizations in order to be able to complete these adjustments. Even in solution following methods such as the present one, a smaller step size is required in the interaction region than in the asymptotic region. It is therefore profitable to take small steps in the interaction region and change to a larger step size farther out. The number and location of step size changes is heavily dependent on the amount of experimentation the investigator is willing to do. This is by far the most time consuming phase of the diddling process. Once x_0, x_N and the (h_i, x_{n_i}) have been determined, it is a simple matter to add sufficient stabilizations (the criterion for this being the symmetry of the reactance matrix or the unitarity of the scattering matrix). Generally, less than half a dozen stabilizing transformations are necessary for potentials with moderate range. Asymptotically closed channels, if they are present, can be dropped some distance away from the classical turning point. Once they have been eliminated, stabilization is no longer necessary. Generally one does all the diddling for

a small basis set but this leads to difficulty for extremely anisotropic potentials or when one wants extreme accuracy for transitions of low probability. Accordingly, it is a good idea to perturb the parameters optimized for a small basis set to ensure convergence for larger basis sets. In most practical calculations, one is usually not worried about low accuracy in small scattering matrix elements, hence, single channel diddling is sufficient for potentials of moderate range. Single channel convergence tests on the long range Li^+-CO system (Test 2) give one or two figures in the scattering matrix with $x_N \sim 200$ bohr whereas the multichannel problem is not converged to this accuracy until about $x_N \sim 1500$ bohr. The reason for this is the very anisotropic interaction potential, the matrix elements of which decay as R^{-4} for diagonal elements, but as R^{-2} for off-diagonal elements. Similarly, a single channel convergence test on the He-H_2 system (Test 1) produces nearly three figure accuracy at $x_N \sim 15$ bohr, but the $v=0$ to $v'=1$ vibrationally inelastic transition probability ($j=j'=0$), which is very small ($\sim 10^{-10}$), is not converged to even one significant figure for a basis set consisting of only these two channels. This inelastic transition has converged to two figures by $x_N \sim 50$ bohr, but this much accuracy is not really necessary in a practical calculation since the more probable transitions will dominate anyway. It is interesting to note that larger bases will give higher accuracy for this transition for $x_N \sim 15$ bohr. In a production run consisting of, say, 100 total J's, one does the diddling only two or three times, the resulting parameters being satisfactory for many J's. Indeed, the parameters which work for low J are more than ample for high J. Diddling at high J is purely an economic measure since these angular momenta correspond to grazing collisions and

the low J integration parameters may be unduly strict. For example, one can choose a larger x_0, drop closed channels sooner, etc.

Diddling with parameters in this method is both an advantage and a disadvantage. It is an advantage because the investigator, and not the machine, is in full control of the quality of the calculation and it is possible to carefully observe the effect of changes in the various parameters. This is particularly useful in the case of potentials with unusual features. The investigator can determine the optimum choice of the parameters using his resourcefulness and ingenuity. There is no guarantee that the more automatic methods will choose the parameters correctly and efficiently and in applications where the execution time is enormous this is a major concern. Obviously, diddling is tedious and some measure of experience is necessary in order to choose the parameters economically. A novice working remotely on the LBL system may find diddling an experience tortuous beyond description. Table 1 gives some typical integration parameters which give two significant figure accuracy in the transition probabilities, $|S_{mn}|^2$. These parameters produce execution times which are competitive with all of the other methods investigated for the Workshop. Further experiments would give even better execution times, but the present parameters are sufficient to illustrate the efficacy of this method.

C. Accuracy Criteria

A large source of ambiguity in scattering calculations involves the question of accuracy. The accuracy criteria used for a particular calculation depend on what observable quantity one is trying to calculate. For example, if one is interested only in integral cross sections, an adequate accuracy criterion might be the number of significant figures in the

transition probabilities, or absolute squares of the scattering matrix elements, $|S_{mn}|^2$. On the other hand, if one is interested in the differential cross sections, the phase of the scattering matrix is important and a more strict accuracy criterion (because the magnitude converges before the phase) might be the number of significant figures in the larger of $Re(S_{mn})$ and $Im(S_{mn})$. Hence, it is useful to decide in advance for what purpose (integral or differential cross sections) the calculation is to be performed in order to be as economical as possible.

D. Recent Modifications of the Computer Program

There are two important changes which have been made to the original code (cf. Part I). The first is concerned with testing to see what sort of activity is to be performed on a given step, namely stabilization, closed channel deletion and integration termination. The old code made a separate test for each activity on every step of the integration. It is more efficient to make one test per step (rather than three or more) to determine if anything at all is to be done on that step. If so, the other tests are made. This "next-most-important step" testing is also more flexible for we can easily and efficiently provide other options without significantly affecting the execution time. The second change is concerned with step size modification. It is well known that in the interaction region a different step size is necessary than in the asymptotic region. Without the option to change step size one must continue the integration into the asymptotic region with inappropriately tiny step sizes consequently taking an enormous number of steps. Although the execution time per step is low, it is possible to cut execution times by at least a factor of five by changing the step size a number of times in the integration. The "next-most-important step"

algorithm made the implementation of the step size changes a nearly trivial task, both from the point of view of programming and execution.

In changing the step size, one merely changes the quadrature weights and increments. We are doing an integral numerically, thus,

$$\int_a^b f(x)dx = \sum_{i=0}^{N} f(x_i)w_i^N$$

where, for the trapezoid rule,

$$w_i^N = \begin{cases} \frac{h}{2} & \text{for } i=0 \text{ or } i=N \\ h & \text{otherwise.} \end{cases}$$

If we change step size from h to $\bar{h}$ at the point x_c, then

$$\int_a^b f(x)dx = \sum_{i=0}^{c} f(x_i)w_i^c + \sum_{j=0}^{N-c} f(x_{j+c})\bar{w}_j^{N-c}$$

It follows that,

$$\int_a^b f(x)dx = \sum_{i=0}^{c-1} f(x_i)w_i^c + f(x_c)w_c^c + f(x_c)\bar{w}_0^{N-c} + \sum_{j=1}^{N-c} f(x_{j+c})\bar{w}_j^{N-c}$$

$$= \sum_{i=0}^{c-1} f(x_i)w_i^c + \sum_{j=1}^{N-c} f(x_{j+c})\bar{w}_j^{N-c} + f(x_c)\tilde{w}_c.$$

where

$$\tilde{w}_c = \tfrac{1}{2}(h+\bar{h}).$$

Hence, when the integration reaches $x = x_c$, the quadrature weight is changed from h to $(h+\bar{h})/2$ for one step. On the very next step, the quadrature weight is changed to $\bar{h}$. Caution: The integration variable is incremented by $\bar{h}$ not $(h+\bar{h})/2$. That is,

$$x_{c+1} = x_c + \bar{h}.$$

Extension to more step size changes is trivial. Introduction of the above ideas into the integral equation formalism clearly shows on what step the changes are to be made. In summary, if the current point is the one after which a new step size is to be used, the computer will make two passes through the quadrature weight changing algorithm, one for the current step and another on the very next one.

E. Conclusion

The results show that with proper diddling the Sams and Kouri method is competitive with all other single energy methods studied. It performs extremely well for the electron scattering problem, rivaling the execution time for the second energy by methods which are fast for more than one energy. As expected, however, the method becomes time consuming for long range potentials, as in the Li^+-CO system, and other methods are better suited for these problems.

The principal drawback is the somewhat tedious experimental optimization of the numerical integration parameters. The program is extremely simple. In fact, it was written by a graduate student having absolutely no prior knowledge of FORTRAN as his very first exercise in close coupling research. Investigators who are primarily concerned with applications will find this program extremely useful as it readily gives the user an intuitive idea for what is going on in a calculation and how it is accomplished. For unusual potential functions this method is the one of choice since potential following methods may become too time consuming or unreliable in some cases.

Due to its extreme simplicity, this program is readily portable. Investigators eager to get results painlessly will find its simplicity a

decisive factor. After some practice in choosing the numerical integration parameters, which is an educational experience in itself, most users will be able to apply the method economically and with confidence.

Note Added in Proof. Some explanation for our early results should be made. These early results are listed as the first entry for each of the tests (see Appendix A: The Sams-Kouri Method). We intended these only as preliminary results for the October Workshop meeting. They do not represent the optimal choice of integration parameters and are typical of the kind of results that would be obtained by a novice (indeed they actually were obtained by one). In particular, the small basis Test 1 results are not converged with respect to the $(vj\ell) = (004) \rightarrow (v'j'\ell') = (104)$ transition. It was originally requested that two or three figure accuracy be attained in the S-matrix elements, consequently extreme accuracy was obtained in the S-matrix absolute squares (transition probabilities), especially for Tests 3 and 4. The latest results (given at the end of our article) are accurate to two (and only two) figures in $|S|^2$. Test 3 was not rerun due to the lack of interest expressed in it at the October meeting.

Table 1: Typical Integration Parameters[a]

Workshop Test	System	Total Energy	Total Angular Momentum	Integration Start	Integration Stop	Initial Step Size	Final Step Size	Drop Closed Channels[b]
1	$He-H_2$	2.24×10^{-2}	4	2.25	40	0.003	0.05	8
2	Li^+-CO	7.79×10^{-5}	5	3.5	1000	.01	1	150
2	Li^+-CO	1.95×10^{-3}	25	3.5	500	0.005	0.1	---
4	e^-N_2	1.1025 (30 eV)	5	0.05	50	0.05	0.5	---

[a] All quantities are expressed in atomic units.

[b] For largest basis set used.

TEST i: $He-H_2$

$J = 4$, even parity

$E = 2.24 \times 10^{-2}$ hartree

Basis 1: $\{0,0\}^a$ 2 channels

Basis 2: $\{2,2\}$ 8 channels

Basis 3: $\{6,2\}$ 18 channels

Basis 4: $\{8,4\}$ 28 channels

$$P_i = |S(1,0,4 \leftarrow 0,0,4)|^{2b}$$

$$P_e = |S(1,0,4 \leftarrow 1,0,4)|^2$$

RESULTS:

Basis	P_i	P_e	t,sec	N
1	9.201×10^{-11}	1.000	0.39	3050
2	1.679×10^{-9}	9.551×10^{-1}	3.17	3050
3	1.181×10^{-9}	9.551×10^{-1}	20.21	3050
4	1.110×10^{-9}	9.547×10^{-1}	56.64	3050

---

[a] This notation gives the maximum rotor state carried in each vibrational manifold, $\{j^{max}_{v=0}, j^{max}_{v=1}, \ldots\}$.

[b] $S(v'j'\ell' \leftarrow vj\ell)$.

TEST 2: Li^+-CO

J = 5, odd parity

E = 7.79×10^{-5} hartree

Basis 1:	{1}[a]	3 channels
Basis 2:	{2}	6 channels
Basis 3:	{4}	15 channels
Basis 4:	{6}	27 channels

For basis 1,

$$P_i = |S(1,6\leftarrow 0,5)|^2$$ [b]

$$P_e = |S(1,6\leftarrow 1,6)|^2$$

For all others,

$$P_i = |S(2,3\leftarrow 0,5)|^2$$

$$P_e = |S(2,3\leftarrow 2,3)|^2$$

RESULTS:

Basis	P_i	P_e	t,sec	N
1	2.269×10^{-1}	3.087×10^{-1}	1.11	2900
2	1.412×10^{-2}	4.889×10^{-2}	2.09	2900
3	7.574×10^{-3}	4.053×10^{-1}	54.17	11575
4	1.618×10^{-2}	1.167×10^{-1}	214.36	11575

---

[a] This notation gives the maximum rotor state carried in each vibrational manifold $\{j^{max}_{v=0}, j^{max}_{v=1}, \ldots\}$.

[b] $S(j'\ell' \leftarrow j\ell)$.

TEST 2: Li^+-CO

J = 25, odd parity

E = 1.95×10^{-3} hartree

Basis 1: {1}[a] 3 channels

Basis 2: {3} 10 channels

Basis 3: {6} 22 channels

For basis 1,

$$P_i = |S(1,26 \leftarrow 0,25)|^2$$ [b]

$$P_e = |S(1,25 \leftarrow 1,26)|^2$$

For all others,

$$P_i = |S(2,23 \leftarrow 0,25)|^2$$

$$P_e = |S(2,23 \leftarrow 2,23)|^2$$

RESULTS:

Basis	P_i	P_e	t,sec	N
1	4.003×10^{-1}	4.886×10^{-1}	2.63	7100
2	4.372×10^{-3}	2.238×10^{-1}	12.13	7100
3	1.753×10^{-2}	3.778×10^{-1}	75.83	7100

[a] This notation gives the maximum rotor state in each vibrational manifold $\{j^{max}_{v=0}, j^{max}_{v=1}, \ldots\}$.

[b] $S(j'\ell' \leftarrow j\ell)$.

TEST 4: $e^- - N_2$

J = 5, odd parity

E = 30 eV = 1.1025 hartree

Basis 1: $\{2\}^a$ 4 channels

Basis 2: $\{6\}$ 15 channels

Basis 3: $\{8\}$ 21 channels

Basis 4: $\{10\}$ 27 channels

$$P_i = |S(2,3\leftarrow 0,5)|^{2b}$$

$$P_e = |S(2,3\leftarrow 2,3)|^2$$

Basis	P_i	P_e	t,sec	N
1	4.387×10^{-3}	9.922×10^{-1}	0.07	189
2	2.914×10^{-3}	6.344×10^{-1}	0.92	189
3	2.876×10^{-3}	5.534×10^{-1}	2.16	189
4	2.870×10^{-3}	5.178×10^{-1}	4.26	189

[a] This notation gives the maximum rotor state carried in each vibrational manifold, $\{j^{max}_{v=0}, j^{max}_{v=1}, \ldots\}$.

[b] $S(j'\ell'\leftarrow j\ell)$.

Applications of Integral Equations With Reference Potentials To the NRCC Close-Coupling Test Problems (INSCAT)

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There have been two major changes in the integral equation code INSCAT since its description in the proceedings of the NRCC workshop on algorithms and computer codes held at Argonne in June, 1979. The first change involved the addition of a Newton-Cotes closed integrator (trapezoid rule), and the second involved replacing the original step size selection algorithm using perturbation methods with one that is based on the gradient of the potential. Both of these changes were made with the idea of improving the efficiency of the code.

As of this writing, the revised code is still being tested, and an accurate assessment of the effect of the modifications is difficult. Because one purpose of this workshop was to compare the efficiency of various algorithms, the results reported here used only a very few steps with the Newton-Cotes algorithm, with most of the integration carried out with the reference potential integrator. Comparison of the timing histograms for this code and the Sams-Kouri integrator will provide the user with sufficient information to allow optimal switching between algorithms.

The $He-H_2$ problem, Test 1, proved difficult for this method, particularly for the two channel basis, J4B1. The first few runs resulted in inelastic probabilities varying over a range of several orders of magnitude with small changes in integration parameters. The difficulty in converging this very small probability led to the abandonment of the original step-size algorithm in favor of the simple expression $H_{i+1} = T\ (\nabla V_i)^{1/3}$. With this selector the step sizes varied smoothly from step to step for this problem and it was possible to converge the result. Initial and final values of "R" were 2.25 and 16.5 bohrs, for all basis sets. Convergence of the larger basis sets was considerably easier than the two channel basis.

The change in step size selector was detrimental for Test 2, as previous experience with the reference potential method has shown that much larger steps can be taken for larger"R" than were allowed by the present step size algorithm. It seems at this time that the previous algorithm might lead to more efficient integration for long-range potentials and relatively large transition probabilities. This will be tested in the near future. The relevant information for Test 3 is contained in the timing histograms for Test 2. Integration for Test 2 was started at $R = 3a_0$ and carried out for 500 a_0, with the tolerance parameter Tset at 0.12.

Test 4 was relatively straightforward. The integration range was 0.02 to 75 bohrs, with an initial step size of 0.007. The tolerance parameter "T" was set at 0.12.

The current version of the program is satisfactory for many applications, but it could be improved by using a more sophisticated method of selecting the step size. It should be possible to use one selector at large "R" and the present one at small "R".

The current program is highly portable, and has been run on CDC, UNIVAC, IBM, AND VAX computer systems. Input is straightforward, and it is relatively easy to change potentials. This method does not diagonalize the interaction matrix, and is rather efficient at the first energy, although it loses ground to other methods at subsequent energies. It should be most attractive in applications to energy dependent potentials.

Application of the Gordon Algorithm to Test Problems in Ro-Vibrationally Inelastic Molecular Collisions (GORDON)

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As discussed in our contribution[1] to the proceedings of the first NRCC Workshop on Algorithms and Scattering Codes for Atomic and Molecular Scattering Theory our intention was the acceleration of the Gordon code[2-4] by elimination of the determination of the first order perturbation corrections to the linear reference potential. In the modified code, described previously and denoted QCOL/MK2,[1] the step sizes were determined from an analysis of the coupling potential matrix. For some of the test problems, notably TEST4 and TEST1, the step-size algorithm[1] proved to be unreliable in that the accuracy of the S-matrix was not a consistent function of the input tolerance parameters. Moreover, even for TEST2 and TEST3, where QCOL/MK2 appeared to work best, the times were greater than or at best equal to those for a subsequent code, denoted QCOL/NEWFLAT.

In the latter we decided to return anew to the original algorithm[2-3] which uses the first order perturbation corrections to predict the step size for the next interval. However, in keeping with our desire to minimize the time required for the initial energy calculation, we modified the original Gordon code[4] so that only the off-diagonal perturbation corrections were computed. In our experience the largest off-diagonal corrections, which arise from terms linear in the expansion of the potential matrix about the midpoint of each interval, are consistently larger than the largest diagonal corrections, which arise only from the quartic and higher order terms in this expansion.[3] An additional gain in computer time was achieved by determining the off-diagonal perturbation corrections

using the simpler formulas for solutions based on a constant reference potential (Subroutine FLAT[4]). The error so introduced is unimportant, since in our modified code the perturbation corrections are used only in the step size determination. In particular these corrections are *not* added on to the zeroth order solutions for the diagonalized potential. Thus the modified code performs only zeroth-order calculations,[3] even at the initial energy. The usage of this modified code, denoted QCOL/NEWFLAT, is described in detail in the program documentation.

Since the NEWFLAT code is a low-order method,[3] the global rate of convergence of the S-matrix is expected to be proportional only to a low power of the step size, or equivalently, inversely proportional to a low power of the number of steps. At the BASIS1 and BASIS2 level we carried out for each test problem an investigation of the convergence of the S-matrix as a function of the number of steps, which can be varied by changing the input tolerance parameter TOLHI.[4] From this study we have found that the relative accuracy of the particular S-matrix elements which were the subject of the workshop comparison between various scattering codes could be fit reasonably well with the functional dependences listed in Table 1. The low order of the present method is particularly apparent for TEST2, TEST3, and TEST4 where large off-diagonal coupling exists due to strong anisotropies in the potential.

By examining the output of each run, one can easily determine the number of steps in a given integration range. This value can be used to obtain discretized values of the "integrator velocity",

dt/dr, which is the direct measure of the speed of the scattering code as a function of the center-of-mass separation between the collision partners. Specifically, we have

$$dt/dr\,|_{r=r_i} = \frac{N_i\, t_{tot}}{2N_{tot}\,\Delta r_i}$$

where N_i is the number of steps required to cover the range $r_i - \Delta r_i$ to $r_i + \Delta r_i$, and N_{tot} and t_{tot} denote the total number of steps and the total time required for the scattering calculation. The values of dt/dr so obtained are plotted in Fig. 1 for the four TEST problems at the BASIS3 level. As one would expect for the present method, the integration proceeds fastest at large distances where the potential is slowly varying.

The comparison[5] with other scattering codes performed at this workshop indicates that although the present method requires the fewest evaluations of the potential matrix, it is by no means the fastest. There are several factors which may contribute to this relative slowness. First, the gain in time achieved by the simplification in the calculation of the perturbation corrections does not compensate for the inaccuracy introduced by the neglect of these corrections in the zeroth-order solution propagation. Secondly, all of the matrix operations are performed using sophisticated algorithms, chosen especially for their numerical stability.[2,3] It may well be that most typical problems in molecular collisions are stable enough that a large degree of computational overhead could be eliminated by the use of considerable faster and simpler, albeit less stable, matrix algorithms.[6]

In all fairness, the reader should recognize that in the

original Gordon code[4] the first-order perturbation corrections are computed fairly exactly using a linear reference potential[3] and are then added to the propogated zeroth-order solutions. Thus, in principle, the first criticism in the preceeding paragraph would not apply to the original Gordon code. Unfortunately, we were unable to integrate the test problems TEST1 and TEST2/3 with this code (TEST4 was not attempted). Typically, due probably to the hyperexponential behavior of the Airy functions in the classically forbidden region, one of the perturbation corrections would suddenly become abnormally large. This would then result in a predicted step size so small that the calculation would grind to a halt.

It is also worth stating that in our experience and as one might expect from mathematical considerations[2,3] the Gordon algorithm and code is truly suited for high energy collisions dominated by long-range forces where the de Broglie wavelengths are much shorter than the range of the potential. This situation would arise, for example, in ion-molecule and polar molecule collisions at hyperthermal energies (0.5 - 2 eV).[7,8] For this type of problem typically only $\sim$20 integration steps are required to determine a reliable S-matrix. Unfortunately, this collision regime was not explored by the NRCC workshop test problems.

We close with some more general conclusions and observations. Gordon's method[2,3] provides an innovative approach to the solution of the close-coupling equations for inelastic collisions which is based on approximation of the potential rather than the wavefunction. Improvements to the method, both in terms of speed, stability, or

accuracy can be achived in three possible ways:

1) Development of the efficient generation of solutions to quadratic reference potentials (Weber Functions)[9] and development of new algorithms and codes for the stable computation of first-order perturbation corrections using Airy[10] and/or Weber functions.[9] This approach will presumably result in an higher degree of accuracy with a fewer number of integration steps.

2) Reduction in the computation time, albeit at the expense of accuracy, by simplifying the determination of step sizes and by ignoring all the perturbation corrections to the propagated solutions. This is the approach we have followed in the development of the QCOL/MK2[1] and QCOL/NEWFLAT codes.

3) Achievement of higher-order convergence by computing zeroth- and first-order solutions by accurate propagation using constant reference potentials over a relatively dense grid of steps. The diagonalization of the potential matrix is carried out on a coarser grid. This is the approach developed by Parker, Schmalz and Light[11] and is equivalent to modification (1) above. However, the solution propagation and determination of perturbation corrections is done using the simple and numerical stable formulas appropriate to the constant reference potential solutions.

Although the workshop study has been restricted to only four test problems and although the recent versions of approach (1) were not tested, we have to conclude that approach (3) offers a very attractive combination of simplicity, speed, and accuracy.

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6. As an example of this, all the matrix inversions in the log-derivative method of B. R. Johnson (this volume, p. 47) are performed using classical Gaussian elimination without pivoting.

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10. A. Rosenthal and R. G. Gordon, J. Chem. Phys. 64, 1621 (1976).

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Table 1. Convergence of S-matrix elements; QCCL/NEWFLAT.

Problem	S-matrix element v j ℓ	v' j' ℓ'	$\lvert S-S_{exact}\rvert/\lvert S_{exact}\rvert$
TEST1/J4B2	0 4 4	1 4 4	$1.15\cdot10^{5}\ N^{-2.34}$
TEST2/J25B1	0 25	1 24	$946\ N^{-1.5}$
TEST3/J25B2	0 5	2 23	$10.3\ N^{-1.37}$
TEST3/J5B2	0 5	2 3	$5.8\ N^{-1.37}$
TEST4/J5B2	0 5	2 3	$5.0\ N^{-1.02}$

a) Variation with the number of steps of relative error in indicated S-matrix element. The indicated proportionalities apply over a range in relative errors of 0.005-0.5.

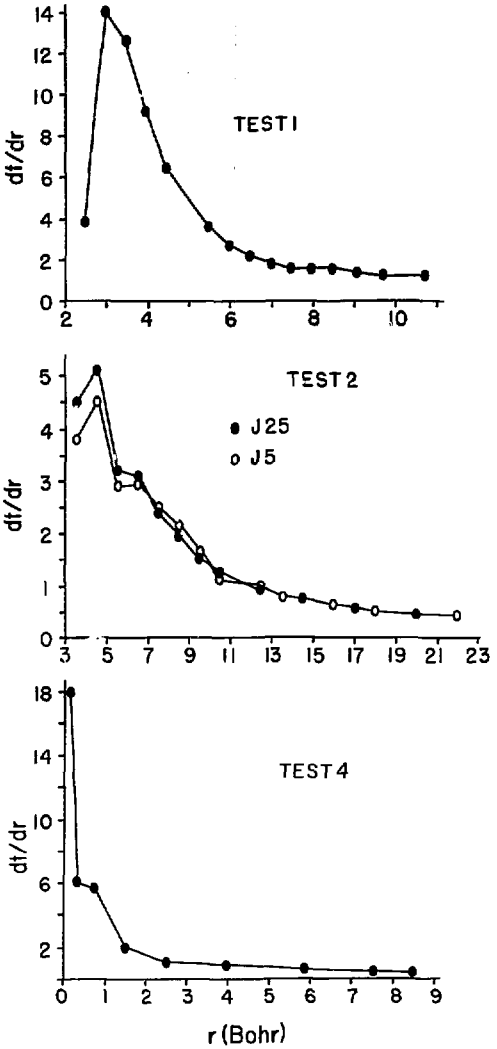

Fig. 1.

A Variable Interval Variable Step Method for the Solution of Linear Second Order Coupled Differential Equations (VIVS)

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Modifications and Discussion of Results

The only modifications to the variable interval variable step method as given in the earlier NRCC workshop report are in the determination of the interval and step sizes.

Since this method is a potential following method the largest intervals are taken where the potential is relatively flat, the coupling relatively constant, and/or the energy is high. We have found that the best way of controlling the interval size is to look directly at the perturbation corrections to the wavefunction and its derivative. Since we want perturbation theory to be valid it is necessary to keep the perturbative correction small compared to the maximum magnitude of the unperturbed quantities. With the choice of a constant reference potential within each step the largest perturbative corrections are proportional to the cube of the interval length (had we used Airy functions or Weber functions the off-diag corrections are still proportional to the cube of the interval length). Therefore we predict the length of next interval ℓ_{i-1} using

$$\ell_{i+1} = \left\{ \frac{\epsilon}{MAX\left[|\Delta g_1^i/\bar{g}_1^i|, |\Delta g_2^i/\bar{g}_2^i|, |\Delta g_1^{i\prime}/\bar{g}_1^{i\prime}|, |\Delta g_2^{i\prime}/\bar{g}_2^{i\prime}| \right]} \right\}^{1/3} \ell_i$$

where the Δg's are the calculated perturbation corrections for interval i, the bar above the zeroth order solutions indicates the maximum magnitude of the solution over the interval and ϵ is an input tolerance parameter controlling the error in the solutions. Since we have included first order perturbation corrections and the second order perturbation corrections are roughly proportional to the square of these, our experience has shown that the error in the final S-matrix elements is roughly proportional to ϵ^2.

Step sizes are somewhat more difficult to determine since we want a fixed interval size. An approach that we have used is to have a fixed number of steps, N_s, per interval and determine the step size within an interval based on a geometric progression. The length of the first step within the interval is

$$h_1 = \begin{cases} \ell_i \left[\frac{1-\alpha_i}{1-\alpha_i^{N_s}}\right] & \alpha_i \neq 1 \\ \ell_i / N_s & \alpha_i = 1 \end{cases}$$

and the length of step s is

$$h_s = \alpha_i h_{s-1} = h_1 \alpha_i^{s-1}$$

The optimum α_{i+1} is one that would result in the same maximum perturbation correction for each step. The errors for each step in interval i can thus be used to predict α_{i+1} for interval i+1. We therefore determine the geometric progression parameter α_{i+1} from a linear least squares fit to the perturbations corrections for interval i, i.e.,

$$\alpha_{i+1} = \begin{cases} \alpha_i \left[\frac{\bar{\epsilon}_o + \ell_i \bar{\epsilon}_1}{\bar{\epsilon}_o}\right]^{1/3(N_s-1)} & N_s > 1 \\ 1 & N_s = 1 \end{cases}$$

where $\bar{\epsilon}_0$ and $\bar{\epsilon}_1$ are coefficients of the constant and linear term, respectively, for a best fit to the maximum perturbation errors for the steps. The least squares fitting procedure gives

$$\bar{\epsilon}_1 = \frac{(\sum_s h_s)(\sum_s \epsilon_s) - N \sum_s h_s \epsilon_s}{(\sum_s h_s)^2 - N \sum_s h_s^2}$$

and

$$\bar{\epsilon}_o = \frac{1}{N}\left[\sum_s \epsilon_s - \bar{\epsilon}_1 \sum_s h_s\right]$$

wnere ϵ_s is the maximum magnitude of the perturbation corrections for step s in interval i.

For all the test problems we used the default input parameters and adjusted only the starting and ending position of the integration ranges as well as the initial interval size. This gave satisfactory accuracy for all test cases except TEST 1 where it was necessary to reduce the input tolerance parameter ϵ governing the interval sizes. The starting and ending positions for each of the test cases are as follows: TEST 1 (RMIN = 2.3 a_0, RMAX = 40 a_0), TEST 2-J5 Basis sets (RMIN = 3.3 a_0, RMAX = 700 a_0), TEST 2-J25 Basis sets (RMIN = 3.3 a_0, RMAX = 5000 a_0), TEST 3 (RMIN = 3.3 a_0, RMAX = 7.0 a_0), and TEST 4 (RMIN = 0.15 a_0, RMAX = 160 a_0). The potential was evaluated much more often than necessary for ease of implementation of the test problems. The current program obtains the answers reported herein and requires only 3/8 the number of potential evaluations.

Although we are quite happy with our trial test times on subsequent energies there were several inefficiencies in the computer program which have now been eliminated. The incorporation of more efficient FORTRAN mathematical routines for matrix multiplication, solution of linear systems of equations and the evaluation of perturbation corrections have increased the efficiency of the program. With these new routines the first and subsequent energy timings can be multiplied by roughly a factor of .7. Currently the evaluation of the perturbation integrals is probably still the most inefficient part of the code. However, as the number of coupled channels increase the evaluation of these integrals becomes a smaller fraction of the total computer time used. However, even for the largest number of channels used in the test problems (N = 32) the evaluation of these perturbation integrals required a substantial fraction of the total computation time ($\sim$25% for subsequent energies). The method of matrix diagonalization that we are currently using is also probably not optimal and a more efficient algorithm could help

considerably. At the first energy the majority the computer time is used in transforming the potential into the local basis (~30%) and in the diagonalization of the potential energy matrix at the midpoint of the interval (~20%).

Speculations

Although our results demonstrate that this approach succeeds admirably in increasing the accuracy while reducing the number of matrix operations required for scattering problems, we may speculate on the further improvements. The present method has a large overhead at the first energy (primarily in transforming the potential and derivative matrices at each step). In common with all other quasi-adiabatic basis methods it must also take small intervals where the potential matrix is rapidly varying, even in the non-classical regions.

This suggests two changes in the algorithm. To reduce the potential transformation overhead at the first energy, it would proably be advantageous to evaluate the Taylor series expansion of the potential at fewer points than at every step. One requires that the potential matrix be accurately represented at each step but the current practice of evaluating and transforming $V(R_s)$, $V'(R_s)$, $V''(R_s)$ at each step, requiring 4.5 N_s matrix multiplications per step at the first energy may be overkill.

The second problem, small steps and intervals in (typically) the non-classical repulsive region, might be overcome by the use of a different sort of algorithm. In this region the potentials are typically varying more rapidly than the wavefunctions, and a high order numerical (nonpropagation) method would seem advantageous. Since the renormalized Numerov derivative methods are high order, require only 3 matrix inversions (which are symmetric matrices) per step and produce the log derivative matrix (R^{-1}), a hybrid using these two methods would seem to be optimal.

Noting the success of Johnson log-derivative method we have incorporated this later modification into the program and succeeded in substantially reducing the computational time for both the first energy and subsequent energy calculations. Preliminary tests using this modification on the Lester-Berstein 9-state rigid rotor problem indicate that the timing for the first energy can be multiplied by a factor of $\sim$.5 and subsequent energy times can be multiplied by a factor of $\sim$.7. These are in addition to the savings mentioned before which implies that the current program is nearly 3 times as fast for the first energy and 2 times as fast for subsequent energies as that reported for the test results reported herein.

Portability and Use

The integrator portion of the program is quite easy to use and is highly portable having basically 6 parameters (RMIN, NSTEPS, RSWTCH, RMAX, TOFF, DRFRST) that are necessary for its efficient use. The second and third parameters are only necessary if both the Johnson log-derivative and variable interval variable step methods are used simultaneously. Test runs have been made on the CDC 7600, IBM 370, and VAX 11/780 requiring only minor modifications for its implementation on the VAX 11/780 (replacement of the input namelist statements).

TABLE I: Test 1 (J4B3)

	# Intervals = ΔN_i	R_i	ΔR_i	F_1[a]	F_2[a]
2.300 → 2.863	5	2.58	.563	1.64	.417
2.863 → 3.209	5	3.04	.346	2.66	.678
3.209 → 3.430	5	3.32	.221	4.17	1.06
3.430 → 3.613	5	3.52	.183	5.04	1.28
3.613 → 3.815	5	3.71	.202	4.56	1.16
3.815 → 4.249	5	4.03	.434	2.12	.541
4.249 → 4.597	5	4.42	.348	2.64	.674
4.597 → 5.522	5	5.06	.925	.996	.253
5.522 → 12.73	5	9.13	7.208	128	.0326
12.73 → 40.00	4	26.37	27.27	.0270	.00689

[a] $F_1 = \frac{t_1 \Delta N}{N_{TOT} \Delta R}$ and $F_2 = \frac{t_2 \Delta N}{N_{TOT} \Delta R}$ where $t_1 = 9.03$ and $t_2 = 2.03$ are the total times for the first energy and subsequent energies, respectively, and $N_{TOT} = 49$ is the total number of intervals.

TABLE II: Test 2 (J583)

	# Intervals = ΔN_i	R_i	ΔR_i	F_1[a]	F_2[a]
3.300 → 4.237	13	3.77	.937	1.62	.410
4.237 → 7.530	13	5.88	3.293	.460	.117
7.530 → 16.80	13	12.17	9.27	.164	.0414
16.80 → 31.53	13	24.17	14.73	.103	.0261
31.53 → 60.78	13	46.16	29.25	.0519	.0131
60.78 → 104.2	13	82.49	43.42	.0349	.00884
104.2 → 160.4	13	132.3	56.2	.0270	.00683
160.4 → 225.9	13	193.2	65.5	.0232	.00586
225.9 → 301.6	13	263.8	75.7	.0200	.00507
301.6 → 381.7	13	341.7	80.1	.0189	.00479
381.7 → 475.7	13	428.7	94.0	.0161	.00408
475.7 → 580.4	13	528.1	104.7	.0145	.00367
580.4 → 700.0	13	640.2	119.6	.0127	.00321

[a] $F_1 = \frac{t_1 \Delta N}{N_{TOT} \Delta R}$ and $F_2 = \frac{t_2 \Delta N}{N_{TOT} \Delta R}$ where $t_1 = 19.72$ and $t_2 = 4.99$ are the total times for the first and subsequent energies, respectively, and $N_{TOT} = 169$ is the total number of intervals.

TABLE III: Test 2 (J25B3)

	# Intervals = ΔN_i	R_i	ΔR_i	F_1[a]	F_2[a]
3.30 → 3.578	3	3.44	.278	3.14	.821
3.578 → 3.831	3	3.70	.253	3.44	.902
3.831 → 3.927	3	3.88	.096	9.08	2.38
3.927 → 4.029	3	3.98	.102	8.55	2.24
4.029 → 4.206	3	4.12	.177	4.93	1.29
4.206 → 4.401	3	4.30	.195	4.47	1.17
4.401 → 4.581	3	4.49	.180	4.84	1.27
4.581 → 5.013	3	4.80	.432	2.02	.528
5.013 → 6.279	3	5.65	1.266	.688	.180
6.279 → 8.464	3	7.37	2.185	.399	.105
8.464 → 11.52	3	9.99	3.056	.285	.0747
11.52 → 17.49	3	14.51	5.97	.146	.0382
17.49 → 30.57	3	24.03	13.08	.0666	.0174
30.57 → 64.36	3	47.47	33.79	.0258	.00675
64.36 → 181.4	3	122.9	117.04	.00745	.00195
181.4 → 659.5	3	420.5	478.1	.00182	.000477
659.5 → 3000.0	3	2829.8	4340.5	.000201	.0000526

[a] $F_1 = \frac{t_1}{N_{TOT}} \frac{\Delta N}{\Delta R}$ and $F_2 = \frac{t_2}{N_{TOT}} \frac{\Delta N}{\Delta R}$ where $t_1 = 14.82$ and $t_2 = 3.88$ are the total times for the first energy and subsequent energies, respectively, and $N_{TOT} = 51$ is the total number of intervals.

TABLE IV: Test 4 (J5B3)

	# Intervals $= \Delta N_i$	R_i	ΔR_i	F_1[a]	F_2[a]
.15 → .6859	3	.418	.5359	1.56	.380
.6859 → .9874	3	.837	.3015	2.77	.675
.9874 → 1.211	3	1.10	.2236	3.74	.911
1.211 → 1.580	3	1.40	.369	2.27	.552
1.580 → 2.293	3	1.94	.713	1.17	.286
2.293 → 3.322	3	2.76	1.029	.813	.198
3.322 → 5.228	3	4.28	1.906	.439	.107
5.228 → 8.522	3	6.88	3.294	.254	.0618
8.522 → 16.59	3	12.56	8.068	.103	.0252
16.59 → 51.59	3	34.09	35.00	.0239	.00581
51.59 → 160.0	3	105.8	108.41	.00771	.00188

[a] $F_1 = \frac{t_2\ \Delta N}{N_{TOT}\ \Delta R}$ and $F_2 = \frac{t_2\ \Delta N}{N_{TOT}\ \Delta R}$ where $t_1 = 9.20$ and $t_2 = 2.24$ are the total times for the first energy and subsequent energies, respectively, and $N_{TOT} = 33$ is the total number of intervals.

The R-matrix Propagation Method with Continuous Perturbation Corrections (RMAT)

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All calculations were performed using the R-matrix method with all perturbation corrections through the second derivative included. The method was essentially unchanged from that described by John Light at the Argonne meeting. Only continuous perturbation corrections to the R-matrix were employed.

TEST1 was integrated from 1.7 bohr to 45 bohr. Quite a small value of the step size parameter (BETA = 0.1) was required to obtain adequate convergence. Although no difficulties were encountered in handling the very small transition probabilities of the problem, this seemed to be a particularly difficult problem for the program. As can be seen from the histograms, this problem was not as completely dominated by the hard wall part of the potential as the others.

TEST2 was integrated from 3.0 bohr to 2000 bohr. (Some J5 runs were begun at 3.2 bohr.) The J25 results show almost four figure agreement with the log derivative results, so these are probably very accurate. Moderate values of the step size parameter (BETA = 0.6-0.7) were required for convergence.

TEST3 was integrated from 3.0 bohr to 7.0 bohr. Only B1 and B3 of each J were integrated to check convergence. Times for B2 and B4 were taken from the TEST2 runs.

TEST4 was integrated from 0.1 bohr to 250 bohr. This, somewhat surprisingly, seemed to be the easiest problem for the method, requiring a step size parameter of only BETA = 0.8-1.0. From the histograms it can be seen that almost all the steps were spent at very small interparticle separation.

The method did not seem to suffer from irregular convergence, as has sometimes been found for other problems, but no detailed studies of this question were performed. Generally, the integration parameters were optimized on the B1 problems and used unchanged for the others.

All times accompanying computed S-matrices are first energy times. However, a second energy calculation is identical to one subsection of the first energy calculation so that second energy times could always be obtained from the output of a first energy calculation. They are generally 1/2 to 1/3 as great.

The times reported here are certainly not optimum for the method. The same can probably be said for most of the other methods used for these test problems, so that comparisons between methods may not change much, but the absolute times required for these problems can probably be reduced by a factor of two at least. The program used here had a FORTRAN dot product subroutine rather than an assembly language version and used the TRED2-TQL2 EISPACK diagonalization path, which is known not to be optimum. The matrix inversion routine is also not particularly efficient. Some time also could be saved by more efficient coding of the algebraically complex perturbation formulas.

The obvious way to improve the method is to pair it with an efficient method for integrating the steeply repulsive part of the potential wall. Because of the compatibility of information required, a likely choice would be the log derivative method. This should result in a significantly faster overall method.

The program as it now stands should be relatively transportable. It was written originally for an IBM system and then moved to the LBL CDC system. It should therefore be adaptable to most machines. When used on an IBM machine it should, however, be run in double precision.

AN L^2 APPROACH TO R-MATRIX PROPAGATION: FOLLOWUP REPORT

(L2RMAT)

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ABSTRACT

A hybridized R-matrix propagation program was used to solve the four test problems presented by the NRCC workshop on close coupling methods. The hybrid method used both the L^2 approach reported earlier and the analytic (constant reference potential) method. This report presents observations on the utility of the hybrid approach.

I. INTRODUCTION

In order to solve the test problems presented by the NRCC close coupling workshop, a program was written which combined the L^2 R-matrix propagation method discussed earlier[1] with the "standard" (analytic) R-matrix propagation technique.[2] The L^2 method is used to initiate the integration in the hard wall region of the potential, because it is independent of the potential variation within an R-matrix sector. We then switch over to the analytic method as the potential flattens out to take advantage of the cheaper (first energy) solution of the coupled equations in this region.

II. DISCUSSION

Because of the hybrid nature of the method used, it is significant to report in Table I the integration regions covered by each method for each of the test problems. The L^2 method is used in the interval from R_1 to R_2, and the analytic method is used from R_2 to R_3. The number of L^2 boxes is N_{BOX}, and the sector width of each box is $(R_2-R_1)/NBOX$. The analytic R-matrix propagation method is used from R_2 to R_3, and in this interval, N_{PROP} steps were taken. The L^2 method requires diagonalizing a matrix of size $N_D \times N_D$ once in each box at the first energy whereas the analytic method requires diagonalizing only a matrix of size $N_{CHAN} \times N_{CHAN}$ once each step at the first energy. Because these diagonalizations are not done after the first energy, the second energy timing is substantially faster than the first. The extremely large matrix which must be diagonalized in the L^2 region effectively limited the total number of coupled equations which could be handled by this program in SCM on the CDC 7600. For this reason, only the first three basis sets for each test problem were solved. The number of

translation functions associated with each coupled channel can be figured out from Table I as $N_{TF} = N_D/N_{CHAN}$.

A more detailed analysis of the timing for the hybrid method is presented in Table II for the third basis set of test problems 1,2a (J=5), 2b (J=25), and 4. These tables show clearly that the principal effort for this method is expended near the beginning of the integration region. For this reason, it is essential to remember to optimize the starting point (R_1 in Table I) of the integration when using this method. In all the problems used here, R_1 could have been made larger than it was, with a significant decrease in execution times. For example, in the 18-channel basis of test problem 1, fully one-third of the total execution time would have been eliminated by setting $R_1 = 2.5$ instead of $R_1 = 1.7$. With $R_1 = 2.5$, it is still possible to obtain between three and four significant figure accuracy in the S-matrix elements obtained. If I were to rerun all the test problems, this is the integration parameter I would most carefully optimize.

In the analytic R-matrix propagation portion of each problem, two parameters governed the selection of step size. One parameter is BSTEP, which chooses step sizes according to the rate of change of the trace of the coupling matrix,[2] and the other is CUPMAX, which limits step sizes by the rate of change of the locally adiabatic basis.[2] Only in the second test problem was CUPMAX set to a value which affected any of the step sizes. The effect can be seen in Table IIB in that more time was expended from $6a_o$ to $7a_o$ than on either side of this region. The step size algorithm used a very small value of STPMIN and a large value of STPMAX.

My experience with the step size algorithm based on BSTEP[2] has been that it tends to take too small a step in the hard wall region of the potential, when BSTEP is set so that proper step sizes are used in the long-range region of the potential. Once again, if I were to rerun the test problems, I would more carefully optimize (increase) the STPMIN parameter.

In conclusion, the test problems selected by the NRCC workshop on close coupling methods have fulfilled the criterion of presenting potentials which would be encountered in realistic research problems. The L^2/analytic hybrid method used here is not the optimal choice for these problems. The L^2 method needs further work to reduce, if possible, the effort expended at the first scattering energy. The program used is limited to fairly small systems of coupled equations because of computer core restrictions. The L^2 method seems also to get comparatively worse as the number of coupled channels increases.

A copy of the computer program used for these test problems is on file with the National Resource for Computation in Chemistry. The program is written entirely in FORTRAN; no special care was taken to ensure that only standard FORTRAN usage was employed, although there should be no difficulties using the program within a CDC environment. The primary source of difficulty in moving this program is likely to be with its usage of input through the NAMELIST format. Although NAMELIST is a standard FORTRAN construct, it frequently seems to be implemented in a nonstandard fashion. A set of documentation appropriate for using this program will be filed with the NRCC.

Table I. Integration Regions for the Hybrid R-matrix Method.

Problem	J_{TOTAL}	N_{CHAN}	N_D	N_{BOX}	N_{PROP}	$R_1(a_o)$	$R_2(a_o)$	$R_3(a_o)$	T_1(sec)	T_2(sec)
1	4	2	12	33	252	1.7	11.60	35	0.53	0.13
1	4	8	48	15	356	1.7	6.20	35	6.96	1.08
1	4	18	108	5	382	1.7	3.20	35	22.52	3.69
2(3)	5	3	18	5	950(170)	3.3	4.80	700(7)	1.51(0.40)	0.18(0.02)
2(3)	5	6	36	5	1029(168)	3.3	4.80	700(7)	4.51(1.41)	2.37(0.37)
2(3)	5	15	75	6	1296(271)	3.3	4.20	700(7)	41.42(14.04)	21.85(5.88)
2(3)	25	3	18	10	284(12)	3.3	6.20	700(7)	0.67(0.32)	0.56(0.12)
2(3)	25	10	60	7	544(53)	3.3	5.05	700(7)	9.67(4.70)	1.59(0.30)
2(3)	25	22	110	3	733(183)	3.3	3.90	700(7)	63.33(23.55)	14.14(3.15)
4	5	4	24	8	208	5.0(-6)	2.40	50	0.82	0.19
4	5	15	60	6	85	5.0(-6)	1.80	50	6.60	1.23
4	5	19	76	4	96	5.0(-6)	1.20	50	13.33	3.03

Table IIA. Details of Timing for Test Problem 1*

R_{left}	Interval(a_o) R_{right}	Method	N_{STEPS}	Total Time (sec)	Time/a_o (sec)
1.7	3.2	L^2	5	14.77(0.47)	9.85(0.31)
3.2	4.0	analytic	47	1.98(0.80)	2.48(1.00)
4.0	5.0	analytic	32	1.35(0.55)	1.35(0.55)
5.0	6.0	analytic	17	0.72(0.29)	0.72(0.29)
6.0	8.0	analytic	14	0.59(0.24)	0.30(0.12)
8.0	10.0	analytic	10	0.42(0.17)	0.21(0.09)
10.0	14.0	analytic	16	0.67(0.27)	0.17(0.07)
14.0	20.0	analytic	18	0.76(0.31)	0.13(0.05)
20.0	35.0	analytic	28	1.19(0.48)	0.08(0.03)

*Total L^2 time was 14.77(0.47) sec; total analytic time was 7.67(3.11) sec; 18 channels.

Table IIB. Details of Timing for Test Problem 2a*

Interval(a_o) R_{left}	R_{right}	Method	N_{STEPS}	Total Time (sec)	Time/a_o (sec)
3.3	4.2	L^2	6	6.71(0.25)	7.45(0.28)
4.2	5.0	analytic	73	1.95(0.78)	2.44(0.98)
5.0	6.3	analytic	127	3.39(1.36)	2.63(1.05)
6.3	7.3	analytic	100	2.67(1.07)	2.67(1.07)
7.3	8.4	analytic	100	2.67(1.07)	2.43(0.97)
8.4	9.8	analytic	100	2.67(1.07)	1.91(0.77)
9.8	11.7	analytic	100	2.67(1.07)	1.41(0.56)
11.7	14.3	analytic	100	2.67(1.07)	1.03(0.41)
14.3	18.2	analytic	100	2.67(1.07)	0.69(0.27)
18.2	25.2	analytic	100	2.67(1.07)	0.38(0.15)
25.2	51.6	analytic	100	2.67(1.07)	0.10(0.04)
51.6	142.8	analytic	100	2.67(1.07)	0.03(0.01)
142.8	700	analytic	196	5.23(2.10)	0.003(0.001)

*Total L^2 time was 6.71(0.25) sec; total analytic time was 34.60(13.87) sec; 15 channels.

Table IIC. Details of Timing for Test Problem 2b*

Interval(a_o) R_{left}	R_{right}	Method	N_{STEPS}	Total Time (sec)	Time/a_o (sec)
3.3	5.0	L^2	3	10.08(0.47)	16.80(0.79)
3.9	5.0	analytic	107	7.72(3.11)	7.02(2.82)
5.0	5.7	analytic	43	3.10(1.25)	4.43(1.78)
5.7	7.5	analytic	50	3.61(1.45)	2.01(0.81)
7.5	10.1	analytic	50	3.61(1.45)	1.39(0.56)
10.1	12.3	analytic	50	3.61(1.45)	1.64(0.66)
12.3	14.6	analytic	50	3.61(1.45)	1.57(0.63)
14.6	17.1	analytic	50	3.61(1.45)	1.44(0.58)
17.1	21.3	analytic	50	3.61(1.45)	0.86(0.35)
21.3	34.9	analytic	50	3.61(1.45)	0.27(0.11)
34.9	72.7	analytic	50	3.61(1.45)	0.10(0.04)
72.7	146.7	analytic	50	3.61(1.45)	0.05(0.02)
146.7	700	analytic	183	13.21(5.32)	0.02(0.01)

*Total L^2 time was 10.080(0.47) sec; total analytic time was 52.91(21.29) sec; 22 channels.

Table IID. Details of Timing for Test Problem 4*

R_{left}	Interval(a_o) R_{right}	Method	N_{STEP}	Total Time (sec)	Time/a_o (sec)
0	1.2	L^2	3	7.09(0.47)	5.91(0.39)
1.2	2.0	analytic	15	0.96(0.38)	1.12(0.48)
2.0	3.0	analytic	10	0.64(0.26)	0.64(0.26)
3.0	4.6	analytic	10	0.64(0.26)	0.41(0.16)
4.6	6.8	analytic	10	0.64(0.26)	0.29(0.12)
6.8	10.1	analytic	10	0.64(0.26)	0.19(0.078)
10.1	15.0	analytic	10	0.64(0.26)	0.13(0.052)
15.0	22.2	analytic	10	0.64(0.26)	0.088(0.035)
22.2	32.9	analytic	10	0.64(0.26)	0.060(0.024)
32.9	50.0	analytic	11	0.70(0.28)	0.041(0.016)

*Total L^2 time was 7.09(0.47) sec; total analytic time was 6.12(2.45) sec; 19 channels.

References

1. R. B. Walker and B. I. Schneider, "An L^2 approach to R-matrix propagation," Proceedings of the NRCC Workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory," Lawrence Berkeley Laboratory report LBL-9501 (1979) Vol. I, p.376. See also B. I. Schneider and R. B. Walker, J. Chem. Phys. 70, 2466 (1979).

2. E. B. Stechel, R. B. Walker, and J. C. Light, J. Chem. Phys. 69, 3518 (1978).

The Logarithmic Derivative, Variable-interval Variable-step Hybrid Method for the Solution of Coupled Linear Second Order Differential Equations (VIVAS)

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At the second meeting of the workshop the advantages of the LOGD method at short range and of VIVS at long-range became obvious. As described earlier by Johnson[1-3], the log-derivative method is essentially a stabilized wave-function following method in which the linear second order Schrödinger differential equation is transformed to a non-linear first order equation (Ricatti equation) for the matrix logrithmic derivative,

$$\underset{\approx}{Y}(x) = \underset{\approx}{\psi}'(x)\ \underset{\approx}{\psi}^{-1}(x).$$

The LOGD solution algorithm requires only 1.5 matrix inversions per step and is just a two term recurrence relation. Thus it is extremely simple and fast per step. The step size must be some fraction of the wavelength and the error is fourth order in the step size. As shown by the test problems (dt/dr plots), this method is effective in the non-classical region or wherever the potential is rapidly varying or the wavelength large.

The variable-interval variable-steps method of Parker et al.,[4,5] is a potential following method which basically uses piecewise constant approximations to the potential, generates diagonal zeroth order solutions over a step and corrects these solutions over the steps in an interval by perturbation theory. Again, as shown by the test problems, it is very effective whenever the potential is slowly varying or the wavelength small. For small steps VIVS is also a fourth order method.

Figures 1-4 (pp. 33-36), showing dt/dr for test problems 1, 2, and 4, indicate that a hybrid code using LOGD at short distances and VIVS at large distances should be significantly faster than either. Since the LOGD method produces the log derivative matrix and VIVS propagates its inverse, the R-matrix, the Parker-Johnson (P-J) hybrid method was easily obtained by integrating with LOGD to a switchover point, inverting the log derivative matrix, transforming it to the

local diagonal basis, and continuing the propagation of the R-matrix with VIVS. It should be noted that both methods are numerically stable.

Applications

The P-J hybrid code was checked out on the 9-state rigid rotor problem of Lester and Bernstein[6] and more detailed results will be published elsewhere. We found, however, that there is a relatively broad minimum for total computation time vs switchover point at a given level of accuracy.

Three of the test problems for this workshop were also run with the P-J hybrid code shortly after the second meeting. As can be seen from Table 4 (p. 25), the hybrid code at the second energy is significantly (approximately a factor of 2) faster than any other code tested, including both LOGD and VIVS. (This, however, is partially due to improvements in the VIVS code itself.) In these tests the switchover point was given as input, and only one step size was used in the LOGD region. Even in this form, however, the code performed extremely well.

There are two aspects of the current P-J hybrid code which can probably be improved. First, the LOGD portion could use a variable step size provided a simple algorithm can be determined to choose the largest step consistent with a given level of accuracy. Second, the choice of switchover point could probably be determined within the code, probably using the local wavelengths and their spatial derivatives as a guide. As it stands now, however, the hybrid code leaves these decisions in the hands of the user.

References

1. B. R. Johnson, J. Comp. Phys. 13, 445 (1973).

2. B. R. Johnson, J. Chem. Phys. 67, 4086 (1977).

3. B. R. Johnson, "The Log Derivative and Renormalized Numerov Algorithms," proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory", Lawrence Berkeley Laboratory Report LBL-9501 (1979), Vol. I, p. 86.

4. G. A. Parker, T. G. Schmalz, and J. C. Light, J. Chem. Phys. (accepted for publication).

5. G. A. Parker, T. G. Schmalz, and J. C. Light, "A Variable Interval Variable Step Method for the Solution of Linear Second Order Coupled Equations," proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory," Lawrence Berkeley Laboratory Report LBL-9501 (1979), Vol. I, p. 172.

6. W. A. Lester, Jr., and R. B. Bernstein, J. Chem. Phys. 48, 4868).

SECTION V

WORKSHOP RECOMMENDATIONS TO THE NRCC

Discussions at the second meeting of the workshop yielded a number of suggestions for the NRCC to consider for future activity in the area of quantum mechanical scattering calculations. These fall into two categories — 1) recommendations for implementation of the results of this workshop and 2) recommendations for longer term projects for the advancement of the field.

In the first category we would recommend the following:

1) Adopt a combined Johnson(LOGD) - Parker(VIVS) program (see VIVAS test results) for documentation, further testing, optimization and distribution as a "support level A" NRCC software library code.

2) Incorporate this code into a more complete scattering program such as MOLSCAT.

3. Optimize this and perhaps other workshop codes for use at LBL with assembly language routines.

In the second category we recommend that the NRCC undertake several low-level, long-term projects.

1) Testing and code development by the external scientific community

   a. Starting from the current set of test problems, develop a standard set of test problems with exact answers and performance tables for all available codes.

b. Encourage the scientific community to try any new or improved methods on this standard set of problems and to contribute to the NRCC documented versions of any codes with significant advantages.

c. Invite the scientific community to contribute new and significantly different test problems to the NRCC in the appropriate format and with appropriate documentation.

2) Service to the user community

a. Make available to the user community documented versions of all the codes used in this workshop.

c. Collect a library of potential programs; for example, a flexible DIM package.

d. Collect and maintain a library of standard scattering modules or "tools." A suggested list of such modules is:

1. Matching of wavefunctions to boundary conditions.
2. Interconversion among the log derivative, R-, K-, and S-matrices
3. Clebsch-Gordan coefficients and 3-j, 6-j, and 9-j symbols
4. Bessel functions for high angular momentum
5. Rotation matrices
6. Programs for specific problems such as atom-diatom collisions
7. Programs for expanding a 3-dimensional potential energy surface in Legendre polynomials
8. Generators for lists of quantum numbers for specific problems
9. Generators for potential matrix elements from a list of quantum numbers

10. Optimized matrix algebra programs for symmetric, diagonally-dominant matrices
11. Versatile differential and integral cross-section programs for computing total, rotationally averaged and fully state-selected (m - dependent) cross sections
12. Transformation of cross sections from the center-of-mass to the laboratory frame of reference

SECTION VI

SUMMARY

This workshop has succeeded in bringing up 11 different coupled equation codes on the NRCC computer, testing them against a set of 24 different test problems and making them available to the user community. These codes span a wide variety of methodologies, and factors of up to 300 were observed in the spread of computer times on specific problems. A very effective method was devised for examining the performance of the individual codes in the different regions of the integration range. Many of the strengths and weaknesses of the codes have been identified. Based on these observations, a hybrid code has been developed which is significantly superior to any single code tested. Thus, not only have the original goals been fully met, the workshop has resulted directly in an advancement of the field.

All of the computer programs except VIVS are available upon request from the NRCC. Since an improved version of VIVS is contained in the hybrid program, VIVAS, it was not made available for distribution. The individual program LOGD is, however, available. The program names in the NRCC software library are identical to those in Table 1 (p. 22). Each library program has documentation on its use, a test input file and a listing of the output generated by that input file.

In addition, programs which compute the potential energy matrices of the test problems are also available. The software library names for Tests 1, 2 and 4 are HEH2, LICO, and EN2, respectively.

APPENDIX A

Selected S-matrix Information From All Tests and Methods

This appendix lists information from all of the S-matrices saved on tape during the workshop. The column headings are:

COUNT	- the number of potential evaluations.
TIME	- the computer time in seconds.
(I, F)	- the squared magnitude of the S-matrix element for the initial (I) and final (F) states specified in Table 2, page 23
RE(I, F)	- real part of the above S-matrix element.
IM(I, F)	- imaginary part of the above S-matrix element.
(I, I)	- squared magnitude of the elastic S-matrix element in the Channel I.
(F, F)	- squared magnitude of the elastic S-matrix element in the Channel F.

The results for the different tests are separated by the test name, the numerical values of I and F and the values of r_{min} and r_{max} used for the run reported in Tables 3-6, pages 24-27.

Many of the runs reported in this appendix were experimental and all of the input parameters for each run are not readily available. Some specific comments, when appropriate, will precede the results for each method.

The Variable-Order, Variable-Stepsize Predictor-Corrector Method (PC)

L. D. Thomas

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	2.500	, 45.00)
3116	1.57	.9167E-10	.6690E-05	-.6849E-05	1.000	1.000
2699	1.34	.9167E-10	.6690E-05	-.6849E-05	1.000	1.000
TEST1/J4B2		(I,F)=(1, 5)		(RMIN,RMAX)=(	2.500	, 45.00)
3954	22.53	.1681E-08	.2422E-04	.3308E-04	.4917	.9551
3326	18.90	.1681E-08	.2422E-04	.3308E-04	.4917	.9551
2771	15.31	.1681E-08	.2422E-04	.3309E-04	.4917	.9551
TEST1/J4B3		(I,F)=(1,15)		(RMIN,RMAX)=(	2.500	, 45.00)
4005	105.74	.1184E-08	-.5391E-05	.3398E-04	.4699	.9551
3544	92.07	.1184E-08	-.5391E-05	.3398E-04	.4699	.9551
2996	75.64	.1184E-08	-.5393E-05	.3398E-04	.4699	.9551
TEST1/J4B4		(I,F)=(1,20)		(RMIN,RMAX)=(	2.500	, 45.00)
4180	350.56	.1112E-08	.1245E-04	.3094E-04	.4702	.9547
3745	308.93	.1112E-08	.1245E-04	.3094E-04	.4702	.9547
3181	256.45	.1112E-08	.1244E-04	.3094E-04	.4702	.9547
TEST2/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000	, 150.0)
4895	4.30	.4073	.3670	.5221	.1404	.4920
4005	3.53	.4073	.3682	.5212	.1405	.4920
3329	2.83	.4055	.3723	.5166	.1412	.4926
2588	2.13	.4058	.1238	.6249	.1364	.4887
2113	1.68	.5369	-.6513	-.3357	.1229	.4766
TEST2/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000	, 150.0)
6174	43.41	.5903E-02	-.6938E-01	-.3301E-01	.7857	.2289
5140	34.62	.5904E-02	-.6939E-01	-.3299E-01	.7857	.2289
4295	28.21	.5911E-02	-.6950E-01	-.3287E-01	.7858	.2289
3497	22.21	.5899E-02	-.6971E-01	-.3224E-01	.7852	.2292
2819	17.18	.5643E-02	-.5375E-01	-.5248E-01	.7709	.2308
TEST2/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000	, 150.0)
7007	276.47	.2036E-01	.8650E-01	-.1135	.7293	.3775
5991	229.22	.2036E-01	.8650E-01	-.1135	.7293	.3776
5025	187.48	.2036E-01	.8646E-01	-.1135	.7293	.3776
4243	154.58	.2033E-01	.8602E-01	-.1137	.7293	.3776
3388	121.63	.2024E-01	.8710E-01	-.1125	.7295	.3775
TEST2/J25B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000	, 150.0)
5881	603.10	.3755E-01	.2680E-01	.1919	.6775	.4769E-01
TEST2/J5R1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000	, 150.0)
1653	1.44	.2253	-.1809E-01	.4743	.4949	.3690
1423	1.21	.2253	-.1792E-01	.4743	.4950	.3690
1168	.98	.2238	-.1619E-01	.4728	.4950	.3691
932	.76	.2199	-.4977E-01	.4663	.4868	.3654
702	.55	.6233	-.3276	.7184	.4235	.3394
TEST2/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000	, 150.0)
2112	5.18	.1777E-01	-.5442E-02	-.1332	.4344	.1948E-01
1687	4.11	.1777E-01	-.5449E-02	-.1332	.4343	.1948E-01

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
1489	3.44	.1768E-01	-.5777E-02	-.1328	.4354	.1947E-01
1147	2.59	.1734E-01	-.4524E-02	-.1316	.4350	.1947E-01
913	1.99	.2326E-01	.2647E-01	-.1502	.4325	.1955E-01
TEST2/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	150.0)
3068	45.82	.1025E-01	.9863E-01	.2296E-01	.8300	.2905
2527	36.96	.1026E-01	.9864E-01	.2295E-01	.8300	.2905
2298	31.95	.1025E-01	.9862E-01	.2286E-01	.8300	.2905
1854	25.70	.9661E-02	.9500E-01	.2521E-01	.8306	.2902
1560	20.60	.1174E-01	.1036	.3173E-01	.8270	.2907
TEST2/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	150.0)
3896	233.12	.1465E-01	.1138	.4124E-01	.9251	.1366
3270	189.49	.1465E-01	.1138	.4123E-01	.9251	.1366
2842	160.07	.1466E-01	.1138	.4120E-01	.9251	.1366
2406	132.27	.1460E-01	.1136	.4108E-01	.9251	.1366
2075	110.56	.1465E-01	.1118	.4621E-01	.9252	.1369
TEST3/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	7.000)
619	.52	.4727	-.2816	-.6272	.4193E-01	.3293
526	.43	.4727	-.2816	-.6273	.4193E-01	.3293
439	.35	.4732	-.2821	-.6274	.4189E-01	.3293
355	.28	.4761	-.2855	-.6281	.4066E-01	.3272
308	.23	.4470	-.3333	-.5795	.4326E-01	.3255
TEST3/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
935	5.81	.1710	-.3951	.1219	.3965	.2026E-01
804	4.76	.1710	-.3951	.1219	.3965	.2026E-01
695	4.00	.1709	-.3951	.1220	.3965	.2026E-01
564	3.11	.1708	-.3943	.1237	.3968	.2064E-01
481	2.57	.1728	-.3921	.1379	.4000	.2363E-01
TEST3/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
1162	41.86	.6569E-01	-.2300	-.1131	.3694	.3118
1022	36.32	.6569E-01	-.2300	-.1131	.3694	.3118
827	28.70	.6569E-01	-.2300	-.1131	.3694	.3118
740	24.90	.6568E-01	-.2300	-.1131	.3694	.3118
595	19.48	.6562E-01	-.2299	-.1129	.3695	.3120
TEST3/J25B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
1169	116.33	.6266E-02	-.8239E-02	.7873E-01	.1283	.2901E-01
968	94.67	.6268E-02	-.8242E-02	.7874E-01	.1283	.2901E-01
835	79.40	.6269E-02	-.8251E-02	.7875E-01	.1283	.2900E-01
TEST3/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	7.000)
604	.50	.4185E-01	.1186	.1667	.9099	.9575
519	.43	.4184E-01	.1186	.1667	.9100	.9575
434	.35	.4184E-01	.1187	.1666	.9101	.9576
357	.29	.4205E-01	.1188	.1671	.9102	.9576
286	.22	.3354E-01	.1113	.1454	.9258	.9652
TEST3/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
796	1.81	.2056	-.2517	.3772	.7005	.7646
645	1.45	.2056	-.2517	.3772	.7005	.7646
555	1.20	.2059	-.2516	.3776	.7001	.7644

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
485	1.00	.2058	-.2518	.3774	.7006	.7646
382	.77	.2036	-.2522	.3742	.7036	.7652
TEST3/J5B3		(I,F)=(1, 4)	(RMIN,RMAX)=(	3.000	, 7.000	)
1068	15.43	.1039E-02	-.1703E-01	-.2737E-01	.9207	.9497
879	12.49	.1039E-02	-.1703E-01	-.2737E-01	.9207	.9497
767	10.80	.1040E-02	-.1704E-01	-.2738E-01	.9207	.9497
641	8.79	.1039E-02	-.1699E-01	-.2740E-01	.9204	.9497
551	7.15	.9917E-03	-.1653E-01	-.2680E-01	.9214	.9498
TEST3/J5B4		(I,F)=(1, 4)	(RMIN,RMAX)=(	3.000	, 7.000	)
1221	71.05	.6097E-02	.6903E-01	.3649E-01	.9784	.9856
1030	58.61	.6097E-02	.6903E-01	.3649E-01	.9784	.9856
885	49.51	.6097E-02	.6903E-01	.3649E-01	.9784	.9856
805	43.04	.6095E-02	.6902E-01	.3649E-01	.9784	.9856
717	37.53	.6092E-02	.6901E-01	.3647E-01	.9784	.9856
TEST4/J5B1		(I,F)=(1, 2)	(RMIN,RMAX)=(	.1000E-01,	120.0	)
1353	1.75	.4330E-02	-.4844E-01	.4453E-01	.9956	.9923
1078	1.38	.4330E-02	-.4842E-01	.4455E-01	.9956	.9923
858	1.09	.4329E-02	-.4840E-01	.4457E-01	.9956	.9923
646	.79	.4326E-02	-.5015E-01	.4255E-01	.9956	.9923
520	.59	.4474E-02	-.6139E-01	.2654E-01	.9957	.9924
TEST4/J5B2		(I,F)=(1, 2)	(RMIN,RMAX)=(	.1000E-01,	120.0	)
2114	30.25	.2912E-02	-.3937E-01	.3691E-01	.9963	.6412
1612	23.08	.2912E-02	-.3937E-01	.3691E-01	.9963	.6412
1291	18.44	.2912E-02	-.3935E-01	.3693E-01	.9963	.6412
1022	14.48	.2913E-02	-.3933E-01	.3696E-01	.9963	.6411
737	10.19	.2904E-02	-.4155E-01	.3432E-01	.9963	.6414
TEST4/J5B3		(I,F)=(1, 2)	(RMIN,RMAX)=(	.1000E-01,	120.0	)
2358	74.33	.2873E-02	-.4043E-01	.3519E-01	.9962	.5766
1906	58.30	.2873E-02	-.4043E-01	.3519E-01	.9962	.5766
1362	42.56	.2873E-02	-.4042E-01	.3520E-01	.9962	.5766
1125	34.03	.2872E-02	-.4037E-01	.3526E-01	.9962	.5764
857	26.01	.2864E-02	-.4045E-01	.3505E-01	.9962	.5768
TEST4/J5B4		(I,F)=(1, 2)	(RMIN,RMAX)=(	.1000E-01,	120.0	)
2584	147.78	.2882E-02	-.4162E-01	.3390E-01	.9961	.5323
1966	112.30	.2882E-02	-.4162E-01	.3390E-01	.9961	.5323
1595	90.82	.2882E-02	-.4162E-01	.3391E-01	.9961	.5323
1193	67.24	.2882E-02	-.4158E-01	.3395E-01	.9961	.5323
933	51.51	.2883E-02	-.4176E-01	.3375E-01	.9961	.5317

DeVogelaere's Method (DEVOG)

L. D. Thomas

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	2.500 ,	45.00)
6791	.80	.9203E-10	.6700E-05	-.6866E-05	1.000	1.000
TEST1/J4B2		(I,F)=(1, 5)		(RMIN,RMAX)=(	2.500 ,	45.00)
6791	7.14	.1681E-08	.2425E-04	.3306E-04	.4917	.9551
TEST1/J4B3		(I,F)=(1,15)		(RMIN,RMAX)=(	2.500 ,	45.00)
6791	45.35	.1183E-08	-.5367E-05	.3397E-04	.4699	.9551
TEST1/J4B4		(I,F)=(1,20)		(RMIN,RMAX)=(	2.500 ,	45.00)
6791	151.74	.1111E-08	.1247E-04	.3092E-04	.4702	.9547
TEST2/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	1000.)
50171	18.11	.3948	.4258	.4621	.1781	.4998
TEST2/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1000.)
50171	82.17	.5991E-02	-.7601E-01	-.1458E-01	.8356	.2255
TEST2/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1000.)
50171	541.30	.1722E-01	.6011E-01	-.1166	.6892	.3755
TEST2/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	1000.)
10595	3.89	.2285	-.8312E-01	.4707	.4613	.3141
TEST2/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1000.)
10595	7.37	.1394E-01	.7223E-02	-.1176	.3971	.4942E-01
TEST2/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1000.)
10595	45.09	.7885E-02	.8261E-01	.3258E-01	.9017	.4107
TEST2/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1000.)
10595	203.49	.1593E-01	.1196	.4043E-01	.9489	.1830
TEST3/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	7.000)
497	.19	.4728	-.2829	-.6268	.4173E-01	.3292
TEST3/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
497	.92	.1700	-.3922	.1272	.3982	.2118E-01
TEST3/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
497	6.08	.6594E-01	-.2309	-.1124	.3683	.3101
TEST3/J25B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
497	21.20	.3973E-02	-.5990E-02	.7705E-01	.1288	.2945E-01
TEST3/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	7.000)
477	.19	.4151E-01	.1184	.1658	.9107	.9579
TEST3/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
477	.36	.2066	-.2509	.3790	.6987	.7640
TEST3/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
477	2.09	.9381E-03	-.1606E-01	-.2608E-01	.9229	.9500

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,1)	(F,F)	
TEST3/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000	)
477	9.56	.6124E-02	.6923E-01	.3648E-01	.9783	.9854	
TEST4/J5B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-01,	120.0	)
1591	.44	.4334E-02	-.4826E-01	.4477E-01	.9956	.9923	
TEST4/J5B2		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-01,	120.0	)
1591	6.77	.2914E-02	-.3920E-01	.3711E-01	.9963	.6410	
TEST4/J5B3		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-01,	120.0	)
1591	16.50	.2874E-02	-.4028E-01	.3538E-01	.9962	.5763	
TEST4/J5B4		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-01,	120.0	)
1591	33.27	.2883E-02	-.4148E-01	.3409E-01	.9961	.5317	

Numerov's Method (MNN)

L. D. Thomas

There are two runs for each test. The runs with the larger COUNT were done with δ = - .15E-8. The runs with the smaller COUNT were done with δ = - .1E-6. HSTART = .125E-3 for all runs.

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	2.500 ,	45.00)
2701	.75	.9169E-10	.6695E-05	-.6845E-05	1.000	1.000
1343	.39	.9648E-10	.6945E-05	-.6946E-05	1.000	1.000
TEST1/J4B2		(I,F)=(1, 5)		(RMIN,RMAX)=(	2.500 ,	45.00)
2705	5.91	.1681E-08	.2420E-04	.3310E-04	.4917	.9551
1347	2.99	.1683E-08	.2393E-04	.3333E-04	.4917	.9551
TEST1/J4B3		(I,F)=(1,15)		(RMIN,RMAX)=(	2.500 ,	45.00)
2705	37.02	.1184E-08	-.5415E-05	.3398E-04	.4699	.9551
1347	18.92	.1181E-08	-.5700E-05	.3389E-04	.4699	.9551
TEST1/J4B4		(I,F)=(1,20)		(RMIN,RMAX)=(	2.500 ,	45.00)
2712	136.05	.1112E-08	.1242E-04	.3094E-04	.4702	.9547
1349	67.86	.1112E-08	.1211E-04	.3107E-04	.4702	.9547
TEST2/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	1000.)
62693	37.05	.4024	.3525	.5274	.1649	.4893
31351	17.87	.4026	.3307	.5415	.1643	.4888
TEST2/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1000.)
62731	205.76	.5025E-02	-.6597E-01	-.2594E-01	.8316	.2218
31370	101.96	.4931E-02	-.6420E-01	-.2845E-01	.8311	.2216
TEST2/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1000.)
62739	1411.11	.1663E-01	.7899E-01	-.1020	.6834	.3735
31373	705.55	.1667E-01	.8350E-01	-.9845E-01	.6829	.3735
TEST2/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	1000.)
8702	5.46	.2295	-.6461E-01	.4746	.4586	.3858
4353	2.56	.2294	-.8454E-01	.4714	.4587	.3856
TEST2/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1000.)
8293	13.53	.1397E-01	.2263E-01	-.1160	.3891	.3817E-01
4364	5.49	.1397E-01	.2630E-01	-.1152	.3891	.3819E-01
TEST2/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1000.)
8306	75.67	.7396E-02	.7424E-01	.4341E-01	.9047	.3918
8171	74.45	.7375E-02	.7382E-01	.4388E-01	.9047	.3919
TEST4/J5B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-05,	120.0)
1251	.84	.4330E-02	-.4849E-01	.4449E-01	.9956	.9923
557	.38	.4338E-02	-.4942E-01	.4354E-01	.9956	.9923
TEST4/J5B2		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-05,	120.0)
1523	13.89	.2913E-02	-.3941E-01	.3688E-01	.9963	.6411
721	6.85	.2913E-02	-.3991E-01	.3634E-01	.9963	.6412
TEST4/J5B3		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-05,	120.0)
1635	34.86	.2873E-02	-.4046E-01	.3515E-01	.9962	.5766
672	15.34	.2874E-02	-.4096E-01	.3458E-01	.9962	.5763
TEST4/J5B4		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-05,	120.0)
1746	74.60	.2882E-02	-.4166E-01	.3386E-01	.9961	.5321
703	30.46	.2884E-02	-.4216E-01	.3326E-01	.9961	.5314

The Log Derivative Method (LOGD)

B. R. Johnson

For Test 2, a multichannel WKB method was used for the long-range potential region. In order to test the accuracy of this, some runs were done using the log derivative method over the entire integration range. Those runs with COUNT > 10,000 were done without the WKB method.

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	1.500 ,	30.00)
901	.10	.1156E-09	.7507E-05	-.7697E-05	1.000	1.000
379	.10	.9144E-10	.6822E-05	-.6701E-05	1.000	1.000
TEST1/J4B2		(I,F)=(1, 5)		(RMIN,RMAX)=(	1.500 ,	30.00)
901	.89	.1677E-08	.2485E-04	.3254E-04	.4917	.9551
879	.89	.1681E-08	.2351E-04	.3358E-04	.4918	.9551
TEST1/J4B3		(I,F)=(1,15)		(RMIN,RMAX)=(	1.500 ,	30.00)
901	5.70	.1143E-08	-.4772E-05	.3347E-04	.4699	.9551
879	5.76	.1185E-08	-.6171E-05	.3387E-04	.4699	.9551
TEST1/J4B4		(I,F)=(1,20)		(RMIN,RMAX)=(	1.500 ,	30.00)
901	19.26	.1096E-08	.1306E-04	.3041E-04	.4701	.9547
879	18.79	.1112E-08	.1178E-04	.3119E-04	.4702	.9547
TEST2/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	800.0)
1347	.54	.3954	.3484	.5234	.1772	.4997
32297	11.34	.3957	.3310	.5349	.1764	.4991
53281	18.57	.3956	.3463	.5251	.1764	.4991
TEST2/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	800.0)
1143	2.61	.5571E-02	-.7027E-01	-.2516E-01	.8364	.2248
53281	85.95	.5523E-02	-.6993E-01	-.2544E-01	.8353	.2249
TEST2/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	800.0)
1143	18.08	.1715E-01	.7783E-01	-.1053	.6891	.3750
TEST2/J25B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	800.0)
1143	47.29	.3446E-01	.1865E-01	.1847	.6336	.4385E-01
TEST2/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	1500.)
1171	.47	.2308	-.9903E-01	.4701	.4571	.3130
27643	9.78	.2302	-.9952E-01	.4694	.4585	.3132
TEST2/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1500.)
1171	1.03	.1385E-01	.1137E-01	-.1171	.3879	.5051E-01
27643	18.23	.1415E-01	.1198E-01	-.1184	.3894	.5014E-01
TEST2/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1500.)
1171	4.68	.8819E-02	.9389E-01	-.1687E-02	.9115	.3314
27643	109.44	.7770E-02	.8014E-01	.3670E-01	.9044	.4109
1687	6.72	.7810E-02	.8224E-01	.3237E-01	.9034	.3897
1753	6.96	.7720E-02	.8142E-01	.3302E-01	.9046	.4032
TEST2/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	1500.)
1171	19.65	.1422E-01	.1192	.4199E-03	.9566	.1593
1687	29.39	.1613E-01	.1197	.4233E-01	.9469	.1638
1753	29.87	.1608E-01	.1195	.4248E-01	.9492	.1739
TEST3/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	7.000)
401	.15	.4727	-.2815	-.6273	.4193E-01	.3293

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST3/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
401	.68	.1710	-.3952	.1217	.3964	.2025E-01
TEST3/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
401	4.31	.6568E-01	-.2299	-.1132	.3695	.3120
TEST3/J25B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
401	11.70	.6277E-02	-.8315E-02	.7879E-01	.1283	.2898E-01
TEST3/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000 ,	7.000)
401	.15	.4186E-01	.1186	.1667	.9099	.9575
201	.08	.4202E-01	.1187	.1671	.9096	.9573
TEST3/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
401	.28	.2056	-.2517	.3771	.7005	.7646
TEST3/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
401	1.62	.1041E-02	-.1705E-01	-.2740E-01	.9207	.9497
TEST3/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
401	7.21	.6097E-02	.6903E-01	.3649E-01	.9784	.9856
TEST4/J5B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-03,	50.00)
1003	.25	.4329E-02	-.4847E-01	.4449E-01	.9956	.9923
503	.13	.4324E-02	-.4843E-01	.4448E-01	.9956	.9923
TEST4/J5B2		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-03,	50.00)
503	2.04	.2908E-02	-.3938E-01	.3684E-01	.9963	.6406
527	2.16	.2907E-02	-.3935E-01	.3686E-01	.9963	.6411
TEST4/J5B3		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-03,	50.00)
503	5.14	.2866E-02	-.4046E-01	.3506E-01	.9962	.5739
527	5.35	.2868E-02	-.4041E-01	.3513E-01	.9962	.5764
TEST4/J5B4		(I,F)=(1, 2)		(RMIN,RMAX)=(	.1000E-03,	50.00)
503	10.07	.2873E-02	-.4167E-01	.3371E-01	.9961	.5275
527	10.58	.2877E-02	-.4161E-01	.3385E-01	.9961	.5320

The Sams-Kouri Method (SAMS)

K. D. McLenithan and D. Secrest

The r_{max} values here are correct only for the runs reported in Tables 3-6. For Test 1, all runs with COUNT = 451 had $r_{max} = 10$. For Test 2, all runs with COUNT = 31501 had $r_{max} = 800$. For Test 4, all runs with COUNT = 1050 had $r_{max} = 100$.

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	2.250 ,	40.00)
451	.06	.7848E-09	.1949E-04	-.2012E-04	1.000	1.000
3384	.44	.9235E-10	.6717E-05	-.6873E-05	1.000	1.000
3051	.39	.9201E-10	.6704E-05	-.6860E-05	1.000	1.000
TEST1/J4B2		(I,F)=(1, 5)		(RMIN,RMAX)=(	2.250 ,	40.00)
451	.50	.2100E-08	.3255E-04	.3227E-04	.4914	.9551
3384	3.61	.1678E-08	.2422E-04	.3304E-04	.4917	.9551
3051	3.17	.1679E-08	.2421E-04	.3306E-04	.4917	.9551
TEST1/J4B3		(I,F)=(1,15)		(RMIN,RMAX)=(	2.250 ,	40.00)
451	3.08	.1113E-08	.1915E-05	.3331E-04	.4694	.9551
3384	22.85	.1180E-08	-.5387E-05	.3393E-04	.4699	.9551
3051	20.21	.1181E-08	-.5397E-05	.3394E-04	.4699	.9551
TEST1/J4B4		(I,F)=(1,20)		(RMIN,RMAX)=(	2.250 ,	40.00)
451	8.00	.1182E-08	.1759E-04	.2953E-04	.4697	.9547
3384	51.20	.1137E-08	.3083E-04	.1363E-04	.4702	.9551
3051	56.64	.1110E-08	.1243E-04	.3091E-04	.4702	.9547
TEST2/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.500 ,	500.0)
31501	11.62	.3968	.3433	.5282	.1734	.4964
7101	2.63	.4003	.3411	.5329	.1690	.4886
TEST2/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	500.0)
31501	52.89	.5088E-02	-.6647E-01	-.2589E-01	.8324	.2244
7101	12.13	.4372E-02	-.6103E-01	-.2543E-01	.8296	.2238
TEST2/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	500.0)
31501	337.85	.1753E-01	.8258E-01	-.1035	.6872	.3763
7101	77.04	.1752E-01	.8731E-01	-.9950E-01	.6771	.3776
TEST2/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.500 ,	1000.)
31501	11.78	.2296	-.1027	.4680	.4608	.3139
2901	1.11	.2269	-.1512	.4517	.4656	.3087
TEST2/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	1000.)
31501	22.15	.1432E-01	.1452E-01	-.1188	.3914	.4843E-01
2901	2.09	.1412E-01	.3425E-01	-.1138	.3749	.4889E-01
TEST2/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	1000.)
31501	58.10	.3323E-01	.1550	-.9599E-01	.8116	.3346
11576	54.17	.7574E-02	.7802E-01	.3856E-01	.9017	.4053
TEST2/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	1000.)
31501	169.24	.1937E-01	.1144	-.7932E-01	.9383	.4605E-01
11576	214.36	.1618E-01	.1154	.5354E-01	.9506	.1167
TEST3/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.500 ,	7.000)

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
5001	1.86	.4735	-.2779	-.6295	.4035E-01	.3288
TEST3/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	7.000)
5001	8.74	.1715	-.3970	.1176	.3949	.2002E-01
TEST3/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	7.000)
5001	54.82	.6572E-01	-.2293	-.1147	.3705	.3137
TEST3/J25B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	7.000)
5001	147.73	.6434E-02	-.1119E-01	.7943E-01	.1267	.2842E-01
TEST3/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.500 ,	7.000)
3501	1.30	.4237E-01	.1188	.1681	.9088	.9570
TEST3/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	7.000)
3501	2.48	.2062	-.2587	.3732	.6996	.7627
TEST3/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	7.000)
5001	24.81	.1099E-02	-.1752E-01	-.2814E-01	.9196	.9495
TEST3/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.500 ,	7.000)
5001	105.33	.6344E-02	.7029E-01	.3745E-01	.9789	.9857
TEST4/J5B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	.5000E-01,	50.00)
1050	.29	.4395E-02	-.4911E-01	.4452E-01	.9956	.9922
550	.17	.4389E-02	-.4908E-01	.4450E-01	.9956	.9922
190	.07	.4387E-02	-.4909E-01	.4446E-01	.9956	.9922
TEST4/J5B2		(I,F)=(1, 2)		(RMIN,RMAX)=(	.5000E-01,	50.00)
1050	4.49	.2921E-02	-.3960E-01	.3678E-01	.9963	.6348
550	2.40	.2916E-02	-.3958E-01	.3675E-01	.9963	.6348
190	.92	.2914E-02	-.3958E-01	.3670E-01	.9963	.6344
TEST4/J5B3		(I,F)=(1, 2)		(RMIN,RMAX)=(	.5000E-01,	50.00)
1050	10.92	.2883E-02	-.4108E-01	.3458E-01	.9961	.5538
550	5.94	.2879E-02	-.4106E-01	.3454E-01	.9961	.5538
190	2.16	.2876E-02	-.4106E-01	.3450E-01	.9961	.5534
TEST4/J5B4		(I,F)=(1, 2)		(RMIN,RMAX)=(	.5000E-01,	50.00)
1050	21.74	.2877E-02	-.4190E-01	.3349E-01	.9960	.5182
550	11.74	.2873E-02	-.4188E-01	.3345E-01	.9960	.5182
190	4.26	.2870E-02	-.4188E-01	.3340E-01	.9960	.5178

The Method of Integral Equations with Reference Potentials (INSCAT)

M. J. Redmon

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	2.250 ,	16.00)
318	.18	.9094E-10	.6661E-05	-.6824E-05	1.000	1.000
TEST1/J4B2		(I,F)=(1, 5)		(RMIN,RMAX)=(	2.250 ,	16.00)
248	.84	.1699E-08	.2268E-04	.3442E-04	.4946	.9552
TEST1/J4B3		(I,F)=(1,15)		(RMIN,RMAX)=(	2.250 ,	16.00)
198	3.73	.1149E-08	-.5244E-05	.3350E-04	.4747	.9553
TEST1/J4B4		(I,F)=(1,20)		(RMIN,RMAX)=(	2.250 ,	16.00)
197	11.71	.3264E-06	.5591E-03	-.1173E-03	.4753	.9948E-08
TEST2/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	500.0)
999	5.74	.5645E-02	.7312E-01	.1726E-01	.5698	.1751
TEST2/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	500.0)
1008	31.62	.2154E-01	.1301	.6789E-01	.6007	.3906
TEST2/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	500.0)
850	1.94	.1755E-01	.1094	-.7468E-01	.3564	.8362E-01
TEST4/J5B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	.2000E-01,	75.00)
328	.36	.4305E-02	-.4900E-01	.4363E-01	.9957	.9923
TEST4/J5B2		(I,F)=(1, 2)		(RMIN,RMAX)=(	.2000E-01,	75.00)
347	4.42	.2928E-02	-.3966E-01	.3681E-01	.9963	.6358
TEST4/J5B3		(I,F)=(1, 2)		(RMIN,RMAX)=(	.2000E-01,	75.00)
382	10.74	.2887E-02	-.4076E-01	.3501E-01	.9961	.5687
TEST4/J5B4		(I,F)=(1, 2)		(RMIN,RMAX)=(	.2000E-01,	75.00)
415	22.66	.2872E-02	-.4181E-01	.3352E-01	.9960	.5219

Gordon's Method (GORDON)

M. H. Alexander

The results are given in pairs, the second member of which has COUNT = 0. These are for the second-energy runs which do no potential evaluations.

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	2.100 ,	19.00)
233	.65	.3757E-08	-.4240E-04	.4426E-04	1.000	1.000
0	.22	.3757E-08	-.4240E-04	.4426E-04	1.000	1.000
373	1.05	.1338E-09	.8032E-05	-.8324E-05	1.000	1.000
0	.36	.1338E-09	.8032E-05	-.8324E-05	1.000	1.000
493	1.38	.9443E-10	.6758E-05	-.6983E-05	1.000	1.000
0	.47	.9443E-10	.6758E-05	-.6983E-05	1.000	1.000
618	1.76	.1096E-09	.7287E-05	-.7517E-05	1.000	1.000
0	.59	.1096E-09	.7287E-05	-.7517E-05	1.000	1.000
TEST1/J4B2		(I,F)=(1, 5)		(RMIN,RMAX)=(	2.100 ,	19.00)
246	3.36	.1892E-08	.1755E-04	.3981E-04	.4898	.9554
0	.72	.1892E-08	.1755E-04	.3981E-04	.4898	.9554
394	5.42	.1734E-08	.2098E-04	.3597E-04	.4905	.9553
0	1.17	.1734E-08	.2098E-04	.3597E-04	.4905	.9553
519	7.13	.1695E-08	.2176E-04	.3495E-04	.4908	.9552
0	1.53	.1695E-08	.2176E-04	.3495E-04	.4908	.9552
650	8.91	.1685E-08	.2253E-04	.3431E-04	.4910	.9552
0	1.90	.1684E-08	.2253E-04	.3430E-04	.4910	.9552
869	11.63	.1677E-08	.2308E-04	.3383E-04	.4912	.9552
0	2.48	.1677E-08	.2308E-04	.3383E-04	.4912	.9552
1125	15.13	.1678E-08	.2363E-04	.3345E-04	.4913	.9552
0	3.20	.1678E-08	.2363E-04	.3346E-04	.4913	.9552
1811	24.66	.1677E-08	.2404E-04	.3316E-04	.4915	.9551
0	5.26	.1677E-08	.2404E-04	.3316E-04	.4915	.9551
TEST1/J4B3		(I,F)=(1,15)		(RMIN,RMAX)=(	2.100 ,	19.00)
258	16.27	.2076E-08	-.1396E-04	.4338E-04	.4688	.9554
0	3.06	.2076E-08	-.1396E-04	.4338E-04	.4688	.9554
401	25.97	.1503E-08	-.9531E-05	.3758E-04	.4692	.9553
0	5.04	.1503E-08	-.9531E-05	.3758E-04	.4692	.9553
524	33.92	.1352E-08	-.7859E-05	.3592E-04	.4694	.9552
0	6.61	.1352E-08	-.7859E-05	.3592E-04	.4694	.9552
680	43.40	.1278E-08	-.6939E-05	.3507E-04	.4695	.9552
0	8.54	.1278E-08	-.6939E-05	.3507E-04	.4695	.9552
TEST1/J4B4		(I,F)=(1,20)		(RMIN,RMAX)=(	2.100 ,	19.00)
272	49.62	.1408E-08	.2414E-06	.3753E-04	.4668	.9550
0	11.19	.1408E-08	.2414E-06	.3753E-04	.4668	.9550
432	78.95	.1208E-08	.5950E-05	.3425E-04	.4681	.9549
0	18.14	.1208E-08	.5950E-05	.3425E-04	.4681	.9549
570	104.18	.1177E-08	.7311E-05	.3352E-04	.4686	.9549
0	24.06	.1177E-08	.7311E-05	.3352E-04	.4686	.9549
716	130.13	.1156E-08	.8331E-05	.3297E-04	.4689	.9549
0	30.20	.1156E-08	.8331E-05	.3297E-04	.4689	.9549
TEST2/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.040 ,	1000.)
1098	4.93	.2833E-05	-.1196E-02	-.1184E-02	1.000	.9948
0	1.31	.2833E-05	-.1196E-02	-.1184E-02	1.000	.9948
1527	6.81	.1846E-05	-.9775E-03	-.9435E-03	1.000	.9950
0	1.83	.5611E-08	.4114E-04	.6260E-04	1.000	1.000
TEST2/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.040 ,	1000.)

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
899	18.34	.4714E-02	-.6401E-01	-.2484E-01	.8309	.2277
0	3.36	.4714E-02	-.6401E-01	-.2484E-01	.8309	.2277
1369	27.81	.4960E-02	-.6581E-01	-.2509E-01	.8324	.2265
0	5.08	.4960E-02	-.6581E-01	-.2509E-01	.8324	.2265

TEST2/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.040	, 1000.)
424	43.16	.1702E-01	.8531E-01	-.9872E-01	.6867	.3770
0	7.49	.1702E-01	.8531E-01	-.9872E-01	.6867	.3770
597	61.22	.1714E-01	.8288E-01	-.1014	.6883	.3756
0	10.81	.1714E-01	.8288E-01	-.1014	.6883	.3756

TEST2/J25B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.040	, 1000.)
937	232.75	.3490E-01	.3530E-02	.1868	.6425	.4744E-01
1102	278.73	.3485E-01	.7997E-02	.1865	.6393	.4643E-01
0	46.83	.3485E-01	.7997E-02	.1865	.6393	.4643E-01

TEST2/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	2.800	, 1000.)
1207	5.07	.2279	-.1208	.4619	.4641	.3250
0	1.31	.2279	-.1208	.4619	.4641	.3250
1484	6.46	.2282	-.1162	.4633	.4635	.3227
0	1.66	.2282	-.1162	.4633	.4635	.3227

TEST2/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	2.800	, 1000.)
1221	11.21	.1439E-01	.1801E-01	-.1186	.3836	.4386E-01
0	2.39	.1439E-01	.1801E-01	-.1186	.3836	.4386E-01
1562	14.21	.1435E-01	.1651E-01	-.1186	.3855	.4496E-01
0	3.02	.1435E-01	.1651E-01	-.1186	.3855	.4496E-01

TEST2/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	2.800	, 1000.)
1622	74.90	.7470E-02	.7538E-01	.4229E-01	.9023	.4119
0	15.99	.7470E-02	.7538E-01	.4229E-01	.9023	.4119
1395	64.05	.7349E-02	.7352E-01	.4409E-01	.9026	.4129
0	13.47	.7349E-02	.7352E-01	.4409E-01	.9026	.4129

TEST2/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	2.800	, 1000.)
1767	298.65	.1492E-01	.1046	.6303E-01	.9525	.1519
0	65.83	.1492E-01	.1046	.6303E-01	.9525	.1519

TEST3/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.000	, 7.000)
198	.89	.4677	-.2897	-.6195	.5116E-01	.3343
0	.24	.4677	-.2897	-.6195	.5116E-01	.3343
288	1.31	.4694	-.2870	-.6221	.4798E-01	.3325
0	.35	.4694	-.2870	-.6221	.4798E-01	.3325
462	1.93	.4705	-.2854	-.6237	.4608E-01	.3315
0	.51	.4705	-.2854	-.6237	.4608E-01	.3315

TEST3/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000	, 7.000)
230	5.01	.1707	-.3956	.1191	.3948	.1872E-01
0	1.04	.1707	-.3956	.1191	.3948	.1872E-01
337	7.42	.1708	-.3955	.1199	.3953	.1918E-01
0	1.53	.1708	-.3955	.1199	.3953	.1918E-01
511	11.10	.1709	-.3954	.1205	.3956	.1949E-01
0	2.27	.1709	-.3954	.1205	.3956	.1949E-01

TEST3/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000	, 7.000)

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
139	14.24	.6350E-01	-.2284	-.1065	.3632	.3092
0	2.90	.6350E-01	-.2284	-.1065	.3632	.3092
178	17.70	.6400E-01	-.2287	-.1082	.3647	.3100
0	3.50	.6400E-01	-.2287	-.1082	.3647	.3100
230	23.30	.6444E-01	-.2290	-.1095	.3659	.3106
0	4.66	.6444E-01	-.2290	-.1095	.3659	.3106
326	34.02	.6484E-01	-.2293	-.1107	.3671	.3110
0	6.88	.6484E-01	-.2293	-.1107	.3671	.3110
150	40.60	.7221E-02	-.1024E-01	.8436E-01	.1271	.2970E-01
0	9.18	.7221E-02	-.1024E-01	.8436E-01	.1271	.2970E-01
TEST3/J25B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.000 ,	7.000)
186	50.08	.7148E-02	-.1036E-01	.8391E-01	.1267	.2947E-01
0	11.32	.7148E-02	-.1036E-01	.8391E-01	.1267	.2947E-01
237	65.41	.7073E-02	-.1047E-01	.8344E-01	.1265	.2938E-01
98	.45	.3496E-01	.1859	-.2019E-01	.8995	.1048E-01
0	.13	.3496E-01	.1859	-.2019E-01	.8995	.1048E-01
TEST3/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	2.780 ,	7.000)
154	.66	.4523E-01	.1221	.1742	.9026	.9540
0	.18	.4523E-01	.1221	.1742	.9026	.9540
273	1.11	.4378E-01	.1206	.1710	.9058	.9555
0	.29	.4378E-01	.1206	.1710	.9058	.9555
128	1.13	.3922E-02	.5609E-01	-.2785E-01	.6894	.9669
0	.25	.3922E-02	.5609E-01	-.2785E-01	.6894	.9669
TEST3/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	2.780 ,	7.000)
174	1.57	.2104	-.2567	.3802	.6931	.7602
0	.34	.2104	-.2567	.3802	.6931	.7602
292	2.67	.2086	-.2548	.3791	.6959	.7619
0	.59	.2086	-.2548	.3791	.6959	.7619
108	5.07	.1750	-.4060	.1009	.7228	.1470
0	1.01	.1750	-.4060	.1009	.7228	.1470
TEST3/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	2.780 ,	7.000)
155	7.21	.8900E-03	-.1377E-01	-.2647E-01	.9296	.9553
0	1.45	.8900E-03	-.1377E-01	-.2647E-01	.9296	.9553
253	11.67	.8706E-03	-.1352E-01	-.2623E-01	.9301	.9545
0	2.32	.8706E-03	-.1352E-01	-.2623E-01	.9301	.9545
110	18.33	.8187	-.3261	.8440	.2543E-01	.8326E-01
0	3.79	.8187	-.3260	.8440	.2543E-01	.8326E-01
TEST3/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(	2.780 ,	7.000)
158	26.60	.3014E-01	.1321	.1126	.9400	.9608
0	5.66	.3014E-01	.1321	.1126	.9400	.9608
258	43.61	.1253E-01	-.2192E-01	.1098	.7263	.5747
0	8.98	.1252E-01	-.2194E-01	.1097	.7265	.5747
124	.69	.9813E-05	-.1050E-03	.3131E-02	.9955	1.000
0	.19	.1039E-04	-.9841E-04	.3221E-02	.9955	1.000
TEST4/J5B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	.0300 ,	70.00)
299	1.67	.4403E-02	-.4993E-01	.4370E-01	.9956	.9922
0	.45	.4403E-02	-.4993E-01	.4370E-01	.9956	.9922
579	3.24	.4366E-02	-.4920E-01	.4411E-01	.9956	.9922
0	.89	.4366E-02	-.4920E-01	.4411E-01	.9956	.9922

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
109	4.90	.2886E-02	-.3757E-01	.3840E-01	.9957	.6466
0	.96	.2887E-02	-.3758E-01	.3841E-01	.9957	.6466
TEST4/J5B2		(I,F)=(1, 2)		(RMIN,RMAX)=(	.0300 ,	70.00)
255	11.50	.2900E-02	-.3859E-01	.3755E-01	.9962	.6443
0	2.29	.2900E-02	-.3859E-01	.3755E-01	.9962	.6443
494	22.62	.2905E-02	-.3897E-01	.3724E-01	.9963	.6430
0	4.71	.2905E-02	-.3897E-01	.3724E-01	.9963	.6430
111	10.27	.2837E-02	-.3915E-01	.3611E-01	.9958	.5832
0	1.89	.2837E-02	-.3916E-01	.3611E-01	.9958	.5832
TEST4/J5B3		(I,F)=(1, 2)		(RMIN,RMAX)=(	.0300 ,	70.00)
266	24.85	.2860E-02	-.3989E-01	.3561E-01	.9961	.5805
0	4.83	.2860E-02	-.3989E-01	.3561E-01	.9961	.5805
511	48.73	.2865E-02	-.4014E-01	.3541E-01	.9962	.5790
0	9.96	.2865E-02	-.4014E-01	.3541E-01	.9962	.5790
149	23.71	.2854E-02	-.4027E-01	.3511E-01	.9958	.5245
0	4.02	.2854E-02	-.4028E-01	.3510E-01	.9958	.5245
TEST4/J5B4		(I,F)=(1, 2)		(RMIN,RMAX)=(	.0300 ,	70.00)
356	58.36	.2871E-02	-.4102E-01	.3447E-01	.9960	.5320
0	11.06	.2871E-02	-.4102E-01	.3447E-01	.9960	.5320
680	113.68	.2876E-02	-.4129E-01	.3421E-01	.9961	.5329

The Variable-Interval, Variable-Step Method (VIVS)

G. A. Parker

The runs are in pairs, the second member of which has COUNT = 0. These were second-energy runs for which no potential evaluations were made.

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	2.300 ,	40.00)
675	.24	.1408E-09	.8292E-05	-.8491E-05	1.000	1.000
0	.06	.1408E-09	.8292E-05	-.8491E-05	1.000	1.000
775	.24	.1058E-09	.7187E-05	-.7358E-05	1.000	1.000
0	.05	.1058E-09	.7187E-05	-.7358E-05	1.000	1.000
1525	.54	.8833E-10	.6567E-05	-.6723E-05	1.000	1.000
0	.13	.8833E-10	.6567E-05	-.6723E-05	1.000	1.000
1127	.34	.7803E-10	.6172E-05	-.6319E-05	1.000	1.000
0	.05	.7803E-10	.6172E-05	-.6319E-05	1.000	1.000
1460	.43	.2349E-06	.3343E-03	-.3509E-03	1.000	1.000
0	.07	.2349E-06	.3343E-03	-.3509E-03	1.000	1.000
1746	.50	.9393E-10	.6772E-05	-.6934E-05	1.000	1.000
0	.09	.9393E-10	.6772E-05	-.6934E-05	1.000	1.000
2178	.62	.9458E-10	.6795E-05	-.6958E-05	1.000	1.000
0	.11	.9458E-10	.6795E-05	-.6958E-05	1.000	1.000
TEST1/J4B2		(I,F)=(1, 5)		(RMIN,RMAX)=(	2.300 ,	40.00)
775	1.05	.1549E-08	.2188E-04	.3272E-04	.4917	.9551
0	.25	.1549E-08	.2188E-04	.3272E-04	.4917	.9551
950	1.29	.1607E-08	.2411E-04	.3203E-04	.4917	.9551
0	.30	.1607E-08	.2411E-04	.3203E-04	.4917	.9551
2025	2.70	.1679E-08	.2414E-04	.3311E-04	.4916	.9551
0	.61	.1679E-08	.2414E-04	.3311E-04	.4916	.9551
TEST1/J4B3		(I,F)=(1,15)		(RMIN,RMAX)=(	2.300 ,	40.00)
1000	9.45	.1213E-08	-.5796E-05	.3434E-04	.4699	.9551
0	3.29	.1213E-08	-.5796E-05	.3434E-04	.4699	.9551
1225	9.03	.1206E-08	-.5470E-05	.3430E-04	.4699	.9551
0	2.30	.1206E-08	-.5470E-05	.3430E-04	.4699	.9551
2450	23.32	.1183E-08	-.5395E-05	.3396E-04	.4699	.9551
0	8.09	.1183E-08	-.5395E-05	.3396E-04	.4699	.9551
1971	11.89	.1283E-08	-.5040E-05	.3547E-04	.4698	.9551
0	2.01	.1283E-08	-.5040E-05	.3547E-04	.4698	.9551
2904	16.73	.1208E-08	-.4122E-06	.3476E-04	.4698	.9549
0	2.44	.1208E-08	-.4122E-06	.3476E-04	.4698	.9549
TEST1/J4B4		(I,F)=(1,20)		(RMIN,RMAX)=(	2.300 ,	40.00)
1725	46.95	.5483E-04	-.5190E-02	-.5281E-02	.4692	.8559
0	15.37	.5483E-04	-.5190E-02	-.5281E-02	.4692	.8559
1425	31.67	.1120E-08	.1217E-04	.3118E-04	.4702	.9547
0	7.87	.1120E-08	.1217E-04	.3118E-04	.4702	.9547
3125	85.39	.1110E-08	.1243E-04	.3092E-04	.4702	.9547
0	27.86	.1110E-08	.1243E-04	.3092E-04	.4702	.9547
TEST2/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.300 ,	5000.)
1025	.59	.3953	.3501	.5222	.1779	.4989
0	.09	.3953	.3501	.5222	.1779	.4989
TEST2/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	5000.)
1125	2.30	.5583E-02	-.7055E-01	-.2461E-01	.8377	.2251
0	.53	.5583E-02	-.7055E-01	-.2461E-01	.8377	.2251
TEST2/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	5000.)

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
1275	14.82	.1732E-01	.7886E-01	-.1053	.6867	.3754
0	3.88	.1732E-01	.7886E-01	-.1053	.6867	.3754
TEST2/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(3.300	, 700.0)	
1300	.73	.2291	-.9807E-01	.4685	.4608	.3125
0	.10	.2291	-.9807E-01	.4685	.4608	.3125
1650	.95	.2297	-.9988E-01	.4687	.4594	.3124
0	.14	.2297	-.9988E-01	.4687	.4594	.3124
TEST2/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(3.300	, 700.0)	
1550	1.51	.1423E-01	.1205E-01	-.1187	.3897	.5138E-01
0	.29	.1423E-01	.1205E-01	-.1187	.3897	.5138E-01
TEST2/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(3.300	, 700.0)	
1300	6.02	.4139E-01	-.1946	.5916E-01	.6996	.2900
0	1.55	.4139E-01	-.1946	.5916E-01	.6996	.2900
TEST2/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(3.300	, 700.0)	
1475	27.75	.6035E-02	.7690E-01	-.1097E-01	.5525	.9704E-01
0	7.32	.6035E-02	.7690E-01	-.1097E-01	.5525	.9704E-01
TEST3/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(3.300	, 7.000)	
525	.30	.4725	-.2820	-.6269	.4221E-01	.3294
0	.04	.4725	-.2820	-.6269	.4221E-01	.3294
TEST3/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(3.300	, 7.000)	
650	1.37	.1711	-.3951	.1225	.3963	.2053E-01
0	.32	.1711	-.3951	.1225	.3963	.2053E-01
TEST3/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(3.300	, 7.000)	
625	7.33	.6565E-01	-.2298	-.1134	.3700	.3123
0	1.97	.6565E-01	-.2298	-.1134	.3700	.3123
TEST3/J25B4		(I,F)=(1, 4)		(RMIN,RMAX)=(3.300	, 7.000)	
650	19.85	.6872E-02	-.1040E-01	.8224E-01	.1257	.2891E-01
0	5.30	.6872E-02	-.1040E-01	.8224E-01	.1257	.2891E-01
850	25.84	.6861E-02	-.1040E-01	.8217E-01	.1259	.2903E-01
0	6.85	.6861E-02	-.1040E-01	.8217E-01	.1259	.2903E-01
1250	37.70	.6871E-02	-.1042E-01	.8223E-01	.1259	.2898E-01
0	9.87	.6871E-02	-.1042E-01	.8223E-01	.1259	.2898E-01
TEST3/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(3.300	, 7.000)	
550	.32	.4179E-01	.1186	.1665	.9101	.9576
0	.04	.4179E-01	.1186	.1665	.9101	.9576
TEST3/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(3.300	, 7.000)	
550	.55	.2052	-.2514	.3768	.7011	.7649
0	.11	.2052	-.2514	.3768	.7011	.7649
TEST3/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(3.300	, 7.000)	
675	3.13	.8596E-03	-.1355E-01	-.2600E-01	.9325	.9537
0	.79	.8596E-03	-.1355E-01	-.2600E-01	.9325	.9537
TEST3/J5B4		(I,F)=(1, 4)		(RMIN,RMAX)=(3.300	, 7.000)	
675	12.93	.2903E-01	.1270	.1136	.9463	.9480

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
0	3.37	.2903E-01	.1270	.1136	.9463	.9480
850	16.36	.2902E-01	.1270	.1136	.9463	.9480
0	4.25	.2902E-01	.1270	.1136	.9463	.9480
1425	27.59	.2903E-01	.1270	.1136	.9463	.9480
0	7.16	.2903E-01	.1270	.1136	.9463	.9480

TEST4/J5B1		(I,F)=(1, 2)	(RMIN,RMAX)=(	.1500	,	160.0	)
600	.34	.4319E-02	-.4831E-01	.4455E-01		.9956	.9923
0	.08	.4319E-02	-.4831E-01	.4455E-01		.9956	.9923

TEST4/J5B2		(I,F)=(1, 2)	(RMIN,RMAX)=(	.1500	,	160.0	)
825	3.96	.2904E-02	-.3912E-01	.3706E-01		.9963	.6478
0	1.00	.2904E-02	-.3912E-01	.3706E-01		.9963	.6478

TEST4/J5B3		(I,F)=(1, 2)	(RMIN,RMAX)=(	.1500	,	160.0	)
825	9.20	.2867E-02	-.4007E-01	.3551E-01		.9962	.5888
0	2.24	.2867E-02	-.4007E-01	.3551E-01		.9962	.5888

TEST4/J5B4		(I,F)=(1, 2)	(RMIN,RMAX)=(	.1500	,	160.0	)
925	19.84	.2886E-02	-.4118E-01	.3449E-01		.9961	.5521
0	4.73	.2886E-02	-.4118E-01	.3449E-01		.9961	.5521

The R-matrix Propagator Method (RMAT)

T. G. Schmalz

The S-matrices stored on tape by this program were only correct in the first column due to a program error. As a consequence, the values of I and F are interchanged here, and the values in the (I,I) column should be ignored. That error has been corrected in the version which is now available from the NRCC software library.

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(2, 1)		(RMIN,RMAX)=(	1.700 ,	45.00)
217	.73	.9041E-10	.6644E-05	-.6802E-05	.3602E-03	1.000
TEST1/J4B2		(I,F)=(5, 1)		(RMIN,RMAX)=(	1.700 ,	45.00)
241	4.04	.1682E-08	.2411E-04	.3318E-04	.1752E-08	.4917
TEST1/J4B3		(I,F)=(15, 1)		(RMIN,RMAX)=(	1.700 ,	45.00)
277	28.21	.1193E-08	-.5499E-05	.3409E-04	.1813E-05	.4699
TEST1/J4B4		(I,F)=(20, 1)		(RMIN,RMAX)=(	1.700 ,	45.00)
221	71.64	.1158E-08	.1105E-04	.3218E-04	.2093E-10	.4702
TEST2/J25B1		(I,F)=(3, 1)		(RMIN,RMAX)=(	3.000 ,	2000.)
185	.87	.3959	.3500	.5229	.3236E-09	.1768
TEST2/J25B2		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	2000.)
209	4.57	.5541E-02	-.7034E-01	-.2435E-01	.3362	.8379
TEST2/J25B3		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	2000.)
216	36.51	.1709E-01	.7817E-01	-.1048	.1103	.6864
TEST2/J25B4		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	2000.)
217	108.38	.3450E-01	.1858E-01	.1848	.3450E-01	.6314
TEST2/J5B1		(I,F)=(3, 1)		(RMIN,RMAX)=(	3.000 ,	2000.)
175	.83	.2287	-.1013	.4674	.3233E-09	.4612
TEST2/J5B2		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	2000.)
189	1.85	.1513E-01	.1294E-01	-.1223	.2767E-08	.3936
TEST2/J5B3		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	2000.)
206	13.17	.7844E-02	.8086E-01	.3614E-01	.3526E-17	.9044
TEST2/J5B4		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	2000.)
202	59.47	.1564E-01	.1160	.4689E-01	.1053E-37	.9498
TEST3/J25B1		(I,F)=(3, 1)		(RMIN,RMAX)=(	3.000 ,	7.000)
45	.22	.4717	-.2852	-.6248	377.6	.4374E-01
TEST3/J25B2		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	7.000)
50	1.24	.1708	-.3943	.1238	.4656	.3977
TEST3/J25B3		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	7.000)
52	9.27	.6585E-01	-.2308	-.1121	.2702E-02	.3681
TEST3/J5B1		(I,F)=(3, 1)		(RMIN,RMAX)=(	3.000 ,	7.000)
41	.20	.4191E-01	.1189	.1666	544.9	.9098
TEST3/J5B2		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	7.000)
45	.55	.2043	-.2513	.3758	452.7	.7023
TEST3/J5B3		(I,F)=(4, 1)		(RMIN,RMAX)=(	3.000 ,	7.000)
68	4.46	.8556E-03	-.1349E-01	-.2595E-01	.7837E-04	.9326

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)	
TEST4/J5B1		(I,F)=(2, 1)		(RMIN,RMAX)=(	.1000 ,	250.0	)
44	.29	.4325E-02	-.4828E-01	.4465E-01	.2354E-07	.9956	
TEST4/J5B2		(I,F)=(2, 1)		(RMIN,RMAX)=(	.1000 ,	250.0	)
55	3.95	.2911E-02	-.3974E-01	.3692E-01	.2279E-07	.9963	
TEST4/J5B3		(I,F)=(2, 1)		(RMIN,RMAX)=(	.1000 ,	250.0	)
69	9.98	.2885E-02	-.4064E-01	.3512E-01	.2631E-07	.9962	
TEST4/J5B4		(I,F)=(2, 1)		(RMIN,RMAX)=(	.1000 ,	250.0	)
76	23.46	.2890E-02	-.4158E-01	.3407E-01	.2481E-07	.9961	

The L^2 Approach to R-matrix Propagation (L2RMAT)

R. B. Walker

The runs here are in pairs, the second member of which is for a second energy. Note that COUNT is listed as the same for both runs even though the second-energy run actually did no potential evaluations. Also, the S-matrix elements for the second energy run are different because a different energy was actually used.

COUNT	TIME	(I,F)	RE(I,F)	IM(I,.	(I,I)	(F,F)
TEST1/J4B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	1.700 ,	35.00)
450	.53	.9071E-10	.6655E-05	-.6814E-05	1.000	1.000
450	.13	.2956E-09	-.1719E-04	.4171E-06	1.000	1.000
TEST1/J4B2		(I,F)=(1, 5)		(RMIN,RMAX)=(	1.700 ,	35.00)
466	6.96	.1683E-08	.2401E-04	.3377E-04	.4917	.9551
466	1.08	.5259E-08	.9544E-05	-.7189E-04	.4740	.9217
TEST1/J4B3		(I,F)=(1,15)		(RMIN,RMAX)=(	1.700 ,	35.00)
217	22.52	.1170E-08	-.5173E-05	.3381E-04	.4699	.9551
217	3.69	.3402E-08	.4733E-04	-.3408E-04	.4506	.9218
TEST2/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.300 ,	700.0)
354	.67	.3959	.3540	.5202	.1788	.4984
354	.18	.3249	.3110	-.4777	.3457	.6317
TEST2/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	700.0)
593	9.67	.5437E-02	-.6972E-01	-.2402E-01	.8381	.2255
593	2.37	.3888E-01	.8061E-01	.1800	.8948	.1867
TEST2/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	700.0)
1003	82.16	.1708E-01	.7840E-01	-.1046	.6840	.3745
1003	29.47	.1707E-01	.7808E-01	-.1048	.6840	.3744
754	63.33	.1718E-01	.7896E-01	-.1046	.6834	.3756
754	21.85	.1717E-01	.7864E-01	-.1048	.6835	.3755
TEST2/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.300 ,	700.0)
995	1.51	.2301	-.9597E-01	.4700	.4584	.3194
995	.58	.2409	.3148	-.3765	.4437	.5653
TEST2/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	700.0)
1064	4.51	.1410E-01	.1112E-01	-.1182	.3927	.4787E-01
1064	1.59	.2326E-01	.1116	.1040	.3622	.1884
1064	1.59	.1307E-01	-.1143	.1988E-02	.3486	.4127
TEST2/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	700.0)
1338	41.42	.7975E-02	.8178E-01	.3589E-01	.9065	.4070
1338	14.14	.7975E-02	.8179E-01	.3585E-01	.9065	.4069
TEST3/J25B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.300 ,	7.000)
82	.32	.4726	-.2847	-.6257	.4214E-01	.3298
82	.02	.4676	-.6795	.7693E-01	.4631E-01	.3438
TEST3/J25B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	7.000)
102	4.70	.1707	-.3944	.1231	.3972	.2040E-01
102	.37	.1937	-.3456E-01	.4388	.3472	.1480E-01
TEST3/J25B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	7.000)
204	23.55	.6571E-01	-.2300	-.1132	.3698	.3122
204	5.88	.6576E-01	-.2302	-.1131	.3696	.3121
TEST3/J5B1		(I,F)=(1, 3)		(RMIN,RMAX)=(	3.300 ,	7.000)
215	.40	.4164E-01	.1185	.1662	.9104	.9577

COUNT	TIME	(I,F)	RE(I,F)	IM(I,F)	(I,I)	(F,F)
215	.12	.5624E-01	.2344	.3624E-01	.8832	.9427
TEST3/J5B2		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	7.000)
203	1.41	.2062	-.2516	.3780	.6997	.7642
203	.30	.2965	.8766E-01	.5374	.4793	.6292
203	.29	.3415	.4542	.3677	.3007	.5259
TEST3/J5B3		(I,F)=(1, 4)		(RMIN,RMAX)=(	3.300 ,	7.000)
313	14.04	.8604E-03	-.1354E-01	-.2602E-01	.9324	.9536
313	3.15	.8604E-03	-.1355E-01	-.2602E-01	.9324	.9536
TEST4/J5B1		(I,F)=(1, 2)		(RMIN,RMAX)=(	.5000E-05,	120.0)
280	.82	.4303E-02	-.4823E-01	.4446E-01	.9957	.9923
280	.19	.6328E-02	-.6456E-01	.4647E-01	.9936	.9887
TEST4/J5B2		(I,F)=(1, 2)		(RMIN,RMAX)=(	.5000E-05,	120.0)
139	6.60	.2892E-02	-.3884E-01	.3719E-01	.9964	.6563
139	1.23	.4104E-02	-.5046E-01	.3947E-01	.9947	.5780
TEST4/J5B3		(I,F)=(1, 2)		(RMIN,RMAX)=(	.5000E-05,	120.0)
132	13.58	.2856E-02	-.3962E-01	.3586E-01	.9963	.6045
132	3.07	.2856E-02	-.3962E-01	.3586E-01	.9963	.6045
102	11.49	.2865E-02	-.3967E-01	.3593E-01	.9963	.6040
102	2.29	.2865E-02	-.3967E-01	.3593E-01	.9963	.6040

APPENDIX B

Full S-matrices For All Test Problems

TEST1/J4B1

ENERGY = .2240E-01
RMIN = 2.500
RMAX = 45.00

COL	1		2	
ROW	REAL	IMAG	REAL	IMAG
1	.6422	-.7665	.6690E-05	-.6849E-05
2	.6690E-05	-.6849E-05	-.7512	.8601

TEST1/J4B2

ENERGY = .2240E-01
RMIN = 2.500
RMAX = 45.00

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.6187	-.5300	-.1551E-01	.3956	.8639E-01	.3580	.2911	.3622	-.2422E-04	.1508E-04
2	-.1551E-01	.5956	.2395	.7366	.3768	-.2419	-.1635	-.1268	.4164E-04	-.4084E-05
3	.8639E-01	.3580	.3768	-.2419	.2709	.9225	-.2605E-02	-.3056	.4594E-04	-.1491E-04
4	.2911	.3622	-.1635	-.1268	-.2605E-02	-.3056	.7304	-.3250	.6000E-04	-.4861E-04
5	.2422E-04	-.1508E-04	.4164E-04	-.4084E-05	.4594E-04	-.1491E-04	.6000E-04	-.4861E-04	-.7559	.6070
6	.3491E-05	-.1366E-05	-.6916E-05	-.5768E-05	-.2569E-05	-.1040E-05	-.6377E-05	-.6035E-05	-.3930E-01	.1223
7	.9715E-06	-.4409E-05	-.3199E-05	-.3384E-06	-.6821E-05	-.9180E-05	-.9058E-05	-.7588E-06	.3146E-01	.1076
8	-.3016E-05	-.3931E-05	-.4621E-05	-.1530E-07	-.3321E-05	.1897E-05	-.8431E-05	.7415E-05	.1186	.4261E-01

COL	6		7		8	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.3491E-05	-.3884E-05	.9715E-06	-.4409E-05	-.3016E-05	-.3931E-05
2	-.6916E-06	-.9788E-05	-.3199E-05	-.3384E-06	-.4621E-05	-.1530E-07
3	-.2689E-05	-.1040E-05	-.6821E-05	-.9180E-05	-.3321E-05	.1897E-05
4	-.6377E-05	-.6035E-05	-.5058E-05	-.7588E-06	-.8431E-05	.7415E-05
5	-.3930E-01	.1223	.3148E-01	.1076	.1186	.4261E-01
6	-.1636	-.9705	-.8694E-01	.8599E-01	.1506E-01	.1714E-02
7	-.8694E-01	.8599E-01	-.9320	-.3145	.5184E-01	.5085E-01
8	.1506E-01	.1714E-02	.5184E-01	.5085E-01	.1584	.9796

TEST1/J4B3

ENERGY = .2240E-01
RMIN = 2.500
RMAX = 45.00

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.5965	-.5378	-.5736E-01	.3803	.4574E-01	.3576	.2480	.3077	.6366E-01	-.4017E-01
2	-.5736E-01	.3803	.5635E-01	.6994	.3269	-.1877	-.1594	-.1254	.1198	-.2617
3	.4574E-01	.3576	.3269	-.1877	.9997E-01	.7535	.7585E-02	-.2655	-.8900E-01	-.3613E-01
4	.2480	.3877	-.1594	-.1254	.7585E-02	-.2655	.7078	-.1379	-.8396E-02	.2624E-01
5	.8566E-01	-.4017E-01	.1198	-.2617	-.8900E-01	-.3613E-01	-.8596E-02	.2624E-01	.8168	-.3320E-01
6	.6518E-01	-.5339E-01	.9384E-01	-.2591	-.3432E-01	-.8781E-01	-.2041E-01	.2983E-01	-.7626E-01	-.4306
7	.4801E-01	-.7071E-01	-.6285E-01	-.1360	-.5493E-01	-.1816	-.4769E-01	.2385E-01	-.1011	.4196E-01
8	.1271E-01	-.8804E-01	-.7790E-01	.2423E-01	-.1113	-.1910	-.1205	.1545E-01	.1108E-01	.1775E-01
9	-.5035E-01	-.9800E-01	.1499E-01	.5007E-01	-.2450E-01	.2443E-01	-.3575	.1166	.5382E-02	-.2596E-02
10	.6146E-02	-.5682E-02	-.7187E-03	-.4266E-01	-.9904E-02	-.6455E-02	-.1567E-02	.2275E-02	.9920E-01	-.1360
11	.5349E-02	-.6098E-02	-.1102E-01	-.2290E-01	-.1066E-01	-.1186E-01	-.2997E-02	.2414E-02	-.5360E-01	-.2703E-01
12	-.2856E-04	-.6379E-02	-.1198E-01	-.4160E-02	-.1820E-01	-.1083E-01	-.6135E-02	.5752E-02	-.4449E-02	-.6811E-02
13	-.5866E-02	-.4657E-02	-.2158E-02	-.4642E-02	-.1841E-01	-.2745E-02	-.9327E-02	.1171E-01	.1106E-02	-.471[illegible]E-03
14	-.6677E-02	-.1496E-04	-.1615E-02	-.3857E-03	-.3298E-02	-.3864E-02	-.6561E-03	.5341E-01	-.[illegible]E-04	-.1837E-03
15	-.5391E-03	.3398E-04	-.1680E-04	-.4534E-04	-.3454E-04	-.3849E-04	-.8106E-04	-.2951E-04	-.7859E-04	-.7377E-04
16	-.3348E-05	-.7960E-05	-.4544E-04	-.1105E-05	-.1201E-04	-.5810E-05	-.2243E-05	-.5962E-05	-.1246E-05	-.1528E-04
17	-.6554E-05	-.3193E-05	-.3956E-05	-.8906E-05	-.1803E-04	-.2849E-04	-.7458E-06	-.1118E-04	-.2801E-04	-.6066E-05
18	-.6191E-05	-.4531E-05	-.3517E-05	-.1772E-05	-.5625E-05	-.3997E-05	-.2723E-04	-.2698E-04	-.9271E-05	-.1025E-05

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.6518E-01	-.5339E-01	.4801E-01	-.7071E-01	.1271E-01	-.8804E-01	-.5035E-01	-.9801E-01	.6146E-02	-.5682E-02
2	.5384E-01	-.2531	-.6265E-01	-.1360	-.7790E-01	.2425E-01	.1499E-01	.5007E-01	-.7187E-03	-.4266E-01
3	-.5432E-01	-.6767E-01	-.3493E-01	-.1816	-.1113	-.1910	-.2450E-01	.2443E-01	-.9904E-02	-.6455E-02
4	-.2041E-01	.2983E-01	-.4769E-01	.2385E-01	-.1205	.1545E-01	-.3575	.1166	-.1567E-02	.2275E-02
5	-.7626E-01	-.4306	-.1011	.4196E-01	.1108E-01	.1775E-01	.5382E-02	-.2596E-02	.9920E-01	-.1360
6	.1744	.6304E-02	-.1594	-.1285	-.2803E-01	.5171E-01	.7608E-02	-.1538E-02	.1620E-01	-.9613E-02
7	-.1594	-.2665	.6199	-.9564	.2466	-.1766E-01	.1781E-01	-.1574E-01	-.2020E-01	-.1941E-01
8	-.2607E-01	.5111E-01	-.2466	-.1766E-01	-.3043	-.8528	-.2232E-01	.1146	-.2375E-02	.3379E-02
9	.7606E-02	-.1338E-02	.1781E-01	.1574E-01	-.2232E-01	.1146	-.8463	.2873	.4782E-03	.5694E-04
10	.1820E-01	-.9613E-01	-.2020E-01	-.1941E-01	-.2375E-02	.3379E-02	.4782E-03	.5694E-04	-.4341E-01	.9667
11	.3645E-01	-.1011	-.1662E-01	-.7807E-01	-.1715E-01	.4598E-03	.6256E-03	.1193E-02	.1475	-.5265E-01
12	-.3166E-01	-.4544E-02	-.5305E-01	-.1070	-.6034E-01	-.1444E-01	-.7316E-03	.5615E-02	-.8452E-02	-.1979E-01
13	.1223E-02	.4481E-02	-.1578E-01	.4344E-01	-.1370	.1433E-01	-.7610E-02	.2895E-01	-.2918E-03	.7285E-02
14	.2761E-03	-.3525E-03	.1934E-02	-.2398E-03	-.1125E-01	.8646E-02	.5216E-01	.1549	.3058E-04	-.8889E-05
15	-.8012E-04	.9709E-04	-.5619E-04	.1249E-03	.9735E-03	.1594E-03	.1265E-03	.1919E-03	-.2036E-03	-.1007E-03
16	.1119E-03	-.2167E-05	.4526E-04	-.2329E-04	-.5146E-04	.4576E-06	.1955E-06	.4443E-05	.5718E-06	.4135E-05
17	.2083E-05	-.1676E-04	.6067E-04	-.5871E-04	.1523E-04	-.1513E-03	-.4953E-05	.2345E-04	.1633E-05	-.3495E-04
18	.7291E-05	.2761E-05	.1203E-05	.4259E-05	-.1628E-04	-.6529E-05	-.1432E-03	-.5107E-04	.1848E-05	.1428E-04

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.5349E-02	-.6098E-02	-.2856E-04	-.6379E-02	-.3866E-02	-.4657E-02	-.6677E-02	-.1496E-04	-.5391E-03	.3398E-04
2	-.1102E-01	-.2290E-01	-.1198E-01	-.4160E-02	-.1820E-01	-.1083E-01	-.6135E-02	.5752E-02	-.1680E-04	-.4534E-04
3	-.1066E-01	-.1186E-01	-.1820E-01	-.1083E-01	-.1841E-01	-.2745E-02	-.3298E-02	-.3864E-02	-.5494E-04	-.3849E-04
4	-.2997E-02	.2114E-02	-.6135E-02	.3752E-02	-.9327E-02	.1171E-01	-.6561E-03	-.5341E-01	-.8106E-04	-.2951E-04
5	-.1360E-01	-.2783E-01	-.4449E-02	.6811E-02	.1106E-02	-.4710E-03	-.4449E-04	-.1037E-03	-.1859E-04	-.7372E-04
6	.3645E-01	-.1011	-.3160E-01	-.4344E-02	.1223E-02	-.4487E-02	-.2761E-03	-.3525E-03	-.8012E-04	-.9709E-04
7	-.1862E-01	-.7807E-01	-.5305E-01	-.1070	-.1578E-01	.2151E-01	-.1934E-02	-.2398E-03	-.5619E-04	-.1249E-03
8	-.1715E-01	.4598E-03	-.6034E-01	-.1444E-01	-.1370	.1433E-01	-.1125E-01	.8646E-02	-.5735E-03	-.1594E-03
9	.6236E-03	.1193E-02	-.7316E-03	.5615E-02	-.7610E-02	.2895E-01	-.5216E-01	.1549	-.1265E-03	-.1919E-03
10	.1475	-.5265E-01	-.8452E-02	-.1099E-01	-.2918E-03	.7285E-02	.3058E-04	-.8889E-05	-.2036E-03	-.1007E-03
11	.3585	.8953	.9429E-01	-.1300	-.1066E-01	.2654E-03	.2654E-03	.1781E-02	-.2018E-03	-.2850E-04
12	.9428E-01	-.1300	.9598	.1377	-.6988E-01	.9487E-01	-.1015E-03	.3494E-02	-.1979E-03	.7489E-04

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
13	-.1068E-01	.5655E-03	-.6988E-01	-.9487E-01	.2347	-.9523	-.3866E-01	.3525E-01	-.1176E-03	.2039E-03
14	.2054E-03	.1781E-03	-.1015E-03	.3494E-02	-.3866E-01	.3525E-01	-.9840	.5147E-01	.1091E-03	.5010E-03
15	-.2018E-03	-.2850E-04	-.1979E-03	.7489E-04	-.1176E-03	.2039E-03	.1091E-03	.5010E-03	-.7659	.6070
16	.1244E-03	.2571E-03	.9265E-04	.5023E-04	-.5525E-04	-.1601E-04	.2405E-04	.8618E-05	-.3928E-01	.1222
17	.1178E-03	.6394E-04	.3100E-03	.3307E-04	.3339E-03	-.2025E-03	-.1781E-04	.5382E-04	.3149E-01	.1075
18	-.1105E-03	.6703E-05	-.6061E-05	-.1328E-04	-.1155E-04	-.1103E-03	-.3927E-05	-.3323E-03	.1183	.4259E-01

COL	16		17		18	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.3348E-05	.7960E-05	.6554E-05	.3193E-05	.6191E-05	-.4531E-05
2	.4544E-04	.1105E-05	.3956E-05	.8906E-05	.3517E-05	-.1772E-05
3	.1201E-04	-.5810E-05	.1803E-04	-.2849E-04	.5625E-05	-.3997E-05
4	-.2243E-05	-.9962E-05	-.7468E-06	-.1118E-04	-.2723E-04	-.2698E-04
5	.1246E-05	.1528E-04	-.2801E-04	-.6661E-05	.9271E-05	.1025E-05
6	.1119E-05	-.2167E-05	.2083E-05	-.1676E-04	.7291E-05	.2761E-05
7	.4526E-04	-.2329E-04	.6067E-04	-.5871E-04	.1203E-05	.4259E-05
8	-.5146E-04	.4576E-06	.1395E-04	-.1513E-03	-.1628E-04	-.6529E-05
9	.1955E-06	.4443E-05	-.4953E-05	.2345E-04	-.1432E-03	-.5107E-04
10	.5218E-04	.4755E-03	.7639E-05	-.3495E-04	.1848E-05	.1428E-04
11	.1244E-03	.2571E-03	.1178E-03	.6394E-04	-.1105E-03	.6703E-05
12	.9265E-04	.5023E-04	.3100E-03	.3307E-04	.6061E-05	-.1328E-04
13	-.5525E-04	-.1601E-04	.3339E-03	-.2025E-03	-.1155E-04	-.1103E-03
14	.2405E-04	.8618E-05	-.1781E-04	.5382E-04	-.3927E-05	-.3323E-03
15	-.3928E-01	.1222	.3149E-01	.1075	.1183	.4259E-01
16	-.1638	-.9705	-.8696E-01	.8403E-01	.1306E-01	.1712E-02
17	-.8696E-01	.8403E-01	-.9520	-.3144	.5186E-01	.5086E-01
18	.1306E-01	.1712E-02	.5186E-01	.5086E-01	.1585	.9795

TEST1/J4B4

ENERGY = .22400E-01
RMIN = 2.500
RMAX = 45.00

ROW	COL 1 REAL	1 IMAG	2 REAL	2 IMAG	3 REAL	3 IMAG	4 REAL	4 IMAG	5 REAL	5 IMAG
1	.5967	-.3378	-.5694E-01	.3800	.4598E-01	.3572	.2480	.3872	.6481E-01	-.3927E-01
2	-.5694E-01	.3800	.5764E-01	.6971	.3262	-.1888	-.1397	-.1252	.1282	-.2607
3	.4598E-01	.3572	.3262	-.1888	.1001	.7321	.6990E-02	-.2657	-.8436E-01	-.3826E-01
4	.2480	.3872	-.1397	-.1252	.6990E-02	-.2657	.7057	-.1589	-.8861E-02	.2615E-01
5	.6481E-01	-.3927E-01	.1282	-.2607	-.8436E-01	-.3826E-01	-.8861E-02	.2615E-01	.8220	.4735E-02
6	.6658E-01	-.5256E-01	.6157E-01	-.2537	-.5210E-01	-.8962E-01	-.2095E-01	.2846E-01	-.5786E-01	-.4251
7	.4960E-01	-.7035E-01	-.5903E-01	-.1588	-.3025E-01	-.1645	-.4824E-01	.2270E-01	-.9980E-01	.3682E-01
8	.1433E-01	-.8849E-01	-.7876E-01	.2249E-01	-.1074	-.1963	-.1216	.1222E-01	.1005E-01	.1780E-01
9	-.4916E-01	-.9965E-01	.1460E-01	[illegible]	-.2623E-01	.7416E-01	-.3641	.1080	.3458E-02	-.2471E-02
10	.6221E-02	-.5446E-02	.9526E-03	-.4210E-01	-.9461E-02	-.6705E-02	-.1593E-02	.2195E-02	.1042	-.1277
11	.3467E-02	-.5930E-02	-.9950E-02	-.2299E-01	-.1004E-01	-.1208E-01	-.2993E-02	.1966E-02	-.3056E-01	-.2794E-01
12	.1400E-03	-.6313E-02	-.1158E-01	-.4558E-02	-.1752E-01	-.1134E-01	-.6141E-02	.3432E-02	-.4450E-02	.6116E-02
13	-.3689E-02	-.4671E-02	-.2248E-02	.4457E-02	-.1819E-01	.2002E-02	-.9571E-02	.1114E-01	.1003E-02	.4972E-03
14	-.6573E-02	-.1887E-03	.1571E-02	.4165E-03	.3088E-02	.3878E-02	-.5329E-03	.3276E-01	.5142E-04	-.1756E-03
15	-.5160E-04	-.4905E-04	-.4259E-03	.1181E-03	-.7528E-04	.1032E-03	.1463E-04	.1886E-04	-.2248E-02	-.3891E-03
16	-.4761E-04	-.1840E-05	-.9299E-04	.1760E-03	-.4136E-04	.1474E-03	.2451E-04	.2647E-04	-.2958E-04	.3199E-03
17	-.2055E-04	.2855E-04	.4976E-04	.5739E-04	.8475E-04	.1201E-03	.5959E-04	.1025E-04	.3748E-04	-.1031E-04
18	.1502E-04	.2074E-04	.1039E-04	-.1723E-04	.8752E-04	-.2839E-04	.5514E-04	-.7027E-04	-.2903E-05	-.2740E-05
19	.1736E-04	-.1123E-04	-.4521E-05	.6150E-06	-.1495E-04	-.5515E-05	-.9016E-04	-.9550E-04	-.3486E-07	.4472E-06
20	.1245E-04	.3094E-04	.2725E-04	.1095E-04	.3445E-04	.3212E-05	.5879E-04	-.2063E-04	-.2663E-04	.8939E-05
21	.2278E-05	.7481E-06	.1680E-04	-.5172E-06	.3522E-05	-.5905E-06	-.4323E-05	-.7686E-05	.3555E-04	.3030E-04
22	.2514E-05	-.8379E-06	.5850E-06	-.2339E-05	.4763E-05	-.1381E-04	-.1919E-05	-.4009E-05	-.9851E-05	-.2781E-05
23	.8515E-06	-.3411E-05	-.3768E-05	-.4357E-06	-.3341E-05	-.5543E-06	-.1519E-04	-.9005E-05	.2288E-05	.2050E-05

ROW	COL 6 REAL	6 IMAG	7 REAL	7 IMAG	8 REAL	8 IMAG	9 REAL	9 IMAG	10 REAL	10 IMAG
1	.6658E-01	-.5256E-01	.4960E-01	-.7035E-01	.1433E-01	-.8849E-01	-.4916E-01	-.9965E-01	.6221E-02	-.5446E-02
2	.6157E-01	-.2537	-.5903E-01	-.1588	-.7876E-01	.2249E-01	.1460E-01	.5043E-01	.9526E-03	-.4210E-01
3	-.5210E-01	-.8962E-01	-.3025E-01	-.1643	-.1074	-.1963	-.2623E-01	.7416E-01	-.9461E-02	-.6705E-02
4	-.2095E-01	.2846E-01	-.4824E-01	.2270E-01	-.1216	.1222E-01	-.3641	.1080	-.1593E-02	.2195E-02
5	-.5786E-01	-.4251	-.9980E-01	.3682E-01	.1005E-01	.1780E-01	.3458E-02	-.2471E-02	.1042	-.1277
6	.7803	.3645E-01	-.1460	-.2694	-.2924E-01	.4919E-01	.7521E-02	-.1065E-02	.2329E-01	-.9216E-01
7	-.1460	-.2694	.6479	-.5717	-.2410	-.2732E-01	.1680E-01	.1596E-01	-.1822E-01	-.1586E-01
8	-.2924E-01	.4919E-01	-.2410	-.2732E-01	-.2641	-.8677	-.7659E-01	.1112	-.2398E-02	.3040E-02
9	.7521E-02	-.1065E-02	.1680E-01	.1596E-01	-.2659E-01	.1112	-.8598	.2424	.4534E-03	.7064E-04
10	.2329E-01	-.9216E-01	-.1822E-01	-.1586E-01	-.2398E-02	.3040E-02	.4534E-03	.7064E-04	-.9671E-01	.9648
11	.4062E-01	-.9752E-01	-.1401E-01	-.7689E-01	-.1632E-01	-.5703E-03	.5295E-03	.1144E-02	.1403	-.2421E-01
12	-.2978E-01	-.5489E-02	-.4697E-01	-.1070	-.5763E-01	-.1720E-01	-.1029E-02	.5456E-02	-.7413E-02	-.9973E-02
13	.9408E-03	.4213E-02	-.1586E-01	.1964E-01	-.1338	.7865E-02	-.8936E-02	.2745E-01	-.2450E-03	.6236E-03
14	.2737E-03	-.3013E-03	.1808E-02	-.1437E-03	.1022E-01	.8645E-02	.2407E-01	.1514	.2669E-04	-.7462E-05
15	-.1544E-02	.1112E-03	-.3704E-03	.2961E-03	.1140E-04	.6832E-04	.4116E-05	-.1978E-05	.2220E-01	-.1305E-01
16	-.9118E-03	.6278E-03	-.6264E-03	.8929E-03	.5892E-04	.3124E-03	.2345E-04	.1543E-05	-.1415E-02	-.1265E-02
17	.1587E-03	.1118E-03	.2791E-03	.9420E-03	.5757E-03	.4728E-03	.9499E-04	-.3482E-04	-.8053E-05	.1010E-03
18	-.1435E-05	-.1843E-04	.7576E-04	-.1102E-03	.8450E-03	-.3919E-03	.8399E-04	-.3114E-03	.2349E-05	-.2922E-05
19	-.5186E-06	[illegible]	-.5511E-05	.2981E-05	-.5874E-04	-.3581E-05	-.7948E-03	-.4053E-03	-.7660E-07	.2651E-07
20	-.2930E-04	[illegible]	-.2638E-04	.2378E-04	-.1556E-04	.3835E-04	.1366E-04	.5759E-04	-.1350E-05	.1168E-04
21	.3517E-04	.2297E-04	.1626E-04	.4812E-05	-.1538E-04	.1167E-05	.4461E-05	.5604E-05	-.3079E-05	-.1038E-03
22	.1990E-05	-.9927E-06	.2998E-04	-.7831E-05	.4678E-04	-.3663E-04	-.1497E-05	.1220E-04	-.1116E-04	-.6158E-06
23	.1725E-05	.2794E-05	.8472E-06	.3210E-05	-.1049E-05	-.3267E-05	-.4226E-04	-.4110E-04	.1307E-05	.3752E-06

ROW	COL 11 REAL	11 IMAG	12 REAL	12 IMAG	13 REAL	13 IMAG	14 REAL	14 IMAG	15 REAL	15 IMAG
1	.3467E-02	-.5930E-02	.1400E-03	-.6313E-02	-.3689E-02	-.4671E-02	-.6573E-02	-.1887E-03	-.5160E-04	-.4905E-04
2	-.9950E-02	-.2299E-01	[illegible]	-.4558E-02	-.2248E-02	.4457E-02	.1571E-02	.4165E-03	-.4259E-03	.1181E-03

ROW	COL 11 REAL	11 IMAG	12 REAL	12 IMAG	13 REAL	13 IMAG	14 REAL	14 IMAG	15 REAL	15 IMAG
3	-.1004E-01	-.1208E-01	-.1752E-01	-.1134E-01	-.1819E-01	.2002E-02	.3088E-02	.3878E-02	-.7528E-04	.1032E-03
4	-.2993E-02	.1966E-02	-.6141E-02	.3432E-02	-.9571E-02	.1114E-01	-.5329E-03	.3276E-01	.1463E-04	.1886E-04
5	-.3056E-01	-.2794E-01	-.4450E-02	.6116E-02	.1003E-02	.4972E-03	.5142E-04	-.1756E-03	-.2248E-02	-.3891E-03
6	.4062E-01	-.9752E-01	-.2978E-01	-.5489E-02	.9408E-03	.4213E-02	.2737E-03	-.3013E-03	-.1544E-02	.1112E-03
7	-.1401E-01	-.7689E-01	-.4697E-01	-.1070	-.1586E-01	.1964E-01	.1808E-02	-.1437E-03	-.3704E-03	.2961E-03
8	-.1632E-01	-.5703E-03	-.5763E-01	-.1720E-01	-.1338	.7865E-02	.1022E-01	.8645E-02	.1140E-04	.6832E-04
9	.5295E-03	.1144E-02	-.1029E-02	.5456E-02	-.8936E-02	.2745E-01	.2407E-01	.1514	.4116E-05	-.1978E-05
10	.1403	-.2421E-01	-.7413E-02	-.9973E-02	-.2450E-03	.6236E-03	.2669E-04	-.7462E-05	.2220E-01	-.1305E-01
11	.3251	.9119	.9411E-01	-.1195	-.9619E-02	.3938E-03	.1764E-03	.1509E-03	.2481E-02	-.5258E-02
12	.9411E-01	-.1195	.9561	.1760	-.6249E-01	-.9238E-01	-.1349E-03	.3145E-02	-.4007E-03	-.5086E-03
13	-.9619E-02	.3938E-03	-.6249E-01	-.9238E-01	.2736	-.9434	-.3792E-01	.3181E-01	-.2514E-04	.2563E-04
14	.1764E-03	.1509E-03	-.1349E-03	.5143E-02	-.3792E-01	.3181E-01	-.9862	.9657E-02	.7231E-06	.9958E-07
15	.2481E-02	-.5258E-02	-.4007E-03	-.5086E-03	-.2514E-04	.2563E-04	.7231E-06	.9958E-07	.9023	.4290
16	.2037E-02	-.1802E-01	-.3776E-02	-.4746E-02	-.5168E-03	.2155E-03	.9648E-05	.1041E-04	-.8164E-02	-.3233E-01
17	-.1445E-02	.7925E-03	-.1499E-01	-.2788E-02	-.2983E-02	.2969E-02	.1139E-03	.1392E-03	-.1515E-03	.6613E-03
18	.6476E-04	.7669E-05	.6753E-03	.7719E-03	.2896E-02	.1288E-01	.1686E-02	.3258E-03	.1640E-05	-.6797E-05
19	-.8633E-06	-.4336E-06	-.6835E-05	-.1607E-04	.5678E-04	-.3750E-05	.5067E-02	-.9995E-02	.2040E-08	.2332E-07
20	.9803E-06	.9663E-05	.3481E-05	.8285E-05	.6204E-05	.6807E-05	.1248E-04	.5361E-05	.1061E-04	.3914E-05
21	-.2425E-04	-.5858E-04	-.2514E-04	-.1454E-04	-.4337E-06	.6435E-05	.1954E-05	-.6865E-06	-.4683E-04	-.5921E-04
22	-.2697E-04	-.1635E-04	-.5525E-04	-.9703E-05	-.5308E-04	.2831E-04	.5706E-05	.2159E-05	-.7399E-05	.1996E-05
23	.2970E-06	.1790E-05	-.7265E-05	.7261E-05	.7056E-05	.2654E-04	.6199E-04	.5775E-04	.1974E-06	-.4361E-06

ROW	COL 16 REAL	16 IMAG	17 REAL	17 IMAG	18 REAL	18 IMAG	19 REAL	19 IMAG	20 REAL	20 IMAG
1	-.4761E-04	-.1840E-05	-.2055E-04	.2855E-04	.1502E-04	.2074E-04	.1736E-04	-.1123E-04	.1245E-04	.3094E-04
2	-.9299E-04	.1760E-03	.4976E-04	.5739E-04	.1039E-04	-.1723E-04	-.4521E-05	.6150E-06	.2725E-04	.1095E-04
3	-.4136E-04	.1474E-03	.8475E-04	.1201E-03	.8752E-04	-.2839E-04	-.1495E-04	-.5515E-05	.3445E-04	.3212E-05
4	.2451E-04	.2647E-04	.5959E-04	.1025E-04	.5514E-04	-.7027E-04	-.9016E-04	-.9550E-04	.5879E-04	-.2063E-04
5	-.2958E-04	.5199E-03	.3748E-04	-.1031E-04	-.2903E-05	-.2740E-05	-.3486E-07	.4472E-06	-.2663E-04	.8939E-05
6	-.9118E-03	.6278E-03	.1587E-03	.1118E-03	-.1435E-05	-.1843E-04	-.5186E-06	.1013E-05	-.2930E-04	.1403E-04
7	-.6264E-03	.8929E-03	.2791E-03	.9420E-03	.7576E-04	-.1102E-03	-.5511E-05	.2981E-05	-.2638E-04	.2378E-04
8	.5892E-04	.3124E-03	.5757E-03	.4728E-03	.8450E-03	-.3919E-03	-.5874E-04	-.3581E-05	-.1556E-04	.3835E-04
9	.2345E-04	.1543E-05	.9499E-04	-.3482E-04	.8399E-04	-.3114E-03	-.7948E-03	-.4053E-03	.1366E-04	.5759E-04
10	-.1415E-02	-.1265E-02	-.8053E-05	.1010E-03	.2349E-05	-.2922E-05	-.7660E-07	.2651E-07	-.1350E-05	.1168E-04
11	.2037E-02	-.1802E-01	-.1445E-02	.7925E-03	.6476E-04	.7669E-05	-.8633E-06	-.4336E-06	.9803E-06	.9663E-05
12	-.3776E-02	-.4746E-02	-.1499E-01	-.2788E-02	.6753E-03	.7719E-03	-.6835E-05	-.1607E-04	.3481E-05	.8285E-05
13	-.5168E-03	.2155E-03	-.2983E-02	.2969E-02	.2896E-02	.1288E-01	.5678E-04	-.3750E-03	.6204E-05	.6807E-05
14	.9648E-05	.1041E-04	.1139E-03	.1392E-03	.1686E-02	.3258E-03	.5067E-02	-.9995E-02	.1248E-04	.5361E-05
15	-.8164E-02	-.3233E-01	-.1315E-03	.6613E-03	.1640E-05	-.6797E-05	.2040E-08	.2332E-07	.1061E-04	.3914E-05
16	.5930	-.8033	-.5726E-01	.1354E-01	.5627E-03	-.1166E-03	-.2181E-05	.1149E-05	.7752E-05	-.3013E-05
17	-.3726E-01	.1354E-01	-.9699	-.2379	.2413E-01	.1487E-01	-.1554E-03	-.6515E-04	.1446E-05	-.6824E-05
18	.5627E-03	-.1166E-03	.2413E-01	.1487E-01	.6473	.7615	-.7114E-02	-.9124E-02	-.5172E-05	-.2946E-05
19	-.2181E-05	.1149E-05	-.1554E-03	-.6515E-04	-.7114E-02	-.9124E-02	-.5796	-.8147	-.5042E-05	.4940E-05
20	.7752E-05	-.3013E-05	.1446E-05	-.6824E-05	-.5172E-05	-.2946E-05	-.3042E-05	.4940E-05	-.7659	.6067
21	-.3539E-04	-.5245E-05	-.6684E-05	.9768E-05	.6639E-06	-.2465E-05	.2471E-08	.4142E-06	-.3988E-01	.1227
22	-.2234E-04	.1019E-04	-.7783E-05	.3386E-04	.2487E-04	.1566E-04	-.2032E-05	.6490E-06	.3130E-01	.1081
23	.3788E-06	.1093E-05	.4550E-05	.3185E-05	.1328E-04	-.7335E-05	-.1397E-04	-.3476E-04	.1189	.4305E-01

ROW	COL 21 REAL	21 IMAG	22 REAL	22 IMAG	23 REAL	23 IMAG
1	.2278E-05	.7481E-06	.2514E-05	-.8379E-06	.8515E-06	-.3411E-05
2	.1680E-04	-.5172E-06	.5850E-06	-.2339E-05	-.3768E-05	-.4357E-06
3	.3522E-05	-.5905E-06	.4763E-05	-.1381E-04	-.3341E-05	-.5543E-06
4	-.4323E-05	-.7686E-05	-.1919E-05	-.4009E-05	-.1319E-04	-.9005E-05
5	.3555E-04	.3030E-04	-.9851E-05	-.2781E-05	.2288E-05	.2050E-05
6	.3517E-04	.2297E-04	.1990E-05	-.9927E-06	.1725E-05	.2794E-05
7	.1626E-04	.4812E-05	.2998E-04	-.7831E-05	.8472E-06	.3210E-05
8	-.1538E-04	.1167E-05	.4678E-04	-.3663E-04	-.1049E-05	-.3267E-05
9	.4461E-05	.5604E-05	-.1497E-05	.1220E-04	-.4228E-04	-.4110E-04
10	-.3079E-05	-.1038E-03	-.1116E-04	-.6158E-06	.1307E-05	.3752E-06

COL	21		22		23	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG
11	-.2625E-04	-.5638E-04	-.2687E-04	-.1835E-04	.2997E-06	.1790E-05
12	-.2514E-04	-.1454E-04	-.5529E-04	-.9703E-05	-.2265E-05	.7261E-05
13	-.4357E-06	.6455E-05	-.5308E-04	.2851E-04	.2056E-05	.2834E-04
14	.1954E-05	-.6865E-06	.5706E-05	.2159E-05	.6199E-04	.5975E-05
15	-.4685E-04	-.5921E-04	-.7309E-05	.1996E-05	.1974E-06	-.4561E-06
16	-.3559E-04	-.5245E-05	-.2234E-04	.1019E-06	.5788E-06	.1093E-05
17	-.6684E-05	.9768E-05	-.7783E-05	.3386E-04	.4850E-05	.3185E-05
18	.6639E-06	-.2465E-05	.2487E-04	.1566E-04	.1328E-04	-.7335E-05
19	.2471E-08	.4142E-06	-.2052E-05	.6490E-06	-.1597E-04	-.5875E-04
20	-.5988E-01	.1227	.3130E-01	.1681	.1189	.4505E-01
21	-.1502	-.9719	-.8644E-01	.8291E-01	.1504E-01	.1277E-02
22	-.8644E-01	.8291E-01	-.9310	-.3180	.5132E-01	.5056E-01
23	.1504E-01	.1777E-02	.5132E-01	.5056E-01	.1346	.9601

TEST2/J2581

ENERGY = .1950E-02
RMIN = 3.000
RMAX = 800.0

COL	1		2		3	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.4049	-.1148	.1573	.6346	.3484	.5234
2	.1573	.6345	.5927	-.3411	-.8813E-01	.3117
3	.3484	.5234	-.8813E-01	.3117	.2590	-.6655

TEST2/J2582

ENERGY = .1050E-02
RMIN = 3.000
RMAX = 800.0

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.1894	-.8943	.1235	.6620E-01	.1740	.1300	-.1027E-01	-.2516E-01	.2854E-01	.1356E-01
2	.1235	.6620E-01	.5620E-01	-.5783	.5592	-.4251E-01	-.2301E-01	-.1940	-.4387E-01	.7610E-01
3	.1740	.1300	.5592	-.4251E-01	.9444E-01	-.6317	-.2510	-.1561E-01	-.3911E-01	-.8456E-01
4	-.1027E-01	-.2516E-01	-.2397E-01	-.1940	-.2310	-.1561E-01	.3144	-.5549	.3759	-.1142
5	.2854E-01	.1356E-01	-.4387E-01	.7610E-01	-.3911E-01	-.8436E-01	.3759	-.1142	-.6980	-.2658
6	.1649	.1324E-01	.1202	.1717	-.9211E-01	.4457E-01	-.3844	-.4789E-01	.1757	-.2324
7	.1467E-01	.5934E-01	-.1748	-.4280	.1234	.2441	-.2433	-.1150	-.1079	-.3519E-01
8	-.2789E-01	-.3477E-01	-.1054	-.2081E-01	.5261E-02	-.5705E-01	-.1590	-.4819E-01	-.2679	-.1418
9	-.1076	-.3407E-01	.2259E-01	.6564E-01	-.1590	-.4551E-01	-.1920	-.6540E-01	-.2787	-.4328E-01
10	-.2019	.6041E-01	.1032	.2973E-02	-.1975	.1584	-.4929	-.3801E-02	-.1885E-01	.3019E-01

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.1649	.1324E-01	.1467E-01	.5934E-01	-.2789E-01	-.3477E-01	-.1076	-.3407E-01	-.2019	.6041E-01
2	.1202	.1717	-.1748	-.4280	-.1054	-.2081E-01	.2259E-01	.6564E-01	.1032	.2973E-02
3	-.9211E-01	.4457E-01	.1234	.2441	.5261E-02	-.5705E-01	-.1590	-.4551E-01	-.1975	.1584
4	-.3844	-.4789E-01	-.2433	-.1150	-.1227	-.4819E-01	-.1920	-.6540E-01	-.4929	-.3801E-02
5	.1757	-.2324	-.1079	-.3519E-01	-.2679	-.1418	-.2787	-.4328E-01	-.1885E-01	.3019E-01
6	-.3678E-01	-.6152	-.1027	-.4436	-.9754E-01	-.3833E-01	.1768E-01	.1233	.1652	.2046
7	-.1027	-.4436	.1839	.3786	.3024	-.2450	-.1033	-.2431	-.7345E-01	-.1034
8	-.9754E-01	-.3833E-01	.3024	-.2450	-.5965E-01	.4986	.4473	-.3465	-.3721	-.2720E-01
9	.1768E-01	.1233	-.1033	-.2431	.4473	-.3465	.1904	.4468	-.3493	-.2767
10	.1652	.2046	-.7345E-01	-.1034	-.3721	-.2720E-01	-.5493	-.2767	-.4131E-01	-.4665

TEST2/J2583

ENERGY = .1950E-02
RMIN = 3.000
RMAX = 800.0

ROW	COL 1 REAL	COL 1 IMAG	COL 2 REAL	COL 2 IMAG	COL 3 REAL	COL 3 IMAG	COL 4 REAL	COL 4 IMAG	COL 5 REAL	COL 5 IMAG
1	.6255	-.6502E-01	.2326	-.1000	.2182	.5234E-01	.7783E-01	-.1053	.9925E-01	-.6567E-02
2	.2326	-.1000	-.2979E-01	.1937	-.6175E-01	-.3567	.1551	-.2196E-01	-.2822	-.2760
3	.2182	.5234E-01	-.6175E-01	-.3567	-.4221	.2299	-.2429	-.2129	.6876E-02	-.2042
4	.7783E-01	-.1053	.1551	-.2196E-01	-.2429	-.2129	-.1909	.5815	.1959	.1165
5	.9925E-01	-.6567E-02	-.2822	-.2760	.6876E-02	-.2042	.1959	.1165	.5797E-01	.5978
6	-.9926E-01	.2568E-01	-.1805	-.3791	.3097	.1194	-.1072	.8498E-01	.1217	.1361E-01
7	-.1599	.1101	.7148E-01	-.2463	.1350	-.2252	-.7171E-01	-.1916	.1747	.1642
8	.3715E-01	.4298E-01	-.2926E-01	-.2576	-.1049	-.1763	.5680E-01	-.7019E-01	-.9297E-01	-.8149
9	-.1571E-01	.5100E-01	.8835E-01	-.1726E-01	.9703E-03	.5760E-01	-.1100	.1609	-.1591	-.1194
10	.1020	-.1319	.7126E-01	.1677	-.6243E-01	.1044	.1794	.4010	.2229E-02	.8901E-01
11	.9462E-01	-.1680	-.3462E-01	.1904	.6717E-01	-.1067	-.1311E-01	-.1443	-.2098E-02	.1099
12	-.6506E-01	-.2001E-01	.8921E-01	-.3117E-01	.1609	.1639E-01	-.1189	.7035E-01	-.9529E-01	-.3522
13	.7156E-02	-.1773E-01	.1888E-01	.2656E-01	.1053	-.1300	.3084E-02	.1766E-01	.1276	-.1200E-01
14	-.7780E-01	.2987E-01	-.1517E-01	-.6402E-01	.1350	-.4797E-01	.1263	.4933E-01	-.1419E-01	-.2072
15	-.2859E-02	-.4392E-01	-.2870	-.7917E-01	-.2312E-01	.1743	[illegible]	-.1277	-.1798	.9154E-01
16	-.1170	-.2868E-01	.8409E-01	-.2370E-01	-.6974E-02	-.1490	-.1881E-01	.4269E-01	-.1067	-.1129
17	-.7085E-01	-.1486E-01	.1574	-.2721E-01	.7566E-01	.2694E-02	-.7182E-01	.3815E-01	.4742E-01	.7251E-01
18	-.1255E-03	-.5283E-01	-.2468E-01	.3713E-01	-.1459E-01	.1954E-02	-.2903E-01	-.3194E-01	.2021	.1080
19	-.6566E-02	.4521E-03	.3161E-01	-.3025E-01	.5851E-01	-.5438E-01	.7116E-01	.3074E-01	.1754E-01	.1752E-01
20	.4171E-01	.6940E-03	-.5555E-01	.2143	-.1710	.4645E-01	.5205E-03	.2627E-01	-.4750E-01	.4137E-01
21	.7667E-01	-.3714E-01	-.7821E-01	.1499E-01	-.4887E-01	.2471E-01	.7089E-02	.4366E-01	.2444	[illegible]
22	-.6802E-01	-.6200E-02	.3094E-01	.4674E-01	.5799E-01	.8536E-01	-.2886E-01	.3550E-01	.2887E-01	[illegible]

ROW	COL 6 REAL	COL 6 IMAG	COL 7 REAL	COL 7 IMAG	COL 8 REAL	COL 8 IMAG	COL 9 REAL	COL 9 IMAG	COL 10 REAL	COL 10 IMAG
1	-.9926E-01	.2568E-01	-.1599	.1101	.3715E-01	.4298E-01	-.1571E-01	.5100E-01	.1020	[illegible]
2	-.1805	-.3791	.7148E-01	-.2463	-.2926E-01	-.2576	.8835E-01	-.1726E-01	[illegible]	[illegible]
3	.3097	.1194	.1350	-.2252	-.1049	-.1763	.9703E-03	.5760E-01	-.6243E-01	.1044
4	-.1072	.8498E-01	-.7171E-01	-.1916	.5680E-01	-.7019E-01	-.1100	.1609	.1794	[illegible]
5	.1217	.1361E-01	.1747	.1642	-.9297E-01	-.8149E-01	-.1591	-.1194	[illegible]	[illegible]
6	-.3656	.1616	-.5471E-02	-.2335	.2157	.6763E-01	.2097	.5648E-01	[illegible]	[illegible]
7	-.5471E-02	-.2335	-.2989	-.2545	-.1396	-.2937	.1764	[illegible]	[illegible]	[illegible]
8	.2157	.6763E-01	-.1396	-.2937	.3540	.3154	-.1205	-.2451	[illegible]	[illegible]
9	.2097	.5648E-01	.1764	.7793E-01	-.1205	-.2451	.3347	-.3096	[illegible]	[illegible]
10	.4555E-01	.2650E-01	-.4520E-01	-.1946	.7506E-01	.6456E-01	.1609	-.9262E-01	-.3959	-.1264
11	.2373	.2429	-.1986	-.2084	-.1658	.2812E-01	.9528E-01	-.5461E-01	[illegible]	[illegible]
12	-.5996E-01	.2278	-.5531E-01	-.5038E-01	-.1092	-.1134	-.5526	-.7561E-01	[illegible]	[illegible]
13	-.2590E-01	-.2578E-01	.6746E-01	-.5652E-01	-.1630	-.6516E-01	.1006	-.3768E-01	[illegible]	[illegible]
14	-.9760E-01	.7039E-01	.1102	.3848E-02	-.2738	-.9062E-01	-.1814	.2223	[illegible]	[illegible]
15	-.2385	.1840E-01	.1591	-.9560E-01	-.3246E-01	-.7017E-01	-.4492E-01	-.6743E-01	-.1554	[illegible]
16	-.3032E-01	-.1682	.1187	-.1781	.2365	.8443E-01	.5806E-01	.7682E-02	[illegible]	[illegible]
17	.8742E-01	-.3143E-01	.1821	.1570E-01	-.1313	-.2046	-.6140E-01	-.1429	[illegible]	[illegible]
18	.3909E-01	-.1186	-.5563E-01	-.5003E-01	.1498	-.7444E-01	-.5435E-01	.4704E-01	[illegible]	[illegible]
19	.6716E-01	.3565E-02	-.7262E-02	.2965E-01	-.1780	-.1209E-01	.1054	[illegible]	[illegible]	[illegible]
20	-.1470	.1790	.2190	.1914E-01	.2448	-.3215E-01	-.2152E-01	[illegible]	[illegible]	[illegible]
21	-.1727E-01	.1596E-01	.2040	-.1254	-.4518E-01	-.1951E-01	-.6620E-01	[illegible]	[illegible]	[illegible]
22	-.2189E-01	.2205E-02	-.6940E-01	-.6543E-01	.1755E-01	.1078	-.6174E-01	[illegible]	[illegible]	[illegible]

ROW	COL 11 REAL	COL 11 IMAG	COL 12 REAL	COL 12 IMAG	COL 13 REAL	COL 13 IMAG	COL 14 REAL	COL 14 IMAG	COL 15 REAL	COL 15 IMAG
1	.9462E-01	-.1680	-.6506E-01	-.2001E-01	.7156E-02	-.1773E-01	-.7780E-01	[illegible]	[illegible]	[illegible]
2	-.3462E-01	.1904	.8921E-01	-.3117E-01	.1889E-01	.2656E-01	-.1517E-01	[illegible]	[illegible]	[illegible]
3	.6717E-01	-.1067	.1609	.1639E-01	[illegible]	-.1300	.1350	[illegible]	[illegible]	[illegible]
4	-.1311E-01	-.1443	-.1169	.7035E-01	.3084E-02	[illegible]	.1263	[illegible]	[illegible]	[illegible]

ROW	COL 11 REAL	COL 11 IMAG	COL 12 REAL	COL 12 IMAG	COL 13 REAL	COL 13 IMAG	COL 14 REAL	COL 14 IMAG	COL 15 REAL	COL 15 IMAG
5	-.2098E-02	.1099	-.9529E-01	-.3522	.1276	-.1200E-01	-.1419E-01	[illegible]	[illegible]	[illegible]
6	.2323	.2429	-.5996E-01	.2278	-.2590E-01	-.2579E-01	-.9780E-01	[illegible]	[illegible]	[illegible]
7	-.1986	-.2084	-.5531E-01	-.5038E-01	.6746E-01	-.5652E-01	.1102	[illegible]	[illegible]	[illegible]
8	-.1658	.2812E-01	-.1092	-.1134	-.1630	-.6516E-01	-.2738	[illegible]	[illegible]	[illegible]
9	.9528E-01	-.5461E-01	-.5526	-.7561E-01	.1006	-.3768E-01	-.1814	.2223	[illegible]	[illegible]
10	.5376E-01	-.4605E-01	.1065	-.1320	.5657E-01	-.1172	.7984E-01	[illegible]	-.1574	[illegible]
11	.8813E-01	.4558	.6448E-01	.3097E-02	.7585E-01	-.3817E-01	.4600E-01	[illegible]	[illegible]	[illegible]
12	.6448E-01	.3097E-02	-.1199	-.6778E-01	-.1879	.1658	.6069E-01	-.2073	[illegible]	[illegible]
13	.7585E-01	-.3817E-01	-.1879	.1858	.7115E-01	.2450	-.2591E-01	-.4012	[illegible]	[illegible]
14	.4600E-01	.6149E-01	.6069E-01	-.2073	-.2591E-01	-.4012	.2789E-01	[illegible]	.4567E-01	[illegible]
15	.3355	-.2756	.9911E-02	-.1356E-01	.1738	.1499	.4567E-01	-.9429E-01	.1534	-.4597
16	.1084	-.4631E-01	.1056	-.7303E-01	.6239E-01	-.1165	.2829E-01	-.2259	[illegible]	[illegible]
17	-.1332E-01	.3967E-01	.3051	.6218E-01	-.1893	-.8686E-01	-.3148	-.7189E-01	.4730E-02	-.4831E-01
18	.1377	-.5160E-01	.7788E-01	.2487E-01	.3958E-01	-.2462E-01	.1077	.9782E-01	-.1148E-01	-.9714E-01
19	.1555	-.1099	.2280E-01	-.1088E-01	-.3472	-.6025E-02	.3911	-.5634E-01	-.1074E-01	.5905E-01
20	-.2424	-.1232	-.1082	-.3982E-01	-.2131	-.7599E-01	.8754E-02	.1002E-02	.1652	-.2540
21	.1607E-01	.1015	.6335E-01	-.2286	-.4060E-01	.4807E-01	.4140E-01	-.9353E-01	-.6123E-02	-.7611E-01
22	-.1327	.2501E-01	-.1429E-01	-.2561	.4453	.3038	.7979E-01	.6542E-01	-.4699E-01	.6540E-01

ROW	COL 16 REAL	COL 16 IMAG	COL 17 REAL	COL 17 IMAG	COL 18 REAL	COL 18 IMAG	COL 19 REAL	COL 19 IMAG	COL 20 REAL	COL 20 IMAG
1	-.1170	-.2869E-01	-.7085E-01	-.1486E-01	-.1255E-03	-.5283E-01	-.6566E-02	.4521E-03	.4171E-01	.6940E-03
2	.8409E-01	-.2370E-01	.1574	-.2721E-01	-.2468E-01	.3713E-01	.3161E-01	-.3025E-01	-.5555E-01	.2143
3	-.6974E-02	-.1490	.7566E-01	.2694E-02	-.1459E-01	.1954E-02	.5851E-01	-.5438E-01	-.1710	.4645E-01
4	-.1881E-01	.4269E-01	-.7182E-01	.3815E-01	-.2903E-01	-.3194E-01	.7116E-01	.3074E-01	.5205E-03	.2627E-01
5	-.1067	-.1129	.4742E-01	.7251E-01	.2021	.1080	.1754E-01	.1752E-01	-.4750E-01	.4137E-01
6	-.3032E-01	-.1682	.8742E-01	-.3143E-01	.3909E-01	-.1186	.6716E-01	.3565E-02	-.1470	.1790
7	.1187	-.1781	.1821	.1570E-01	-.5563E-01	-.5003E-01	-.7262E-02	.2965E-01	.2190	.1914E-01
8	.2365	.8443E-01	-.1313	-.2046	.1498	-.7444E-01	-.1780	-.1209E-01	.2449	-.3215E-01
9	.5806E-01	.7682E-02	-.6140E-01	-.1429	-.5435E-01	.4704E-01	.1054	.1184	-.2152E-01	[illegible]
10	.1757	-.1632	.2491	-.2265E-02	.8406E-01	-.1464	-.1516	.1625	-.1227	-.2930
11	.1084	-.4631E-01	-.1332E-01	.3967E-01	.1377	-.5160E-01	.1553	-.1099	-.2424	-.1232
12	.1056	-.7303E-01	.3051	.6218E-01	.7788E-01	.2487E-01	.2280E-01	-.1088E-01	-.1082	-.3982E-01
13	.6239E-01	-.1165	-.1893	-.8686E-01	.3958E-01	-.2462E-01	-.3472	-.6025E-02	-.2131	-.7599E-01
14	.2829E-01	-.2259	-.3148	-.7189E-01	.1077	.9782E-01	-.3911	-.5634E-01	.8754E-02	.1002E-02
15	.4494E-01	.6610E-01	.4730E-02	-.4831E-01	-.1148E-01	-.9714E-01	-.1074E-01	.5905E-01	.1692	-.2540
16	-.3738	-.2166	-.2963	-.9224E-01	-.1215	.1023	.2015	-.1785	-.9767E-01	-.4034
17	-.2963	-.9224E-01	.1802	.5763E-01	.1339	-.2439	-.1122	.300[illegible]	.1374	-.1395
18	-.1215	.1023	.1339	-.2439	.4917	.4363	.1138	.12[illegible]7	.4075E-01	-.2289E-01
19	.2015	-.1785	-.1122	.3008	.1158	.1217	.4308	-.2558	.1716	-.8950E-01
20	-.9767E-01	-.4034	.1374	-.1393	.4076E-01	-.2289E-01	.1716	-.8950E-01	.3526E-02	.2522
21	.1137	-.8081E-01	-.1502	.8202E-01	-.3839	-.1378	-.8782E-01	-.1248	.1160	.1655
22	-.1283	-.1886	-.2272	.2854	.2502	-.6871E-01	.1690	.7467E-01	.1233	.2066

ROW	COL 21 REAL	COL 21 IMAG	COL 22 REAL	COL 22 IMAG
1	.7567E-01	-.3714E-01	-.6802E-01	-.6200E-02
2	-.7821E-01	.1499E-01	.3094E-01	.4674E-01
3	-.4887E-01	.2471E-01	.5799E-01	.8536E-01
4	.7089E-02	.4366E-01	-.2886E-01	.3550E-01
5	.2444	.2077	.2887E-01	-.1572
6	-.1727E-01	.1596E-01	-.2189E-01	.2205E-02
7	.2040	-.1254	-.6940E-01	-.6543E-01
8	-.4518E-01	-.1951E-01	.1755E-01	.1078
9	-.6620E-01	-.6145E-01	-.6174E-01	-.1161
10	.4156E-01	-.2262	.6477E-02	-.1305E-01
11	.1607E-01	.1015	-.1327	.2501E-01
12	.6335E-01	-.2286	-.1429E-01	-.2561
13	-.4060E-01	.4807E-01	.4453	.3038
14	.4140E-01	-.9353E-01	.7979E-01	.6542E-01

COL	21		22	
ROW	REAL	IMAG	REAL	IMAG
15	-.6125E-02	-.7611E-01	-.4899E-01	.8340E-01
16	-.1132	-.8081E-01	-.1285	-.1886
17	-.1502	-.8202E-01	-.2272	.2854
18	-.3839	-.1378	.2502	-.6021E-01
19	-.8782E-01	-.1248	.1890	.7487E-01
20	.1160	.1695	.1235	.2966
21	-.5639	-.1390	-.4119E-01	-.2251
22	-.4119E-01	-.2251	-.9793E-01	.5267

TEST2/J2504

ENERGY = .1950E-02
RMIN = 3.000
RMAX = 800.0

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.7934	.6420E-01	-.1934E-01	.2143	-.1069	.1882	.1865E-01	.1847	-.1452E-01	.1246
2	-.1934E-01	.2143	-.3765	.4059	-.1180	-.9994E-01	-.6061E-02	.2993	-.9052E-01	.1039
3	-.1069	.1882	-.1180	-.9994E-01	-.1982	.4607	.1574	-.2984	-.1585	-.1103
4	.1865E-01	.1847	-.6061E-02	.2993	.1574	-.2984	-.2024E-01	.5566E-01	-.2166	-.2166
5	-.1432E-01	.1246	-.9052E-01	.1039	-.1585	-.1503	.9366E-01	-.2166	-.5416E-01	.3093
6	-.4928E-01	.2202	-.6989E-01	-.2906	.1291	.9091E-01	-.6683E-01	.2262	-.2249	-.9377E-01
7	.3719E-01	.1514	-.1882	.4507E-01	-.2071	-.3565E-01	-.1233E-01	.6928E-01	.1517	-.3559
8	.3650E-01	-.9112E-01	.6129E-01	.2573	.6406E-01	.1018	-.8345E-01	.1662E-01	.1115	.1065
9	-.6598E-01	.4159E-01	.2037	.1221	-.1488	-.4407E-01	-.7052E-01	-.1043	-.9262E-01	.2092
10	.1044	-.6899E-01	-.1012	.1760	-.4368E-01	.2879	-.2587E-01	-.8028E-02	.4224E-01	-.3287
11	-.7216E-01	-.2831E-01	.1014	.2004	.8003E-01	-.9322E-01	-.1576	-.3169E-01	.2687E-02	-.3125
12	.9083E-01	.1196	-.6678E-01	.3185E-01	-.1714	.3496E-01	-.2277	-.6021E-01	-.7429E-01	.1211
13	.5915E-01	.3979E-01	-.1185	-.5322E-01	-.7319E-01	.7729E-02	.4195E-01	-.3806E-01	.5805E-01	-.5673E-01
14	-.1585E-01	.1375	-.9683E-01	-.8521E-01	-.6766E-01	-.2409	.1083	-.1235	-.2140	-.7504E-01
15	-.4063E-01	.1135E-01	.5475E-01	-.1297	.1530	-.4301E-01	-.1568	.2275	.7560E-01	-.2539E-01
16	-.8022E-01	.9491E-01	.2741E-01	-.5715E-02	.1837E-01	-.1942	-.2603	-.1840	.1715E-01	-.3575E-02
17	-.4619E-01	.1557E-02	.1020E-01	.4290E-01	-.1398	-.1785E-01	-.2033	-.2280	.8410E-01	.2614E-01
18	.5094E-01	-.9503E-01	.6246E-01	.9729E-01	-.1688E-01	.3052E-01	-.1250E-01	-.6178E-01	.1269	.2171E-01
19	-.3405E-01	-.2906E-01	.3684E-01	.4734E-01	.3295E-01	-.7497E-01	.9606E-01	-.5243E-01	.6985E-01	-.1152
20	-.9208E-01	-.3798E-02	-.6817E-01	.1704E-01	.7755E-01	-.6471E-02	-.2203	-.1177	.8279E-02	-.1934
21	.2057E-01	-.1012	.1796E-01	.1611E-01	.2147E-01	.1301	.4265E-01	.1220	.5784E-01	.1246
22	-.2348E-01	-.2645E-01	-.3937E-01	-.6970E-01	.2860E-01	.1239E-01	.1155	-.1878E-02	.7630E-02	-.9581E-01
23	-.7641E-02	-.1825E-01	.7283E-02	-.2040E-01	.7685E-01	.2055E-01	.4548E-01	-.2209E-01	.1611	.2454E-01
24	-.8640E-02	-.4430E-01	.2845E-01	.1028	.1065	.1148	-.6480E-01	.1170	-.5979E-01	-.1037E-01
25	.8545E-01	.3171E-01	-.1032	.3659E-01	-.1242E-01	-.1571E-01	-.2795E-01	.6582E-01	-.2302	-.3916E-01
26	-.4546E-01	.8018E-01	.3996E-01	-.7973E-01	-.6385E-01	-.1675	-.2365E-01	-.1038	-.1940E-01	.1291E-01
27	-.1540E-01	-.7655E-02	.1076	-.4843E-01	-.8846E-01	.5524E-01	-.8667E-01	.1290	-.2115	-.9366E-03
28	-.4362E-01	.8159E-02	.5117E-01	.2155E-01	.1014	-.5175E-01	.4162E-01	-.5605E-02	.1735E-01	-.1595E-01
29	.2754E-01	-.3329E-01	-.9697E-01	.1062	.5662E-01	-.6067E-02	.1214	-.3896E-02	-.1943	-.2573E-02
30	-.1147E-01	-.7003E-02	.7852E-01	.4710E-01	-.5997E-01	-.3320E-01	-.6156E-01	-.7937E-01	.3622E-01	-.2617E-01
31	.1955E-01	-.1023E-01	-.2477E-01	.1715E-01	-.8717E-02	-.1372E-03	-.4255E-01	.1712E-01	.5745E-02	-.5555E-01

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.4928E-01	.2202	.3719E-01	.1514	.3850E-01	-.9112E-01	-.6598E-01	.4159E-01	.1044	-.6899E-01
2	-.6985E-01	-.7906	-.1882	.4507E-01	.6129E-01	.2573	.2037	.1221	-.1012	.1760
3	.1291	.9091E-01	-.2071	-.3565E-01	.6406E-01	.1018	-.1488	-.4407E-01	-.4368E-01	.2879
4	-.6683E-01	-.1233E-01	.6928E-01	-.8345E-01	.1662E-01	-.7052E-01	-.1043	-.2587E-01	-.8028E-02	.4224E-01
5	-.2220	.9370E-01	.1517	-.3539	.1115	.1063	-.9262E-01	.2092	.4224E-01	-.3287
6	-.2844	.4217	-.9505E-02	-.1785	-.1207	-.2716E-01	.1652	-.2556	.5591E-01	.1451
7	-.9303E-02	-.1785	-.1012	.3474	.6425E-01	-.3479	.8721E-02	-.3267E-01	.1533	-.2725E-01
8	-.1202	-.2716E-01	.6425E-01	-.3479	-.4457	-.9534E-01	-.2568	.3742E-01	.2206E-01	.1580
9	.1652	-.2558	.8721E-02	-.3267E-01	-.2568	.3742E-01	-.4749E-01	-.1925	-.8363E-01	.1298
10	.3591E-01	.1451	.1533	.2725E-01	.1580	-.1298	-.8353E-01	.1298	.1377E-01	-.1585
11	.8576E-01	.6007E-01	-.1034	-.1685	.1741	.1255	-.3166E-03	-.8349E-01	.8477E-01	.1533
12	-.2448E-01	.1071	.1920E-01	-.4739E-01	-.4391E-01	.2022	.5466E-01	-.1293	.7041E-02	-.2596
13	.1098E-01	.2628E-01	.4084E-01	.1079	.2328E-01	.3499E-01	.2447	.1529	.1524	-.1911
14	-.8900E-01	-.1577E-01	-.1415E-01	-.1198	.1309	.2892E-01	-.8226E-01	.1057E-01	.7197E-01	.1052
15	-.9652E-01	-.1065E-01	-.5233E-01	-.2736E-01	.1511	-.1319	-.1073	.2236E-01	.6178E-01	.1430
16	.1715E-01	.1697	-.1071	.1337	.1548	-.1646	-.1964E-01	.3644E-01	-.9226E-01	.3039E-01
17	.7864E-01	.2465E-01	.1576	-.2371E-02	-.7382E-01	.1190	.8361E-01	-.8107E-01	.1450E-01	.1938
18	.8286E-01	.9995E-01	-.6632E-02	.8705E-01	-.2580E-01	-.7620E-01	.5841E-01	.2521	-.8199E-01	.4559E-01
19	.1227	.1149	.6495E-01	.1954E-01	-.7830E-01	-.9939E-01	-.1008	.4777E-01	-.5445E-01	.5634E-02
20	-.4558E-01	-.4235E-01	-.4585E-01	-.7998E-01	-.1404	.5986E-01	.1694	-.3469E-01	.1102	-.2147

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
21	.6954E-01	.1705E-01	.3482E-01	-.1795	.4736E-01	.6305E-01	.1052E-01	-.4515E-01	.1672	-.8567E-01
22	.1723	-.9117E-01	.2554E-02	-.1922	.1401	.7631E-01	-.2186E-01	-.1099	-.1961E-01	-.3072E-02
23	.1084E-01	.1472E-01	.2116E-01	.2940E-02	-.4593E-01	.5583E-02	.1812	.8836E-03	.2310	-.5226E-01
24	.2510E-02	.1938E-01	.2237E-01	-.1624	-.5527E-02	-.2485	-.2230	.6210E-02	-.2126E-01	-.1738
25	-.1526	.1145	.1338	-.6387E-01	.1477	-.4079E-01	-.2455E-01	.4256	-.1637	.1454
26	.1197E-01	-.4051E-01	-.2637	.4576E-01	.3887E-01	-.5086E-02	.1992E-03	-.1241	.1135	-.5240E-01
27	.2316	-.1098	-.1913E-01	-.8289E-01	.5922E-01	.5548E-01	.9673E-02	.5745E-01	.2385	-.1497
28	-.6799E-01	.9840E-02	-.4635E-01	-.3337E-01	.9792E-01	.1357E-01	.2660E-01	-.2734	-.5778E-01	.6239E-01
29	.8975E-01	.6545E-02	.3401E-01	-.1881	.1359	.5860E-01	.7569E-01	.1719E-01	-.1655E-01	.5163E-01
30	.4237E-01	.8112E-01	-.4097E-01	-.5083E-01	.7997E-01	-.1171	-.1899E-01	.1774	.5195E-01	-.2784E-01
31	.3780E-01	.8149E-01	.4018E-01	.5677E-02	.5129E-01	-.1128E-01	.1129E-01	.8050E-02	.1620	-.1817E-02

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.7236E-01	-.2831E-01	.5083E-01	.1194	.5913E-01	.5979E-01	-.1383E-01	.1375	-.4063E-01	.1135E-01
2	.1014	.2004	-.6678E-01	.3183E-01	-.1185	-.5322E-01	-.9683E-01	-.8521E-01	.5475E-01	-.1297
3	.8903E-01	-.5322E-01	-.1714	.5456E-01	-.7319E-01	.7729E-02	-.6768E-01	-.2409	.1530	-.4301E-01
4	-.1576	-.3169E-01	-.2277	-.6010E-01	.4159E-01	-.3836E-01	.1083	-.1255	-.1568	.2273
5	.2887E-02	-.1125	-.7426E-01	.1211	.5805E-01	-.5673E-01	-.2140	-.7304E-01	.7560E-01	.2339E-01
6	.8576E-01	.6007E-01	-.2448E-01	.1071	.1098E-01	.2828E-01	-.8900E-01	-.1677E-01	-.9632E-01	-.1065E-01
7	-.1034	-.1685	.1920E-01	-.4739E-01	.4684E-01	.1079	-.1415E-01	-.1198	-.5233E-01	-.2758E-01
8	.1741	.1255	-.4391E-01	.2022	.2328E-01	.5489E-01	.1309	.2892E-01	.1511	-.1319
9	-.3166E-03	-.8349E-01	.3446E-01	-.1293	.2447	.1526	-.8226E-01	.1057E-01	-.1075	.2236E-01
10	.8477E-01	.1333	.7041E-02	-.2556	.1974	-.1911	.7157E-01	.1052	.6178E-01	.1452
11	.5995E-01	-.8256E-01	.3047E-01	-.8033E-01	.4292E-01	-.7466E-01	.4556E-01	.9309E-01	-.1046	-.4874E-01
12	.3047E-01	-.8033E-01	-.2102	-.1940	-.1970	.4615E-01	.1104	.7153E-01	-.1380	-.8126E-01
13	.4292E-01	-.7466E-01	-.1970	.4615E-01	-.3865E-01	.7651E-01	-.2149	-.1376	.2077E-02	.2229E-02
14	.4556E-01	.9309E-01	.1104	.7153E-01	-.2149	-.1376	.2618E-01	.3355	-.2294E-01	-.7791E-01
15	-.1046	-.4874E-01	-.1380	-.8126E-01	.2077E-02	.2229E-02	-.2294E-01	-.7791E-01	-.3415E-01	-.1116
16	.5130	.5234	-.8195E-01	-.8630E-01	.2265	.1238	-.8852E-01	-.1024	.1304	.1090
17	-.1789	.7268E-01	.8023E-02	.1550	-.2091	-.2341	-.3069	-.1686	-.2706	.2209
18	-.4945E-01	.5068E-01	.7083E-01	.1880	.1395E-01	-.4783E-01	.9607E-01	.2594E-01	-.1253	.6966E-02
19	-.9923E-03	-.7769E-01	.4667E-01	-.2424	-.3170	.7625E-01	-.2671	-.9097E-01	.8947E-01	-.1527
20	.1480	-.2185	.1048	.4135E-01	.3501E-01	.1758E-01	.1890E-01	.3573E-01	.7971E-01	.1484
21	.1591	.9157E-01	-.1833	-.1583	.4524E-01	.3047E-01	-.1269	-.1610	-.1950	.1487E-02
22	-.2301E-01	.1327	-.1371	-.4708E-01	.3719	-.6522E-01	-.1353	.1131	-.2175	-.9039E-01
23	-.2150	.4909E-01	-.2748	.1104	.3990E-01	.8838E-01	.1022	-.1174E-02	.4053	.8182E-01
24	-.2901E-01	.8515E-01	.1416	-.1739	-.1968	-.1489	-.2571	-.2297	-.9282E-01	-.2811E-01
25	-.9512E-01	-.9559E-01	.2694	-.3404E-01	.3210	.1235	-.1270	-.5525E-01	-.2592E-01	.9050E-01
26	-.7413E-01	-.1589E-02	.1172	-.1174E-01	.1537	.3662E-01	-.1145	-.1535	.2039	-.5733E-02
27	.1779E-01	.2012	.1484	.3334E-01	.4184E-02	.1512E-01	[illegible]	-.2357E-01	-.1505	-.7500E-01
28	.2693E-01	.7620E-01	-.4643E-02	-.6680E-01	.6525E-01	.5499E-01	-.1015	-.1779E-01	.4546E-01	-.1273
29	.3253E-01	-.1167	.4021E-01	.6779E-01	.9825E-02	.7485E-01	.1066	-.4259E-01	-.7226E-01	.1415
30	-.1334	.1155	-.2368	-.3679E-01	-.2017E-01	.2247E-02	.1415	.7185E-01	-.4992E-01	-.2564
31	.1071E-02	.6224E-01	-.6816E-01	-.3176E-01	.1500	.1471E-02	.8437E-02	-.1537E-01	.1238	-.6879E-02

COL	16		17		18		19		20	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.8022E-01	.9491E-01	-.4819E-01	.1557E-02	.5094E-01	-.9503E-01	-.3405E-01	-.2996E-01	-.9208E-01	-.3758E-02
2	.2741E-01	-.5716E-02	.1020E-01	.4290E-01	.6246E-01	.9729E-01	.5684E-01	.4754E-01	-.8817E-01	.1704E-01
3	.1837E-01	-.1942	-.1398	-.1785E-01	-.1688E-01	.3052E-01	.5293E-01	-.7487E-01	.7755E-01	-.6471E-02
4	-.2603	-.1840	-.2033	-.2280	-.1250E-01	-.8178E-01	.9608E-01	-.5243E-01	-.2203	-.1177
5	.1715E-01	.3876E-02	.8410E-01	.2614E-01	.1269	.2171E-01	.6985E-01	-.1152	.8279E-02	-.1934
6	.1715E-01	.1697	.7864E-01	.2465E-01	.8286E-01	.9995E-01	.1227	.1149	-.4558E-01	-.4235E-01
7	-.1071	.1537	.1571	-.2371E-02	-.6632E-02	.8709E-01	.6495E-01	.1934E-01	-.4385E-01	-.7996E-01
8	.1548	-.1646	-.7382E-01	.1190	-.2580E-01	-.7620E-01	-.7830E-01	-.3759E-01	-.1404	.5968E-01
9	-.1964E-01	.3644E-01	.8361E-01	-.8107E-01	.3841E-01	.2321	-.1008	.4777E-01	.1694	-.5449E-01
10	-.9726E-01	.3039E-01	.1450E-01	.1939	-.8199E-01	.4359E-01	-.5445E-01	.5654E-02	.1102	-.2147
11	.5130	.3234	-.1789	.7268E-01	-.4945E-01	.5068E-01	-.9923E-03	-.7769E-01	.1480	-.2185
12	-.8195E-01	-.8630E-01	.8023E-02	.1550	.7083E-01	.1880	.4667E-01	-.2424	.1048	.4135E-01

COL	16		17		18		19		20	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
13	.2265	.1238	-.2091	-.2341	.1395E-01	-.4783E-01	-.3170	.7625E-01	.3501E-01	.1758E-01
14	-.8852E-01	-.1024	-.3069	-.1686	.9607E-01	.2594E-01	-.2671	-.9097E-01	.1890E-01	.3573E-01
15	.1304	.1090	-.2706	.2209	-.1253	.6966E-02	.8947E-01	-.1527	.7971E-01	.1484
16	.9436E-01	-.9004E-01	.1321	-.6854E-01	.8468E-01	.7873E-01	-.4374E-01	.4162E-01	.7744E-01	.8373E-01
17	.1321	-.6854E-01	.1453	.8139E-01	-.6761E-01	-.1173	.4600E-01	.1988	.3100E-01	.9705E-01
18	.8468E-01	.7873E-01	-.6761E-01	-.1173	.1845	.3449	.2480	-.5952E-01	.1075	-.5241E-02
19	-.4374E-01	.4162E-01	.4600E-01	.1988	.2480	-.5952E-01	.3692	.4176E-01	-.7398E-01	-.2607E-01
20	.7744E-01	.8373E-01	.3100E-01	.9705E-01	.1075	-.5241E-02	-.7398E-01	-.2607E-01	-.2056	.3963
21	.7404E-02	-.6250E-01	-.5152E-01	-.8287E-01	-.3786	-.2819	-.1524E-01	.7022E-01	-.6042E-01	.4403E-01
22	-.1310	-.6176E-01	-.1380	.2212	.3615	.3980E-01	.9655E-02	.9563E-01	-.1426	.2337
23	.1668E-01	-.3667E-01	.6100E-01	-.1896E-01	.2228	-.7905E-01	.9844E-01	.8498E-01	.2094	.9079E-01
24	-.3866E-01	-.6859E-02	-.5680E-01	-.1466	.1863	.6558E-01	-.2848	-.4548E-01	.2299	.1520
25	.8494E-01	-.1918	-.2717E-01	.1970E-01	-.4142E-01	-.1088	.1335	-.3856E-01	.4900E-01	.5615E-01
26	-.1030	.1471	-.3012E-01	.1714	-.4503E-02	-.1157	-.4091E-02	.5545E-01	-.4078E-01	-.2644
27	-.1294E-01	.4996E-02	.3919E-01	-.2256	.1120	.9195E-01	.1377	.2689	-.6496E-01	-.6609E-01
28	-.1294	-.1054	.5645E-01	.9436E-01	.6242E-01	.1644E-01	-.1787	.3300E-03	.2217E-01	.2206E-01
29	.3757E-01	-.8936E-02	.8035E-01	-.1213	.2653E-01	-.1159	-.4841E-02	.1272	-.5426E-01	.4918E-02
30	.1946E-01	-.8664E-01	-.7265E-01	-.1571	.1257E-01	-.2251E-01	.1952	.1995	.1166	.2358
31	.1280	.1085E-01	.4761E-02	.5555E-02	.5349E-01	-.2792E-01	.6486E-01	.3232E-01	.6045E-01	.1527

COL	21		22		23		24		25	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.2067E-01	-.1012	-.2348E-01	-.2645E-01	-.7641E-02	-.1825E-01	-.8640E-02	-.4430E-01	.6446E-01	.3171E-01
2	.1796E-01	.1611E-01	-.3997E-01	-.6970E-01	.7283E-02	-.2040E-01	.2845E-01	.1028	-.1032	.3659E-01
3	.2147E-01	.1301	.2860E-01	.1239E-01	.7685E-01	.2055E-01	[illegible]	.1148	-.1242E-01	.1571E-01
4	.4265E-01	.1220	.1155	-.1828E-02	.4546E-01	-.2209E-01	-.6460E-01	.1170	-.2795E-01	.8582E-01
5	.5764E-01	.1246	.7630E-02	-.9581E-01	.1611	.2454E-01	.5979E-01	-.1037E-01	-.2302	-.3916E-01
6	.6954E-01	.1705E-01	.1723	-.9117E-01	.1084E-01	.1472E-01	.2510E-02	.1938E-01	-.1526	.1145
7	.3482E-01	-.1795	.2554E-02	-.1922	.2116E-01	.2940E-02	.2237E-01	-.1624	.1338	-.6387E-01
8	.4736E-01	.6305E-01	.1401	.7631E-01	-.4593E-01	.5583E-02	-.5527E-02	-.2485	.1477	-.4079E-01
9	.1052E-01	-.4515E-01	-.2186E-01	-.1099	.1812	.8836E-03	-.2230	.6210E-02	-.2455E-01	.4256
10	.1672	-.8567E-01	-.1961E-01	-.3072E-02	.2310	-.5226E-01	-.2126E-01	-.1738	-.1637	.1454
11	.1591	.9157E-01	-.2301E-01	.1327	-.2150	.4909E-01	-.2901E-01	.8515E-01	-.9512E-01	-.9559E-01
12	-.1833	-.1583	-.1371	-.4708E-01	-.2748	.1104	.1416	-.1739	.2694	-.3404E-01
13	.4524E-01	.3047E-01	.3719	-.6522E-01	.3990E-01	.8838E-01	-.1968	-.1489	.3210	.1235
14	-.1269	-.1610	-.1353	.1131	.1022	-.1174E-02	-.2571	-.2297	-.1270	-.5525E-01
15	-.1950	.1487E-02	-.2175	-.9039E-01	.4053	.8182E-01	-.9282E-01	-.2811E-01	-.2592E-01	.9050E-01
16	.7404E-02	-.6250E-01	-.1310	-.6176E-01	.1668E-01	-.3667E-01	-.3866E-01	-.6859E-02	.8494E-01	-.1918
17	-.5152E-01	-.8287E-01	-.1380	.2212	.6100E-01	-.1896E-01	-.5680E-01	-.1466	-.2717E-01	.1970E-01
18	-.3786	-.2819	.3615	.3980E-01	.2228	-.7905E-01	.1863	.6558E-01	-.4142E-01	-.1088
19	-.1524E-01	.7022E-01	.9655E-02	.9563E-01	.9844E-01	.8498E-01	-.2848	-.4548E-01	.1335	-.3856E-01
20	-.6042E-01	.4403E-01	-.1426	.2337	.2094	.9079E-01	.2299	.1520	.4900E-01	.5615E-01
21	-.3467	-.1975	-.1289E-01	-.4125E-01	-.2255E-01	-.1736	.8281E-01	-.3037E-01	-.1818	-.2510E-01
22	-.1289E-01	-.4125E-01	.2604	.2155	-.2158	-.5028E-02	-.2439E-01	-.1846E-01	-.1173	.2892E-01
23	-.2255E-01	-.1736	-.2156	-.3028E-02	-.2141	.7511E-01	-.1955	.1486E-01	-.2704	.1042
24	.8281E-01	-.3037E-01	-.2439E-01	-.1846E-01	-.1955	.1486E-01	.4339E-01	.3601	-.8585E-01	.1725E-02
25	-.1818	-.2510E-01	-.1173	.2892E-01	-.2704	.1042	-.8585E-01	.1725E-02	.1804	.2063
26	-.1748	-.1015	.3164E-01	.1267	-.1067	-.1560	.1215	-.1276	-.1579E-01	-.9981E-01
27	.1258E-01	.2546	-.1389	-.1865E-01	.1225	.1691	.1380	-.8528E-01	.3355E-01	-.1875E-01
28	-.8048E-01	-.1017E-01	-.1716E-01	-.6075E-01	.1552	-.5037E-02	.5037E-01	-.5243E-01	.1399	.1265
29	-.6339E-02	.6025E-01	-.9020E-01	.1327	.4723E-01	-.7480E-01	.7617E-01	-.3969E-01	.8977E-01	.2377E-01
30	.1003	.2589	-.8767E-01	-.8477E-01	-.2052E-01	-.1539	.1269	-.1129	-.3097E-01	.9708E-01
31	.3352E-01	-.6182E-01	.7101E-01	.2746E-01	.1530	.6566E-01	-.7457E-01	-.9390E-01	.1248E-01	.4684E-01

COL	26		27		28		29		30	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.4546E-01	.6016E-01	.1540E-01	-.7665E-02	-.4362E-01	-.8759E-02	.2754E-01	-.3329E-01	-.1147E-01	-.7003E-02
2	.5996E-01	-.2973E-01	.1076	-.4843E-01	.5117E-01	.2745E-01	-.9697E-01	.1062	.7852E-01	.4710E-01
3	-.6385E-01	-.1673	-.8846E-01	.5574E-01	.1014	-.3175E-01	.5062E-01	.6067E-02	-.5997E-01	-.3320E-01
4	-.2365E-01	-.1038	-.8667E-01	.1290	.4160E-01	-.5605E-02	.1214	.3896E-02	-.6156E-01	-.7972E-01

COL	26		27		28		29		30	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
5	-.1940E-01	.1291E-01	-.2115	-.3668E-03	.1733E-01	.1595E-01	-.1943	-.2579E-02	.3623E-01	-.2617E-01
6	.1197E-01	-.4031E-01	.2316	-.1098	-.6799E-01	.9860E-02	.8973E-01	.8545E-02	.4237E-01	.8133E-01
7	-.2837	.4576E-01	-.1915E-01	-.8298E-01	-.4635E-01	-.3537E-01	.3401E-01	-.1881	-.8097E-01	-.3083E-01
8	.3887E-01	-.5086E-02	.5922E-01	.5348E-01	.9792E-01	.1357E-01	.1539	.3808E-01	.7997E-01	-.1171
9	.1992E-03	-.1241	.9815E-02	.5745E-01	.2660E-01	-.2134	.7568E-01	.1719E-01	-.1898E-01	.1774
10	.1135	-.5240E-01	.2365	-.1697	-.5779E-01	.6239E-01	-.1629E-01	.5183E-01	.5119E-01	-.2798E-01
11	-.7415E-01	-.1589E-02	.1779E-01	.2012	.2693E-01	.7620E-01	.3253E-01	-.1167	-.1334	.1195
12	.1172	-.1174E-01	.1484	.3334E-01	-.4643E-02	-.6680E-01	.4021E-01	.8779E-01	-.2368	-.3679E-01
13	.1531	.3662E-01	.4184E-02	.1515E-01	.6529E-01	.3499E-01	.9823E-02	.7465E-01	-.2817E-01	.2547E-02
14	-.1145	.1539	.8189E-01	-.2557E-01	-.1015	-.1779E-01	.1066	-.6259E-01	.4415	.5182E-01
15	.2039	-.9753E-02	-.1503	-.7508E-01	.4346E-01	-.1270	-.7228E-01	.1416	-.4952E-01	-.2864
16	-.1030	.1471	-.1924E-01	.4986E-02	-.1284	-.1054	.3757E-01	-.8936E-02	.1944E-03	-.9868E-01
17	-.3012E-01	.1714	.5918E-01	-.2256	.5643E-01	.9436E-01	.8053E-01	-.1215	-.7283E-01	-.1571
18	-.4503E-02	-.1157	.1120	.9195E-01	.6242E-01	.1644E-01	-.2853E-01	-.1198	.1257E-01	-.2251E-01
19	-.6091E-02	.5345E-01	.1377	-.2589	-.1787	.5300E-03	-.4861E-02	.1272	.1952	.1995
20	-.4078E-01	-.2844	-.6496E-01	-.6609E-03	.2717E-01	.2209E-01	-.5408E-01	.6918E-02	.1186	.2358
21	-.1748	-.1013	.1258E-01	.2546	-.8048E-01	-.1017E-01	-.6339E-02	.8023E-01	.1063	.2589
22	.3184E-01	.1267	-.1889	-.1865E-01	-.1716E-01	-.6075E-01	-.9029E-01	.1527	-.8787E-01	-.8877E-01
23	-.1067	-.1560	.1229	.1691	.1552	-.3057E-02	.4723E-01	-.7480E-01	-.2052E-01	-.1538
24	.1215	-.1278	.1580	-.8528E-01	.5037E-01	-.5743E-03	.7617E-01	-.3869E-01	.1269	-.1179
25	-.1579E-01	-.9981E-01	.3355E-01	-.1873E-01	.1399	.1265	.8977E-01	.2537E-01	-.3097E-01	.8706E-01
26	.4530	-.8529E-01	-.2453E-01	-.9867E-01	.1727	-.9081E-01	.3558	.1073E-01	.2585	.3698E-01
27	-.2455E-01	-.9867E-01	-.1056E-01	.1700	.2447E-01	.2599	.2570	.2537	-.1984E-02	-.2625
28	.1227	-.9081E-01	.2447E-01	.2599	.1085E-01	.8048	-.1844	-.8533	-.6198E-01	-.5346E-01
29	.3538	.1075E-01	.2570	.2537	-.1844	-.4513	-.2772	-.7268	.8084E-03	-.2867
30	.2585	.3698E-01	-.1984E-02	-.2625	-.6198E-01	-.5346E-01	.8084E-01	.2807	-.1729E-03	.4057
31	-.6712E-01	-.1567E-01	.9530E-01	-.1855E-01	-.2917E-01	.8134E-02	-.3609E-01	.7361E-01	.3853E-01	-.1474E-01

COL	31	
ROW	REAL	IMAG
1	.1955E-01	-.1025E-0
2	-.2477E-01	.1715E-01
3	-.8717E-02	-.1372E-03
4	-.4255E-01	.1712E-01
5	.5745E-02	-.5555E-01
6	.3780E-01	.8149E-01
7	.4018E-01	.3677E-02
8	-.5129E-01	-.1128E-01
9	.1125E-01	.8050E-02
10	.1820	-.1817E-02
11	.1071E-02	.6224E-01
12	-.6816E-01	-.3176E-01
13	.1500	.1471E-02
14	.8443E-02	-.1537E-01
15	.1238	-.6873E-02
16	.1260	.1085E-01
17	.4761E-02	.5335E-02
18	.5349E-01	-.2792E-01
19	.6486E-01	.3232E-01
20	.6045E-01	.1521
21	.3552E-01	-.6162E-01
22	.7101E-01	.2746E-01
23	.1530	.8306E-01
24	-.7457E-01	-.9390E-01
25	.1245E-01	.4654E-01
26	-.6712E-01	-.1767E-01
27	.5550E-01	-.1855E-01
28	-.2917E-01	.8134E-02
29	-.3609E-01	.7361E-01
30	.3853E-01	-.1474E-01

COL	31	
ROW	REAL	IMAG
31	-.6716	-.1668

TEST27.DAT

ENERGY = .7790E-04
RMIN = 3.000
RMAX = 1500.

COL	1		2		3	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.5925	-.5250	-.1905	.5253	-.9903E-01	.4701
2	-.1903	.5253	-.3527	.3479	-.4584	-.4960
3	-.9903E-01	.4701	-.4584	-.4960	-.6516E-01	.5557

TEST2/J582

ENERGY = .7790E-04
RMIN = 3.000
RMAX = 1500.

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.4932	-.3803	-.3529	-.4490	-.3816	-.3366	.1137E-01	-.1171	-.2562E-02	-.8543E-01
2	-.3529	-.4490	.1280	-.5999	.4538	.1980	.1522	-.1044	.2265E-01	-.5631E-01
3	-.3816	-.3366	.4538	.1980	-.1886	-.6141	-.7660E-01	-.9167E-01	.2264E-01	-.1016
4	.1137E-01	-.1171	.1522	-.1044	-.7660E-01	-.9167E-01	-.2242	.1511E-01	-.5632	.6434
5	-.2562E-02	-.8543E-01	.2265E-01	-.5631E-01	.2264E-01	-.1016	-.5632	.6434	.2208	-.4217
6	-.1706E-01	-.7533E-01	-.1189	.2504E-01	.1447	-.1930	.1013	.5754	-.1419	.4307

COL	6	
ROW	REAL	IMAG
1	-.1706E-01	-.7553E-01
2	-.1189	.2504E-01
3	.1447	-.1930
4	.1013	.5754
5	-.1419	.4307
6	-.7938	-.4680

TEST2/J583

ENERGY = .7790E-04
RMIN = 3.000
RMAX = 1500.

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.9349	.1746	.1190	-.2015	.6473E-01	-.1558	.8142E-01	.3302E-01	.5383E-01	[illegible]
2	.1190	-.2015	-.4552	-.7502	.1600	-.2196	.1746E-01	-.1654	.5798E-01	[illegible]
3	.6473E-01	-.1558	.1600	-.2196	-.8005	-.3887	.1152	.2322	.1219E-01	[illegible]
4	.8142E-01	.3302E-01	.1746E-01	-.1654	.1152	.2322	.5875E-01	.6322	.4156	-.2171
5	.5383E-01	.1535E-01	.5798E-01	.5042E-01	.1219E-01	.2438E-01	.4156	-.2171	.1274E-01	.7214
6	.3565E-01	-.9824E-02	.1444	.2559	-.1082	-.1637	.4627	-.2468	.4037	-.2947

COL	6	
ROW	REAL	IMAG
1	.3565E-01	-.9824E-02
2	.1444	.2559
3	-.1082	-.1632
4	.4627	-.2468
5	.4037	-.2947
6	.7510	.5548

TEST2/J584

ENERGY = .7790E-04
RMIN = 3.000
RMAX = 1500.

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.8092	-.5426	-.4401E-01	.5294E-01	-.3079E-01	.1167E-01	.1195	.4248E-01	.1088	[illegible]
2	-.4401E-01	.5294E-01	.4177	.2696	-.1071E-01	.5735	-.9108E-01	-.2102	.1425	.1045
3	-.3079E-01	.1167E-01	-.1071E-01	.5735	.5544	.1129	.2079	.4516	.4922E-02	[illegible]
4	.1195	.4248E-01	-.9108E-01	-.2102	.2079	.4516	.2562	.3290	-.1264	.5565
5	.1088	.2116E-01	.1425	.1045	.4922E-02	.1183	-.1264	-.5565	-.9707E-01	.5556
6	.1289	-.4748E-02	.4686	.3465	-.2486	-.1011	4201	.1180	-.3697	-.4381

COL	6	
ROW	REAL	IMAG
1	.1289	-.4748E-02
2	.4686	.3465
3	-.2486	-.1011
4	-.4201	.1180
5	-.3697	-.4381
6	-.1351	-.1820

TEST3/J2981

ENERGY = .1950E-07
RMIN = 3.000
RMAX = 7.000

COL	1		2		3	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.1323	.1363	.5043	-.4806	-.2816	-.6272
2	.5043	-.4806	.6530E-01	-.5565	.4394	.7000E-01
3	-.2816	-.6272	.4394	.7000E-01	-.4198	.3912

TEST3/J2502

ENERGY = .1950E-02
RMIN = 3.000
RMAX = 7.000

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.1446	.6129	.9949E-01	.2304E-01	-.7969E-01	-.1060	-.3951	.1219	-.8741E-01	.2868
2	.9949E-01	.2304E-01	-.2266	-.6441	.2260E-01	.4214	-.1588	-.2157	-.1867	.3181E-01
3	-.7969E-01	-.1060	.2260E-01	.4214	-.4831	.3750	-.2271	.9684E-01	-.7963E-01	.1891
4	-.3951	.1219	-.1588	-.2157	-.2271	.9684E-01	.4051E-01	-.1364	-.3791E-01	.1006
5	-.8741E-01	.2868	-.1867	.3181E-01	-.7963E-01	.1891	-.3791E-01	.1006	.3267	-.7725
6	.2704	.2396	-.1304	.2938	.3502E-01	.7255E-01	.4660	-.6122	.1823	.1270
7	.2183	-.2264E-01	.7324E-01	-.2015	-.5474E-01	.2395	.1379	-.9563E-01	-.1506	.2542E-01
8	.6544E-01	-.1647	-.1363	-.5595E-01	.3814E-01	.9052E-01	-.8194E-01	-.5411E-01	.1126	-.1534
9	-.1367	-.1268	-.3804E-01	.1324	.6010E-01	.8845E-01	.5148E-01	.1349E-01	-.1096	-.9989E-02
10	-.2214	.1439	.2174	-.1941E-01	.2585	.3859E-01	-.6164E-01	-.1680	.4044E-01	.5067E-02

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.2704	.2396	.2183	-.2264E-01	.6544E-01	-.1647	-.1367	-.1268	-.2214	.1439
2	-.1304	.2938	.7324E-01	-.2015	-.1363	-.5595E-01	-.3804E-01	.1324	.2174	-.1941E-01
3	.3502E-01	.7255E-01	-.5474E-01	.2395	.3814E-01	.9052E-01	.6010E-01	.8845E-01	.2585	.3839E-01
4	.4660	-.6122	.1379	-.9563E-01	-.8194E-01	-.5411E-01	.5148E-01	.1549E-01	-.6164E-01	-.1680
5	.1823	.1270	-.1306	.2542E-01	.1126	-.1534	-.1096	-.9989E-02	.4044E-01	.5067E-02
6	.1581	.1217	.1988	-.6939E-02	.5117E-01	.1390E-01	.7985E-02	.2940E-01	.1878	-.8375E-02
7	.1988	-.6939E-02	-.4457	-.1244E-01	.3917	.3240	.6625E-01	-.4563	-.2973	.4274E-01
8	.5117E-01	.1390E-01	.3917	.3240	-.3965	.1181	.3682	-.3704	-.2581	.3780
9	.7985E-02	.2940E-01	.6625E-01	-.4563	.3682	-.3704	.4594	.1346	-.9757E-01	.4415
10	.1878	-.8375E-02	-.2973	.4274E-01	-.2081	.3780	-.9757E-01	.4415	-.3334E-01	.5132

TEST3/J25B1

ENERGY = .1950E-02
RMIN = 3.000
RMAX = 7.000

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.3526	.5087	-.1068	.8531E-01	-.8581E-01	.8787E-01	-.2300	-.1131	-.2149	-.1256
2	-.1068	.8531E-01	.1706	.2450	-.1997	-.2348	.8132E-01	.2240	-.7485E-01	.1090
3	-.8581E-01	.8787E-01	-.1992	-.2348	-.3755	-.3261	-.1183	.1989	.2347	.3907E-01
4	-.2300	-.1131	.5132E-01	.2240	-.1183	.1909	-.5081	-.4670	-.6220E-01	.2041
5	-.2149	-.1256	-.7486E-01	.1090	.2347	.3907E-01	-.6220E-01	.2041	-.1967	.2247
6	.1684	.2195	.3244	.1256	.5324E-01	.5332E-02	-.1937	-.5349E-01	.1534	-.2437E-01
7	-.8582E-01	.9182E-01	-.1225	-.2351	.1324E-02	.3886E-01	.1028	.1363	.4592E-02	.1022
8	.4480E-01	.5176E-01	.3799E-01	.1014	-.7252E-01	-.1130	.9990E-01	-.3181E-01	.6068E-01	-.9351E-01
9	.2022	.4966E-01	.8586E-01	-.2033E-01	.3050E-01	.2021E-01	.1620	-.4641E-01	.5562E-01	.7663E-01
10	.9519E-02	-.8831E-02	-.9982E-01	-.1035	-.1705E-01	-.1853	-.2354	.8914E-01	-.4678E-01	-.6718E-01
11	-.5822E-02	.1451E-01	-.2761	.1002	.3737E-01	-.1275	-.1851	.1945	-.1541	-.1414
12	.9495E-01	-.1010	.1441	.1845	.1573	.9233E-01	.1147	.1306	-.3579	-.2359
13	.6998E-01	.1404	.1469	-.1064	.6893E-01	-.2538E-01	.1109	-.3024E-01	-.2604	.9751E-01
14	.1084	.6517E-01	.1124	.6742E-01	-.1735	.3046E-01	-.8193E-01	.3662E-01	.9520E-02	.2671
15	-.1788	.2171	.4705E-01	-.4826E-01	-.5439E-01	.3489	-.1582	.2218	-.6255E-01	-.2531
16	.5646E-02	.1641	-.2898E-01	.2193	.3218	-.1398	.3421E-01	-.1215	.2297	-.1092E-01
17	-.3599E-02	.1695	.1414E-01	.1777	-.6649E-01	-.2121	.1043	-.3134E-01	-.1339	-.2148E-01
18	-.2395E-01	.7560E-02	.1212E-01	.1897E-01	-.8159E-01	.7512E-01	.1613E-01	-.6228E-02	-.1653	-.1261E-01
19	-.9208E-01	.1038	-.3689E-02	-.2389	-.3160E-01	-.4337E-01	-.6859E-01	-.1072E-02	-.2957	.1944
20	-.2580	.4250E-01	.1487	-.9876E-01	.7151E-01	.1567	.1947	.2406E-01	.9651E-02	.9205E-01
21	-.2776E-01	.1877	.7897E-01	-.9259E-01	.4949E-01	.1356	.1259	-.3912E-01	-.2437E-01	.2358E-02
22	.9228E-01	-.4708E-01	-.5692E-01	.5246E-01	-.1414	.3397E-01	-.4430E-01	-.7765E-01	.6457E-01	.3811E-01

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.1684	.2195	-.8582E-01	.9182E-01	.4480E-01	.5176E-01	.2022	.4966E-01	.9519E-02	-.8831E-02
2	.3244	.1736	-.1225	-.2351	.3799E-01	.1014	.8586E-01	-.2033E-01	-.9982E-01	-.1035
3	.5524E-01	.5332E-02	.1324E-02	.3886E-01	-.7252E-01	-.1130	.3050E-01	.2021E-01	-.1705E-01	-.1853
4	-.1937	-.5349E-01	.1028	.1363	.9990E-01	-.3181E-01	.1620	-.4641E-01	-.2354	.8914E-01
5	.1534	-.2437E-01	.4592E-02	.1022	.6068E-01	-.9351E-01	.5362E-01	.7663E-01	-.4678E-01	-.6718E-01
6	.1318	-.1722	-.4240E-01	.8883E-01	-.2537E-01	.1449E-01	.7403E-01	-.5686E-02	-.8169E-01	.1841
7	-.4240E-01	.8883E-01	.5258E-01	-.6127E-02	-.9325E-01	.8050E-01	-.4868E-01	-.1187	-.4007	.2677
8	-.2537E-01	.1449E-01	-.9325E-01	.8050E-01	.3856	.1583	.1392	-.2514	-.4385E-01	.8681E-01
9	.7403E-01	-.5686E-02	-.4868E-01	-.1187	.1392	-.2514	-.6826E-01	-.1280E-01	-.1558	.8783E-01
10	-.8169E-01	.1841	-.4007	.2672	-.4385E-01	.8681E-01	-.1558	.8783E-01	-.2429	.3085
11	-.1159E-01	[illegible]	.1686	-.1153	-.1055	.2895E-01	.1315	.6196E-01	-.2785	.1955
12	-.1221	.1125	-.2272E-01	.1461E-01	.2929E-01	-.1785	.9841E-01	.5173	-.1635	.5298E-01
13	-.5567E-02	-.6491E-01	.9454E-02	-.9104E-01	-.4560E-01	.6134E-01	-.2257	.3237	.7850E-01	.1266
14	-.3058E-01	-.1221	-.3394E-01	-.9087E-01	-.2541	-.1477E-01	.3491E-01	.2449	.9032E-01	.1672E-01
15	-.1234	-.2633	-.1455	-.5997E-01	.1099	-.6642E-01	.1125	.6723E-01	.2052	-.2343
16	.3110E-02	-.2717	-.2868	.2467	-.1256	-.9235E-02	-.5002E-01	-.1140	.1376	-.6002E-01
17	-.7943E-01	-.1819	.3054E-01	.2275	-.7285E-02	-.1840	-.1273	.6681E-01	.4790E-01	-.1177
18	.4965E-02	.6564E-01	-.1978	-.3031E-02	-.4963	-.3286	.8869E-01	-.3104E-01	.1602	.4667E-01
19	-.1419	-.1293	-.1963	.1253E-01	.2381	.6099E-01	.4929E-01	.1898	.4353E-01	.4956E-01
20	.9769E-01	-.7495E-01	.1629	.3267	-.2380E-01	.1238E-01	.1416	.1154	-.1626E-01	.1950
21	.1100E-01	.1040	.2635	.4867E-01	-.1086	.6714E-01	-.2750	.4927E-01	-.3770E-01	-.6797E-01
22	.2316E-01	-.1781E-01	-.8582E-01	-.1119	-.2344	.4256E-01	-.1174	-.1950	.5211E-01	.1345

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.5822E-02	.1451E-01	.9495E-01	-.1010	.6998E-01	.1404	.1084	.6517E-01	-.1788	.2171
2	-.2761	.1002	.1441	.1845	.1469	-.1064	.1124	.6742E-01	.4705E-01	-.4826E-01
3	.3737E-01	-.1275	.1573	.9233E-01	.6893E-01	-.2538E-01	-.1735	.3046E-01	-.5439E-01	.3489
4	-.1851	.1945	.1147	.1306	.1109	-.3024E-01	-.8193E-01	.3662E-01	-.1587	.2218

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
5	-.1341	-.1414	.3579	-.2399	-.2604	.9751E-01	.9520E-02	.2671	-.6255E-01	-.2351
6	-.1159E-01	-.3641	-.1721	.1125	-.3367E-02	-.6491E-01	-.3098E-01	-.1221	-.1234	-.2633
7	.1886	-.1133	-.2272E-01	.1481E-01	.9454E-02	-.9104E-01	-.3391E-01	-.9087E-01	-.1453	-.5997E-01
8	-.1055	.2895E-01	.2929E-01	-.1785	-.4560E-01	.6134E-01	-.2541	-.1477E-01	.1099	-.6642E-01
9	.1319	.6196E-01	.9841E-01	.3125	-.2257	.5257	.3491E-01	.2449	.1179	.6723E-01
10	-.2785	.1935	-.1655	.5298E-01	.7850E-01	.1286	.9032E-01	.1672E-01	.2E-02	-.2343
11	-.3273E-02	.1014	-.1509E-01	.9377E-01	.1708E-01	-.1510E-01	.2009E-01	.5758E-01	-.1440E-01	.1490E-01
12	-.1909E-01	.9377E-01	.7490E-01	.1353	.2598E-01	-.2064	.2684E-01	-.7557E-02	-.8704E-01	.4685E-01
13	.1708E-01	-.1510E-01	.2398E-01	-.2064	.3588	-.2241E-02	-.3588	.2844	.2566E-01	.1254E-01
14	.2009E-01	.5758E-01	.2684E-01	-.7557E-02	-.3588	.2844	-.2530	-.6489E-01	.9084E-02	.5118E-01
15	-.1440E-01	.1490E-01	-.8704E-01	.4685E-01	.2566E-01	.1254E-01	.9084E-02	.5118E-01	-.1099	-.2427
16	.9768E-02	.1662	.1909	-.2718E-01	-.2210E-01	-.2928	-.2360	.5172E-01	.6485E-01	-.9981E-01
17	.7033E-01	-.1113E-01	.9822E-01	.6990E-01	.9930E-01	.1067	.1975	-.7551E-01	.1754	.2339E-01
18	-.1343	.8879E-01	-.2962	.3941E-01	-.3473E-01	-.4237E-01	-.6899E-01	-.8412E-01	.1211	.9539E-02
19	.6625E-01	-.1807	.5992E-01	.9189E-01	-.6273E-01	-.1702	.1585	-.8049E-01	.1836	.1016
20	-.9051E-01	-.1640	-.2344	.5446E-01	-.3694E-01	.1572	.4680E-01	.1612	.1972	.2950
21	-.3369	.7910E-02	.1756	-.3376E-01	-.1122	-.1938	.1231	-.4131E-02	.1034	-.3603E-02
22	.2703E-01	-.3957E-01	.3075E-01	-.1871E-01	-.1596	-.1579	.2909	.3783	-.3291	-.4724E-01

COL	16		17		18		19		20	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.5645E-02	.1641	-.3599E-02	.1695	-.2595E-01	.7360E-02	-.9208E-01	.1038	-.2580	.4290E-01
2	-.2898E-01	.2193	.1414E-01	.1777	.1212E-01	.1897E-01	-.3689E-02	-.2589	.1487	-.9878E-01
3	.3218	-.1598	-.6849E-01	.2121	-.6159E-01	.7512E-01	-.3160E-01	-.4337E-01	.7151E-01	.1569
4	.5421E-01	-.1215	.1043	-.3134E-01	.1615E-01	-.6229E-02	-.6859E-01	-.1072E-02	.1947	.2406E-01
5	.2297	-.1092E-01	-.1339	-.2148E-01	-.1033	-.1281E-01	-.2997	.1944	.9651E-02	.9203E-01
6	.3110E-02	-.2717	-.7943E-01	-.1819	.4965E-02	.6564E-01	-.1419	-.1295	.9769E-01	-.7495E-01
7	-.2868	.2467	.3054E-01	.2275	-.1978	-.3031E-02	-.1963	.1255E-01	.1829	.3267
8	-.1256	-.9233E-02	-.7285E-02	-.1840	-.4965	-.3286	.2361	.6099E-01	-.2380E-01	.1238E-01
9	-.5002E-01	-.1140	-.1273	.6681E-01	.8869E-01	-.3104E-01	.8429E-01	.1898	.1416	.1134
10	.1376	-.6002E-01	.6790E-01	-.1177	.1602	.4667E-01	.4955E-01	.4956E-01	-.1626E-01	.1950
11	.9768E-02	.1662	.7033E-01	-.1115E-01	-.1345	.9879E-01	.6825E-01	-.1807	-.9051E-01	-.1640
12	.1305	-.2719E-01	.9822E-01	.6990E-01	-.2962	.3941E-01	.3992E-01	.9189E-01	-.2344	.5446E-01
13	-.2210E-01	-.1778	.9930E-01	.1087	-.3473E-01	-.4237E-01	-.6575E-01	-.1705	-.3694E-01	.1572
14	.2360	.5172E-01	.1975	-.7551E-01	-.6899E-01	-.8412E-01	.1585	-.8049E-01	.4680E-01	.1612
15	.6485E-01	.9991E-01	.1754	.2539E-01	.1211	.9539E-02	.1836	.1016	.1972	.2950
16	-.6551E-01	.1687	-.3015	.1435	.1353	.2057E-01	.4592E-01	-.6098E-01	.1197	.2389
17	-.3015	.1435	.2395E-01	-.4202	-.4634E-01	.4472E-01	-.2586	.1396	-.1385	.3676E-02
18	.1353	.2657E-01	-.4634E-01	.4472E-01	-.5350	-.2418	-.1696	.7002E-01	.1706	-.1943
19	.4592E-01	-.6098E-01	-.2586	.1396	-.1696	.7002E-01	.3878	.7496E-01	-.6550E-01	-.1645
20	.1197	.2389	-.1385	.3676E-02	.1706	-.1943	.6539E-01	-.1645	-.2488	-.2086E-01
21	-.1366E-01	.8863E-01	.2411	-.3183	-.4273E-01	.8882E-01	.2168	-.6752E-01	.1078	.1404
22	.8633E-01	-.2618E-01	-.1048	-.1453	-.3122E-01	-.2728	.2731	-.1715	-.2134	.1498

COL	21		22	
ROW	REAL	IMAG	REAL	IMAG
1	-.2776E-01	.1877	.9228E-01	-.4708E-01
2	.7897E-01	-.9259E-01	-.3692E-01	.5246E-01
3	.4949E-01	-.1356	-.1414	.3397E-01
4	.1239	-.3012E-01	-.4450E-01	-.7963E-01
5	-.2437E-01	.2356E-02	.6457E-01	.3811E-01
6	.1106E-01	.1042	-.2516E-01	-.1781E-01
7	.2655	.4802E-01	-.8582E-01	-.1119
8	-.1686	.6714E-01	-.2544	.4256E-01
9	-.2750	.4927E-01	-.1174	-.1950
10	-.3770E-01	-.6797E-01	.5211E-01	.1345
11	-.3369	-.7910E-02	.2763E-01	-.3957E-01
12	.1756	-.3376E-01	.3075E-01	-.1871E-01
13	-.1122	-.1938	-.1596	-.1579
14	.1231	-.4131E-02	.2909	.3783

COL	21		22	
ROW	REAL	IMAG	REAL	IMAG
15	.1034	-.3603E-02	-.5291	-.4724E-01
16	-.1366E-01	.8863E-01	.8653E-01	-.2618E-01
17	.2411	-.3183	-.1048	-.1453
18	-.4273E-01	.8882E-01	-.3122E-01	-.2728
19	.2168	-.6752E-01	.2731	-. 715
20	.1078	.1404	-.2134	.1498
21	-.1672	.5380	.1524	-.2842
22	.1524	-.2842	-.3876E-01	-.1363

TEST3/J2584

ENERGY = .1950E-02
RMIN = 3.000
RMAX = 7.000

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.1337	.3323	-.2067E-01	.1002	.7899E-01	.4572E-01	-.8239E-02	.7873E-01	-.1072	.6704E-02
2	-.2067E-01	.1002	-.1034	.1085	.1217	-.7163E-01	.2973E-01	-.4289E-01	-.3983E-01	-.4347E-01
3	.7899E-01	.4572E-01	.1217	-.7163E-01	-.3592E-01	.1013	.3577E-02	.9470E-01	.1344	.8579E-01
4	-.8239E-02	.7873E-01	.2973E-01	-.4289E-01	.3577E-02	.9470E-01	-.1090	-.1309	-.2488	-.8043E-01
5	-.1072	.6704E-02	-.3983E-01	-.4347E-01	.1344	.8579E-01	-.2488	-.8043E-01	-.7036E-01	.1461
6	-.3461	.4545E-02	.1800	.1248	.5261E-01	.1651	-.5762E-01	-.1147	.1147	.2247
7	-.2032	-.7223E-01	.5289E-01	-.1728	-.1173	-.1826	.1166	-.1448E-01	-.7795E-01	.4165
8	-.2774E-01	.1004	-.9019E-01	.1757	-.1971	-.5331E-01	-.2546	.1187	-.5382E-02	-.2852E-01
9	.7850E-01	.1469	-.4536E-02	.8309E-01	.2265	-.2577E-03	.1400	.1851E-01	.7920E-01	.2235
10	.1865	-.3326E-01	-.6560E-02	.4192E-01	-.1870E-01	.4407E-01	.7645E-01	.5446E-01	.1562	.1234
11	.9225E-01	.7579E-01	-.5639E-02	.8305E-01	-.2355	.1548	-.1237	-.1155	.1095	-.3174E-01
12	-.1131	-.2888	-.2723E-01	.2572	.1315	.5797E-01	-.6251E-01	.2493	.9457E-01	-.1354
13	.1088E-01	.1009	.2865	.2390E-01	.2636E-01	.1968	.5377E-01	.1635	-.1874	-.1492
14	-.8698E-01	.1145	.2290	.2603	-.2023	-.2587E-01	-.8435E-01	-.4487E-01	-.3649E-01	.6332E-01
15	-.2091E-01	.2142	.5922E-01	-.2744	-.6077E-01	-.9021E-01	-.1485	.2426	.1034	-.2505E-01
16	-.1232	-.1223	-.1021	-.5359E-01	-.9663E-01	.1398	-.2434E-01	.3587	-.1134E-02	-.3425E-01
17	-.2605	.8219E-01	-.9093E-02	-.4170E-01	.2482	.1539	.2711E-01	-.2246E-01	.1236	.1064E-01
18	.8550E-01	-.1255E-01	-.2864E-02	.7006E-01	-.1117	-.1415E-01	-.3268E-01	.5734E-01	-.3934E-01	-.5747E-01
19	.1160	.1380	.1742E-01	.2749E-01	-.6862E-01	-.5531E-01	.6079E-01	.6521E-01	-.1521	.3504
20	.1488	.1635E-02	-.1708	.1218	.1925	.2251E-01	-.1361	.7284E-01	-.1110	.1611
21	-.5064E-01	.1153	.4785E-01	-.7676E-01	.2614	.1211	.5173E-01	-.1750	.1560	-.8116E-01
22	-.3194E-02	.4131E-01	.5717E-02	-.1102E-01	.5296E-02	.8176E-01	.8264E-01	.2309E-01	.7620E-01	.2267
23	.4537E-01	-.1306	-.7573E-01	-.1072	.6784E-01	-.5863E-01	-.2440	.2213	.2387E-01	.1695
24	[illegible]	.2469	-.2855	.1039	-.1092	.1047	.3403E-01	.2037	-.7737E-01	-.2516E-01
25	-.2378	.1154	-.1496	-.5247E-01	-.6692E-01	-.5585E-01	.1276	-.1426	-.4500E-01	.6115E-01
26	-.1361E-01	-.3616E-02	.4533E-01	.1247	-.1975	.1609	-.4771E-01	-.1558	.4404E-01	-.1138
27	.3812E-01	.4978E-01	.1554	.1324	.6938E-01	-.9962E-01	-.2270	.1202	.3233E-01	.1138
28	-.4272E-01	.1361	.1223	-.5681E-01	-.2577	-.3081	.9205E-01	.7941E-01	-.8997E-01	-.9885E-01
29	-.2192E-01	.1277	-.8754E-03	-.1209	-.8622E-02	.7719E-01	-.6158E-01	.1491	.1289	-.1016E-01
30	.3512E-01	.1085E-01	.9262E-01	-.3788	-.9516E-01	.5971E-01	-.2024E-01	-.2428E-01	-.7268E-01	-.8396E-01
31	-.2751E-01	.4248E-01	-.6066E-01	.3389E-01	-.3391E-01	-.3886E-01	-.2387E-01	.6422E-01	.6564E-01	-.2151E-01

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.3461	.4545E-02	-.2032	-.7223E-01	-.2774E-01	.1004	.7850E-01	.1469	.1865	-.3326E-01
2	.1800	.1248	.5289E-01	-.1728	-.9019E-01	.1757	-.4536E-02	.8309E-01	-.6560E-02	.4192E-01
3	.5261E-01	.1651	-.1173	-.1826	-.1971	-.5331E-01	.2265	-.2577E-03	-.1870E-01	.4407E-01
4	-.5762E-01	-.1147	.1166	-.1448E-01	-.2546	.1187	.1400	.1851E-01	.7645E-01	.5446E-01
5	.1147	.2247	-.7795E-01	.4165	-.5382E-02	-.2852E-01	.7920E-01	.2235	.1562	.1234
6	-.1621	-.5909E-01	.1084	.6314E-01	.4715E-01	.2869E-01	.2438E-02	.8651E-01	.9296E-02	.8324E-01
7	.1084	.6314E-01	.1968	.1504E-01	-.1620	.2513E-01	.5573E-01	.4114E-01	.1614	-.5465E-01
8	.4715E-01	.2869E-01	-.1620	.2513E-01	.2674	.1543	.5750E-01	-.2164	-.9709E-01	-.2197E-01
9	.2438E-02	.8651E-01	.5573E-01	.4114E-01	.5750E-01	-.2164	-.8824E-01	.6383E-01	.7918E-01	-.8463E-01
10	.9296E-02	.8324E-01	.1614	-.5465E-01	-.9709E-01	-.2197E-01	.7918E-01	-.8463E-01	.7665E-01	.4068
11	.5599E-01	-.4792E-01	.5523E-01	.1517	.1715E-01	.5621E-01	.2024	.2113	-.2456	-.1413
12	-.1532	-.5514E-01	-.2165E-01	.4731E-01	-.1452	-.5544E-01	.8082E-01	.3821	-.1774E-02	-.3478
13	.1968	.5137E-01	.9248E-01	.3958E-01	-.9470E-01	.1543	-.7853E-01	.2206	-.9539E-02	-.9325E-02
14	.1364	.3050E-01	-.6692E-01	-.6343E-01	-.6849E-01	.1068E-01	-.1765E-01	-.6923E-01	.1058E-01	-.7797E-01
15	-.1570	.4050E-01	-.4756E-01	.1302	-.3548E-01	-.7565E-02	-.6355E-01	.1385	-.2516E-01	.5538E-01
16	.3292	.7428E-02	-.1245	-.1919E-01	-.5137E-01	.1046	.1263	.1643	.4773E-01	.1336
17	-.8363E-01	-.3040E-01	-.2078	-.3079E-01	.5840E-01	-.2346	.2093	-.8514E-01	.1901E-01	-.1372
18	.4918E-02	-.1281	.1668	.9496E-02	-.4124	-.1179	.1125	-.1353	-.6781E-01	.7292E-01
19	.2389E-02	-.2735E-01	-.1361	-.2485	.1614E-01	-.3003E-01	-.2103E-01	.1105	-.1608	-.2596E-02
20	.8057E-01	-.1298	-.2539E-01	.1958	-.1654	.1335	.2416E-01	-.2107	.6892E-01	-.2283

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
21	.3491	.8836E-01	.1168	.8904E-01	-.2345E-01	.3058E-01	-.2418	-.3519E-01	-.1501	-.1691
22	.2747E-01	-.1828	-.1202	.1015E-01	-.4094	-.8185E-01	-.1956	-.5792E-01	-.1470	.4422E-01
23	-.1251	-.1105E-01	.5396E-01	.1081	-.8160E-01	.7607E-01	-.1064E-01	-.1552	-.2530	-.6230E-01
24	.5290E-01	.2849E-01	.4300E-01	-.5231E-01	-.1286	-.5278E-01	-.1195	-.6185E-01	.3458E-01	-.2165E-01
25	.1547	.9401E-01	-.2861	.1685	.6673E-01	.1693	-.4605E-01	.7956E-01	-.1858	.4038E-01
26	-.4003E-01	.1338	.1295	-.5314E-01	.7538E-02	.5846E-01	.1169	-.2208	.3672E-01	-.1127
27	.2343	.1836	-.9781E-01	-.1855	.1458E-01	.1191	-.2943E-01	.6706E-01	.1713	-.2511E-02
28	-.5906E-01	-.5413E-01	-.2420E-01	.2332	-.2103E-02	-.5089E-01	-.7760E-01	-.4586E-01	.2618	-.5772E-01
29	-.1994	-.1010	.6077E-02	-.6500E-01	-.3618E-01	.8238E-01	-.7575E-01	-.2453E-01	.1326	-.1246
30	-.3187E-01	.2015E-01	.5477E-01	-.2717E-01	.3739E-01	.5827E-01	-.7173E-01	-.2652E-01	.1401E-01	-.1173
31	.3321E-01	-.5665E-02	-.7139E-02	-.2391E-02	.1549E-01	.1811E-01	.4013E-01	.7202E-01	-.6073E-02	.1990E-01

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.9225E-01	.7579E-01	-.1131	-.2888	.1088E-01	.1009	-.8698E-01	.1145	-.2091E-01	.2142
2	-.5639E-02	.8305E-01	-.2723E-01	.2572	.2865	.2390E-01	.2290	.2603	.5922E-01	-.2744
3	-.2355	.1548	.1315	.5797E-01	.2636E-01	.1968	-.2023	-.2587E-01	-.6077E-01	-.9021E-01
4	-.1237	-.1155	-.6251E-01	.2493	.5377E-01	.1635	-.8435E-01	-.4487E-01	-.1485	.2426
5	.1095	-.3174E-01	.9457E-01	-.1354	-.1874	-.1492	-.3649E-01	.6332E-01	.1034	-.2505E-01
6	.5599E-01	-.4792E-01	-.1532	-.5514E-01	.1968	.5137E-01	.1364	.3050E-01	-.1570	.4050E-01
7	.5523E-01	.1517	-.2165E-01	.4731E-01	.9248E-01	.3958E-01	-.6692E-01	-.6343E-01	-.4756E-01	.1302
8	.1715E-01	.5621E-01	-.1452	-.5544E-01	-.9470E-01	.1543	-.6849E-01	.1068E-01	-.3548E-01	-.7565E-02
9	.2024	.2113	.8082E-01	.3821	-.7853E-01	.2206	-.1765E-01	-.6923E-01	-.6355E-01	.1385
10	-.2456	-.1413	-.1774E-02	-.3478	-.9539E-02	-.9325E-02	.1058E-01	-.7797E-01	-.2516E-01	.5538E-01
11	.8380E-01	.1955	-.9025E-01	.8088E-01	-.1938E-01	-.6809E-01	-.1929	.1648	-.3701	-.8713E-01
12	-.9025E-01	.8088E-01	.1296	.2049E-01	-.1248	-.9787E-01	.1537	-.4728E-01	.1012	.1169
13	-.1938E-01	-.6809E-01	-.1248	-.9787E-01	.1238	-.2110	-.2853	.1252	.9728E-01	-.2698E-01
14	-.1929	.1648	.1537	-.4728E-01	-.2853	.1252	.2637	.1698	.2023	.1202
15	-.3701	-.8713E-01	.1012	.1169	.9728E-01	-.2698E-01	.2023	.1202	-.1030	-.2761
16	.7702E-01	.2519E-02	.4594E-02	.1761	-.2286E-01	-.5645E-01	-.8537E-01	-.6848E-01	.1644	.1224
17	-.9702E-01	-.1919E-02	-.1045	-.8796E-02	.1707	-.1468	.4850E-01	-.1079	-.3797E-01	-.2456E-02
18	.1443	-.6838E-01	-.1901	.2139	.4517E-01	-.6028E-01	-.6072E-01	-.4340E-01	.5053E-01	-.7427E-01
19	.1121	-.9191E-01	-.1598	-.7584E-02	-.1632	-.2867	-.9790E-01	-.2607E-01	-.2104E-01	.1264E-01
20	-.3165E-01	-.1697	-.7778E-01	-.5310E-01	-.1741E-02	-.3694E-01	.3002E-01	-.2872	-.1565E-01	-.1149
21	-.7742E-01	-.6298E-01	.7283E-02	-.1446	-.1211	-.2079E-01	.9477E-02	.1084	-.1785	.1828
22	-.4321E-01	.1909	-.1072	-.1725	-.1105	-.1222	.2033	.1872	[illegible]	.1244E-01
23	.1608E-02	.1572	-.2522E-01	-.8282E-01	.2276	-.6103E-01	.8367E-01	.7865E-01	-.3904E-01	.1559
24	.7766E-01	-.1887	.1953E-02	.4892E-01	-.1725E-01	.1297	.1300	.8747E-02	-.1258	-.3734E-01
25	-.1858	-.1071	-.3499E-01	.6361E-01	.9661E-01	.1315	.6977E-01	-.1257	.2309E-01	.3203
26	-.1726	-.3527E-01	-.1235	.1163	-.4683E-01	-.1715	.1559	-.3288E-01	.9933E-01	.4605E-01
27	.1646	-.1428	.9105E-02	-.8537E-01	-.1038E-01	.1075	.5266E-01	.1455E-01	-.2055	-.3234E-01
28	.6643E-01	.6568E-01	.1666E-01	.1109E-01	.1184E-01	.5197E-01	.4464E-01	.1749	-.4351E-01	.1536
29	.1343	-.1527E-01	.1205	-.1442E-01	-.1274	-.1577E-01	-.2185	.8589E-01	.7370E-01	.6823E-02
30	.4744E-01	-.8800E-01	.2059E-01	-.8888E-02	-.2617	-.9320E-02	.8751E-02	-.1420	.3474E-01	.8225E-01
31	-.6423E-01	.7930E-01	-.1650E-01	.3931E-01	-.1116E-01	-.3146E-01	-.6942E-01	.1161	-.2633E-01	-.2531E-02

COL	16		17		18		19		20	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.1232	-.1223	-.2605	.8219E-01	.8550E-01	-.1255E-01	.1160	.1380	.1488	.1636E-02
2	-.1021	-.5359E-01	-.9093E-02	-.4170E-01	-.2864E-02	.7006E-01	.1742E-01	.2749E-01	-.1708	.1218
3	-.9663E-01	.1398	.2482	.1539	-.1117	-.1415E-01	-.6862E-01	-.5531E-01	.1925	.2251E-01
4	-.2434E-01	.3587	.2711E-01	-.2246E-01	-.3268E-01	.5734E-01	.6079E-01	.6321E-01	-.1361	.7284E-01
5	-.1134E-02	-.3425E-01	.1236	.1064E-01	-.3934E-01	-.5747E-01	-.1521	.3504	-.1110	.1611
6	.3292	.7427E-02	-.8363E-01	-.3040E-01	.4918E-02	-.1281	.2389E-02	-.2735E-01	.8057E-01	-.1298
7	-.1245	-.1919E-01	-.2078	-.3079E-01	-.1668	.9496E-02	-.1361	-.2485	-.2539E-01	.1958
8	-.5137E-01	.1046	.5840E-01	-.2346	-.4124	-.1179	.1614E-01	-.3003E-01	-.1654	.1335
9	.1263	.1643	.2093	-.8514E-01	.1125	-.1353	-.2103E-01	.1105	.2416E-01	-.2107
10	.4773E-01	.1336	.1901E-01	-.1372	-.6781E-01	.7292E-01	-.1608	-.2596E-02	.6892E-01	-.2283
11	.7702E-01	.2519E-02	-.9702E-01	-.1919E-02	.1443	-.6838E-01	.1121	-.9191E-01	-.3165E-01	-.1697
12	.4594E-02	.1761	-.1045	-.8796E-02	-.1901	.2139	-.1598	-.7584E-02	-.7778E-01	-.5310E-01

ROW	COL 16 REAL	16 IMAG	17 REAL	17 IMAG	18 REAL	18 IMAG	19 REAL	19 IMAG	20 REAL	20 IMAG
13	-.2266E-01	-.5645E-01	.1707	-.1468	.4517E-01	-.6028E-01	-.1632	-.2867	-.1741E-02	-.3694E-01
14	-.8537E-01	-.6848E-01	.4860E-01	-.1079	-.6072E-01	-.4340E-01	-.9290E-01	-.2607E-01	.3002E-01	-.2872
15	.1644	.1224	-.5797E-01	-.2486E-02	.5053E-01	-.7427E-01	-.2104E-01	.1264E-01	-.1565E-01	-.1149
16	.1134	-.7442E-01	-.9690E-01	-.6496E-01	.9464E-01	-.8291E-01	.2354	-.3839E-01	.1889	.3627E-01
17	-.9690E-01	-.6496E-01	.1241	-.3562	-.1048	-.5868E-01	.2164	-.4243E-01	.5621E-01	-.5379E-02
18	.9464E-01	-.8291E-01	-.1048	-.5868E-01	-.1465	-.1880	-.2318	.3557	.2370	-.1100E-01
19	.2354	-.3839E-01	.2164	-.4243E-01	-.2318	.3557	.1356	.2530E-01	-.1768	-.1332
20	.1889	.3627E-01	.5621E-01	-.5379E-02	.2370	-.1100E-01	-.1768	-.1332	-.3384E-01	-.9962E-01
21	.2060E-01	.6627E-01	.2121E-01	.1427	-.8690E-01	.1465	.3430E-01	.8397E-01	.1077	.1012
22	.1256	.3079E-01	-.2197E-01	.2085	-.2409E-01	-.2763	.2601	-.1128	-.1116	.2159
23	-.3207	-.1624	.8640E-01	-.5926E-01	.1757	.1555	-.1170	.5250E-01	.8574E-01	-.2345E-01
24	.3637E-02	-.1845	.1664	.3979E-01	.1025	.8104E-01	-.1517	-.1583E-01	-.2681	.4391E-02
25	-.1479E-01	.6260E-01	-.9325E-01	-.7830E-01	.5086E-02	-.4862E-01	-.1834E-01	-.1921E-01	-.4253E-01	-.9064E-01
26	.1929	.3029E-02	-.2243E-01	-.2513E-01	.1135	.1711E-02	-.4891E-01	-.2402E-01	-.2419E-01	.1676
27	.1587E-01	-.9781E-02	-.2779	.3989E-01	.1155	-.5067E-01	-.1001	-.7852E-01	.2542E-02	-.1351
28	.1438	-.1244	.2377	-.1335E-01	.3647E-01	.2997E-01	-.8756E-01	.2848E-01	.1395	.8542E-01
29	-.9015E-01	.2501	.1348	-.6431E-01	.1236	-.7721E-01	.2188E-02	-.8645E-01	-.2241	.1405
30	.9399E-01	.8727E-01	-.1146	-.1734	.3355E-01	-.1111	.3786E-01	-.6040E-01	.8297E-01	-.2271E-01
31	-.9842E-01	.2003E-01	-.8400E-01	-.5694E-01	.1014E-01	.1215E-02	.5601E-02	-.3947E-01	.5846E-01	-.7910E-01

ROW	COL 21 REAL	21 IMAG	22 REAL	22 IMAG	23 REAL	23 IMAG	24 REAL	24 IMAG	25 REAL	25 IMAG
1	-.5064E-01	.1153	-.3194E-02	.4131E-01	-.4537E-01	-.1306	-.1622	.3469	-.2318	.1154
2	.4785E-01	-.7676E-01	.5718E-02	-.1102E-01	-.7573E-01	-.1072	-.2855	.1039	-.1496	-.5247E-01
3	.2614	.1211	.5296E-02	.8176E-01	.6784E-01	-.3863E-01	-.1092	.1047	-.6692E-01	-.5565E-01
4	.5175E-01	-.1750	.8264E-01	.2510E-01	-.2440	.2215	.5403E-01	.2397	.1276	-.1426
5	.1560	-.8116E-01	.7620E-01	.2267	.2382E-01	.1693	-.7737E-01	-.2516E-01	-.4500E-01	.6115E-01
6	.3491	.8836E-01	.2747E-01	-.1828	-.1251	-.1105E-01	.5290E-01	.2849E-01	.1547	.9401E-01
7	.1168	.8904E-01	-.1202	.1015E-01	.5396E-01	.1081	.4300E-01	-.5231E-01	-.2861	.1685
8	-.2345E-01	.3058E-01	-.4094	-.8185E-01	-.8160E-01	.7667E-01	-.1286	-.5278E-01	.6673E-01	.1695
9	-.2418	-.3519E-01	-.1956	-.5792E-01	-.1064E-01	-.1552	-.1195	-.6185E-01	-.4605E-01	.7956E-01
10	-.1301	-.1691	-.1470	.4422E-01	-.2530	-.6230E-01	.3458E-01	-.2165E-01	-.1858	.4038E-01
11	-.7742E-01	-.6298E-01	-.4321E-01	.1909	.1808E-02	.1572	.7764E-01	-.1887	-.1806	-.1071
12	.7283E-02	-.1446	-.1072	-.1725	-.2522E-01	-.9282E-01	.1953E-02	.4892E-01	-.3499E-01	.6361E-01
13	-.1211	-.2079E-01	-.1105	-.1222	.2276	-.6103E-01	-.1725E-01	.1297	.9661E-01	.1315
14	.9477E-02	.1084	.2033	.1872	.8367E-01	.7865E-01	.1300	.8747E-02	.6977E-01	-.1257
15	-.1785	.1828	.6873E-01	.1244E-01	-.3904E-01	.1559	-.1238	-.3734E-01	.2307E-01	.3203
16	.2060E-01	.6627E-01	.1256	.3079E-01	-.3207	-.1624	.9637E-02	-.1645	-.1479E-01	.6260E-01
17	.2121E-01	.1427	-.2197E-01	.2085	.8640E-01	-.5926E-01	.1664	.3979E-01	-.9325E-01	-.7830E-01
18	-.8690E-01	.1465	-.2409E-01	-.2763	.1757	.1555	[illegible]	.8104E-01	.5086E-02	-.4862E-01
19	.3430E-01	.8397E-01	.2601	-.1128	-.1170	.5250E-01	-.1517	-.1583E-01	-.1834E-01	-.1921E-01
20	.1077	.1012	-.1116	.2159	.8574E-01	-.2345E-01	-.268	.4391E-02	-.4253E-01	-.9064E-01
21	-.1175	.3657	-.8367E-01	-.2446	-.1136	.1286	.1209E-01	.5127E-01	-.1320	-.7962E-01
22	-.8367E-01	-.2446	-.1973	.1111	-.2186E-01	-.7225E-01	-.1059E-01	.6791E-01	.1462	-.2128E-01
23	-.1136	.1286	-.2186E-01	-.7225E-01	-.2484	.5736E-01	-.3602E-01	-.5824E-01	.2010	-.9444E-01
24	.1209E-01	.5127E-01	-.1059E-01	.6791E-01	-.3602E-01	-.5824E-01	.4948	.1180	-.1770	.1853
25	-.1320	-.7962E-01	.1462	[illegible]	.2010	-.9444E-01	-.1770	.1853	.9889E-01	-.1464E-01
26	.1030	.1434	-.1456E-01	[illegible]	-.1086	-.2956	-.1730	-.3445E-01	-.1151	-.9767E-01
27	.2286E-01	-.9586E-02	-.6662E-01	-.3608E-01	.2578E-01	-.4701E-01	.6124E-01	-.2659E-02	.2108	-.2592
28	.1016	-.3191E-01	[illegible]	-.8371E-01	-.1897	-.1030	-.1046	-.1343	.4995E-01	-.9893E-01
29	.7128E-01	.2064	.5095E-01	.3080E-01	-.9777E-01	-.2210E-01	.6183E-01	.8642E-01	.1518	-.1444
30	.1319E-02	-.4165E-01	-.3796E-01	.9753E-02	.2568E-01	-.1383	.5653E-01	.7186E-01	.5792E-01	.1438
31	.9508E-03	.6111E-02	.3220E-01	-.7390E-02	-.7034E-01	-.2966E-01	.5778E-01	.5170E-01	-.1326E-01	-.1306

ROW	COL 26 REAL	26 IMAG	27 REAL	27 IMAG	28 REAL	28 IMAG	29 REAL	29 IMAG	30 REAL	30 IMAG
1	-.1381E-01	-.3616E-02	.3812E-01	.4978E-01	-.4272E-01	.1361	-.2192E-01	.1277	.3512E-01	.1085E-01
2	.4533E-01	.1247	.1554	.1324	.1223	-.5681E-01	-.8734E-03	-.1209	.9262E-01	-.3788
3	-.1975	.1609	.6938E-01	-.9962E-01	-.2577	-.3081	-.8522E-02	.7719E-01	-.9316E-01	.5971E-01
4	-.4771E-01	-.1358	-.2270	.1202	.9203E-01	.7941E-01	-.6158E-01	.1491	-.2024E-01	-.2428E-01

ROW	COL 26 REAL	26 IMAG	27 REAL	27 IMAG	28 REAL	28 IMAG	29 REAL	29 IMAG	30 REAL	30 IMAG
5	.4404E-01	-.1136	.3233E-01	.1158	-.8997E-01	-.9885E-01	.1289	-.1016E-01	-.7266E-01	-.8396E-01
6	-.4003E-01	.1338	.2343	.1836	-.5906E-01	-.5413E-01	-.1994	-.1010	-.3137E-01	.2015E-01
7	.1295	-.5314E-01	-.9281E-01	-.1855	-.2420E-01	.2332	.6077E-02	-.6500E-01	.5477E-01	-.2717E-01
8	.7558E-02	.5846E-01	.1459E-01	.1191	-.2103E-02	-.5089E-01	-.3618E-01	.8258E-01	.5739E-01	.5827E-01
9	.1169	-.2208	-.2943E-01	.6206E-01	-.7760E-01	-.4586E-01	-.7575E-01	-.2453E-01	-.7173E-01	-.2652E-01
10	.3677E-01	-.1127	.1715	-.2511E-02	.2618	-.5772E-01	.1326	-.1246	.1401E-01	-.1173
11	-.1726	-.3527E-01	.1846	-.1428	.6643E-01	.6568E-01	.1345	-.1527E-01	.4244E-01	-.8800E-01
12	-.1253	.1163	.9105E-02	-.8537E-01	.1666E-01	.1109E-01	.1203	-.1442E-01	.2059E-01	-.8888E-02
13	-.4683E-01	-.1715	-.1038E-01	.1075	.1184E-01	.5197E-01	-.1274	-.1577E-01	-.2617	-.9320E-02
14	.1559	-.3288E-01	.5266E-01	.1455E-01	.4464E-01	.1749	-.2185	.8589E-01	.8751E-02	-.1420
15	.9953E-01	.4603E-01	-.2055	-.3234E-01	-.4351E-01	.1536	.7370E-01	.6873E-02	.3474E-01	.8225E-01
16	.1929	.3029E-02	.1587E-01	-.9781E-02	.1438	-.1244	-.9015E-01	.2501	.9399E-01	.8727E-01
17	-.2243E-01	-.2513E-01	-.2779	.3989E-01	.2377	-.1335E-01	.1348	-.6431E-01	-.1146	-.1734
18	.1135	.1711E-02	.1155	-.5067E-01	.3647E-01	.2997E-01	.1236	-.7721E-01	.3355E-01	-.1111
19	-.4891E-01	-.2402E-01	-.1001	-.7852E-01	-.8756E-01	.2848E-01	.2188E-02	-.8645E-01	.3786E-01	-.6040E-01
20	-.2419E-01	.1676	.2543E-02	-.1351	.1395	.8542E-01	-.2241	.1405	.8297E-01	-.2271E-01
21	.1030	.1434	.2286E-01	-.9586E-02	.1016	-.3191E-01	.7128E-01	.2064	.1319E-02	-.4165E-01
22	-.1456E-01	-.1805E-01	-.8662E-01	-.3608E-01	-.2632E-01	-.8371E-01	.5095E-01	.3080E-01	-.3796E-01	.9753E-02
23	-.1086	-.2956	.2578E-01	-.4701E-01	-.1897	-.1030	-.9777E-01	-.2210E-01	.2568E-01	-.1383
24	-.1730	-.3445E-01	.6124E-01	-.2659E-02	-.1046	-.1343	.6183E-01	.8642E-01	.5653E-01	.7186E-01
25	-.1151	-.9767E-01	.2108	-.2592	.4995E-01	-.9893E-01	.1518	-.1444	.5792E-01	.1438
26	.0065E-01	-.3003	.1265E-01	.9839E-02	-.2941	.1618	.3381	.5272E-01	-.1598	.8372E-01
27	.1265E-01	.9839E-02	-.3768	.1202E-01	-.6466E-01	-.1438	.3125	-.1550	.3758E-01	.2758E-01
28	-.2941	.1618	-.6466E-01	-.1438	.2983	-.3126E-01	.1353	.1063E-01	-.2387	-.1115
29	.3381	.5272E-01	.3125	-.1550	.1353	.1063E-01	.1191	-.3480	.2939E-01	.3572E-01
30	-.1598	.8372E-01	.3758E-01	.2758E-01	-.2387	-.1115	.2939E-01	.3572E-01	.2567	-.6076
31	.7783E-01	.2922E-01	-.1055	-.4066E-03	.9550E-02	-.2741E-01	-.6059E-01	-.4084E-01	.2673E-01	-.3618E-01

ROW	COL 31 REAL	31 IMAG
1	-.2961E-01	.4948E-01
2	-.6066E-01	.3389E-01
3	-.3391E-01	-.3886E-01
4	-.2387E-01	.6422E-01
5	.6564E-01	-.2151E-01
6	.3321E-01	-.5665E-02
7	-.7139E-02	-.2391E-02
8	.1349E-01	.1811E-01
9	.4013E-01	.7202E-01
10	-.6073E-02	.1990E-01
11	-.6423E-01	.7950E-01
12	-.1650E-01	.3951E-01
13	-.1116E-01	-.3146E-01
14	-.6942E-01	.1161
15	-.2633E-01	-.2551E-02
16	-.9842E-01	.2003E-01
17	-.8400E-01	-.5694E-01
18	.1014E-01	.1215E-02
19	.5601E-02	-.3947E-01
20	.5846E-01	-.7910E-01
21	.9508E-03	.6111E-02
22	.3220E-01	-.7390E-02
23	-.7034E-01	-.2966E-01
24	.5770E-01	.5170E-01
25	-.1326E-01	-.1306
26	.7783E-01	.2922E-01
27	-.1055	-.4066E-03
28	.9550E-02	-.2741E-01
29	-.6059E-01	-.4084E-01
30	.2673E-01	-.3618E-01

COL 31		
ROW	REAL	IMAG
31	.6887	-.2461

TEST3/J581

ENERGY = .7790E-04
RMIN = 3.000
RMAX = 7.000

COL	1		2		3	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.4945	.8157	-.1755	.1319	.1186	.1667
2	-.1755	.1319	.6682	.7103	-.1005E-01	.2326E-01
3	.1186	.1667	-.1005E-01	.2326E-01	-.6334	-.7458

TEST3/J582

ENERGY = .7790E-04
RMIN = 3.000
RMAX = 7.000

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.6895	-.5022	.6858E-02	-.3171E-02	-.5307E-01	-.2917E-01	-.2917	.3772	.2734	.4987E-01
2	.6858E-02	-.3171E-02	.5531	.8184	-.8606E-01	-.1259	.1415E-01	.1631E-01	.2768E-03	.1119E-01
3	.5307E-01	-.2917E-01	-.8606E-01	-.1259	-.5067	-.6046	-.5330E-01	.3784E-01	.1744E-01	.1616E-01
4	-.2917	.3772	.1415E-01	.1631E-01	-.5330E-01	.3784E-01	-.6022	-.3478	-.1345	-.6151E-01
5	.2734	.4987E-01	.2768E-03	.1119E-01	.1744E-01	.1616E-01	-.1345	-.6151E-01	.8085	-.4952
6	-.1028	-.5131E-01	.9166E-02	-.1790E-01	.4596E-02	-.2200E-02	.4077E-01	.3908E-01	.1152E-01	-.3501E-01

COL	6	
ROW	REAL	IMAG
1	-.1028	-.5131E-01
2	.9166E-02	-.1790E-01
3	.4596E-02	-.2200E-02
4	.4077E-01	.3908E-01
5	.1152E-01	-.3501E-01
6	.9907	-.1856E-01

TEST3/J583

ENERGY = .7790E-04
RMIN = 3.000
RMAX = 7.000

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.4657	.8401	.1807	-.8904E-01	-.9936E-01	-.1653	-.1703E-01	-.2737E-01	-.1033E-01	.1567E-01
2	.1807	-.8904E-01	.3214	.8958	-.5055E-01	-.8898E-01	.1497	.1523	.1524E-01	-.5361E-01
3	-.9936E-01	-.1653	-.5055E-01	-.8898E-01	-.4286	-.8721	-.5363E-01	.5995E-01	-.1049E-01	-.3749E-02
4	-.1703E-01	-.2737E-01	.1497	.1523	-.5363E-01	.5995E-01	-.9644	-.1595	.4476E-01	-.1421E-01
5	-.1033E-01	.1567E-01	.1524E-01	-.5361E-01	-.1049E-01	-.3749E-02	.4476E-01	-.1421E-01	.8519	-.5181
6	.5642E-02	-.4924E-02	.8227E-02	-.1438E-01	.5309E-01	.2044E-01	.2583E-01	-.1395E-02	-.3084E-03	.1709E-02

COL	6	
ROW	REAL	IMAG
1	.5642E-02	-.4924E-02
2	.8227E-02	-.1438E-01
3	.5309E-01	.2044E-01
4	.2583E-01	-.1395E-02
5	-.3084E-03	.1709E-02
6	.9982	-.3270E-01

TEST3/J504

ENERGY = .7790E-04
RMIN = 5.000
RMAX = 7.000

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.6525	.7434	.7501E-01	-.8594E-01	.7449E-03	-.5789E-03	.6903E-01	.3649E-01	.6693E-02	-.4582E-01
2	.7301E-01	-.8594E-01	.8390	.5283	-.2768E-01	-.2193E-01	-.4856E-03	-.2919E-02	-.2495E-02	.5812E-01
3	.7449E-03	-.5789E-03	-.2768E-01	-.2193E-01	-.6862	-.7220	-.2502E-01	.4988E-01	.2729E-01	.1137E-02
4	.6903E-01	.3649E-01	-.4856E-03	-.2919E-02	-.2502E-01	.4988E-01	-.9858	-.1539	.6673E-01	-.1340E-01
5	.6693E-02	-.4582E-01	-.2495E-02	.5812E-01	.2729E-01	.1137E-02	.6673E-01	-.1340E-01	.8362	-.5078
6	-.1008E-01	.1653E-01	.1016E-01	-.3389E-01	-.5850E-03	-.8943E-04	.2126E-01	.2358E-02	.2591E-02	.7445E-02

COL	6	
ROW	REAL	IMAG
1	-.1008E-01	.1653E-01
2	.1016E-01	-.3389E-01
3	-.5850E-03	-.8943E-04
4	.2126E-01	.2358E-02
5	.2591E-02	.7445E-02
6	.9584	-.3340E-01

TEST4/J501

ENERGY = 1.103
RMIN = .1000E-01
RMAX = 120.0

COL	1		2		3		4	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.9869	.1472	-.4844E-01	.4455E-01	.2635E-02	-.4701E-02	-.3697E-05	.3057E-02
2	-.4845E-01	.4453E-01	.6816E-01	.9938	.4280E-01	-.3940E-01	-.1541E-02	.1376E-02
3	.2635E-02	-.4701E-02	.4280E-01	-.3940E-01	.9878	.1447	.1913E-03	-.1281E-02
4	-.3697E-05	.3057E-02	-.1540E-02	.1376E-02	.1913E-03	-.1281E-02	.9989	.4638E-01

TEST4/J582

ENERGY = 1.103
RMIN = .1000E-01
RMAX = 120.0

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.9873	.1470	-.3937E-01	.3691E-01	.2486E-02	-.4489E-02	-.3627E-03	.5055E-02	-.9797E-02	-.1177E-01
2	-.3937E-01	.3691E-01	.2684	.7544	.3865E-01	-.3174E-01	-.1331E-02	.1174E-02	-.2758	-.1823
3	.2486E-02	-.4489E-02	.3865E-01	-.3174E-01	.9876	.1446	.1899E-03	-.1285E-02	.1071E-01	.1237E-01
4	-.3627E-03	.5055E-02	-.1331E-02	.1174E-02	.1899E-03	-.1285E-02	.9989	.4642E-01	-.3014E-03	-.4316E-03
5	-.9797E-02	-.1177E-01	-.2758	-.1823	.1071E-01	.1237E-01	-.3014E-03	-.4316E-03	.1175E-01	.3840
6	.1735E-01	-.2254E-02	.3589	-.8350E-01	-.2280E-01	.1223E-01	.6565E-03	-.2154E-03	.2103	.1106
7	-.1378E-02	.1816E-03	-.2832E-01	.1480E-01	.2042E-02	-.3437E-02	-.5254E-04	.3975E-04	-.1017E-01	-.1057E-01
8	.1898E-04	.2696E-03	.9318E-03	-.6634E-03	-.2795E-03	.2375E-02	-.1143E-03	.2438E-02	.2514E-03	.3372E-03
9	.1875E-05	-.1023E-04	-.1658E-04	.2231E-04	-.1011E-05	.8615E-05	.4302E-04	-.1319E-02	-.4874E-05	-.6557E-05
10	-.9894E-03	-.1148E-01	-.6250E-01	-.2668	.4777E-03	.1212E-01	-.6344E-05	-.3729E-03	-.5724	-.5764
11	-.8078E-02	-.1893E-02	-.1772	-.2280E-01	.1076E-01	.3504E-03	-.3045E-03	-.4249E-04	-.1581	-.3085E-01
12	.7901E-03	.4044E-04	.1665E-01	-.3810E-03	-.1056E-02	.4626E-04	.2826E-04	.1871E-04	.8946E-02	.7455E-02
13	-.2897E-04	-.8873E-05	-.6292E-03	.2593E-03	.1438E-04	.2278E-03	.1363E-05	-.1183E-03	-.2232E-03	-.2685E-03
14	.2329E-06	.3683E-05	.1171E-04	-.1087E-04	.9369E-06	-.4733E-05	-.2234E-05	.1236E-03	.3660E-05	.4615E-05
15	.9766E-08	.2073E-06	-.1429E-06	.2292E-06	-.2109E-08	-.1327E-06	-.4039E-06	-.3038E-04	-.4745E-07	-.5623E-07

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.1735E-01	-.2254E-02	-.1378E-02	.1816E-03	.1898E-04	.2696E-03	.1875E-05	-.1023E-04	-.9894E-03	-.1148E-01
2	.3589	-.8350E-01	-.2832E-01	.1480E-01	.9318E-03	-.6634E-03	-.1858E-04	.2231E-04	-.6250E-01	-.2668
3	-.2280E-01	.1223E-01	.2042E-02	-.3437E-02	-.2795E-03	.2375E-02	-.1011E-05	.8615E-05	.4777E-03	.1212E-01
4	.6565E-03	-.2154E-03	-.5254E-04	.3975E-04	-.1143E-03	.2438E-02	.4302E-04	-.1319E-02	-.6344E-05	-.3729E-03
5	.2103	.1106	-.1017E-01	-.1057E-01	.2514E-03	.3372E-03	-.4874E-05	-.6557E-05	-.5724	-.5764
6	.5401	.6325	.2720E-01	-.2566E-01	-.6728E-03	.1824E-03	.1005E-04	-.5713E-05	-.1968E-02	.1891
7	.2720E-01	-.2566E-01	.9878	.1455	.1718E-03	-.1318E-02	-.1305E-06	-.3692E-05	.9216E-05	-.1055E-01
8	-.6728E-03	.4824E-03	.1715E-03	-.1318E-02	.9987	.4976E-01	-.9715E-05	.3448E-03	-.1853E-04	.2906E-03
9	.1005E-04	-.5713E-05	-.1305E-06	-.3692E-05	-.9715E-05	.3448E-03	.9998	.1956E-01	-.2871E-06	-.5487E-05
10	-.1968E-02	.1891	.9216E-03	-.1055E-01	-.1853E-04	.2906E-03	-.2871E-06	-.5487E-05	-.4247	.1629
11	.2529	-.1122	-.1545E-01	.6797E-02	.3500E-03	-.8525E-04	-.4910E-05	.9473E-07	.7536E-01	-.1270
12	-.2515E-01	.2553E-01	.1723E-02	-.2834E-02	-.3626E-04	.4292E-04	.4008E-06	.7180E-06	-.2729E-02	.8009E-02
13	.6935E-03	-.6540E-03	-.2886E-03	.2564E-02	-.1311E-03	.2694E-02	.8171E-06	-.4630E-04	.5048E-04	-.2315E-03
14	-.9104E-05	.9814E-05	-.1077E-05	.6180E-05	.3349E-04	-.9645E-03	-.2281E-04	.1134E-02	-.2087E-06	.3844E-05
15	.8440E-07	-.6872E-07	-.5057E-08	.3417E-07	.1891E-06	.9307E-05	.2704E-04	-.1853E-02	-.4894E-08	-.4743E-07

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.8078E-02	-.1893E-02	.7901E-03	.4044E-04	-.2897E-04	-.8873E-05	.2329E-06	.3683E-05	.9766E-08	.2073E-06
2	-.1772	-.2280E-01	.1665E-01	-.3810E-03	-.6292E-03	.2593E-03	.1171E-04	-.1087E-04	-.1429E-06	.2292E-06
3	.1076E-01	.3504E-03	-.1056E-02	.4626E-04	.1438E-04	.2278E-03	.9369E-06	-.4733E-05	-.2109E-08	-.1327E-06
4	-.3045E-03	-.4249E-04	.2826E-04	.1871E-04	.1363E-05	-.1183E-03	-.2234E-05	.1236E-03	-.4039E-06	-.3038E-04
5	-.1581	-.3085E-01	.8946E-02	.7455E-02	-.2232E-03	-.2685E-03	.3660E-05	.4615E-05	-.4745E-07	-.3622E-07
6	.2529	-.1122	-.2515E-01	.2553E-01	.6935E-03	-.6340E-03	-.9104E-05	.9814E-05	.8440E-07	-.6872E-07
7	-.1545E-01	.6797E-02	.1723E-02	-.2834E-02	-.2886E-03	.2564E-02	-.1077E-05	.6181E-05	-.5057E-08	.3417E-07
8	.3500E-03	-.8525E-04	-.3626E-04	.4292E-04	-.1311E-03	.2694E-02	.3349E-04	-.9645E-03	.1891E-06	.9307E-05
9	-.4910E-05	.9473E-07	.4008E-06	.7180E-06	.8171E-06	-.4630E-04	-.2281E-04	.1134E-02	.2704E-04	-.1863E-02
10	.7536E-01	-.1270	-.2729E-02	.8009E-02	.5048E-04	-.2315E-03	-.2087E-06	.3844E-05	-.4889E-08	-.4743E-07
11	.5570	.7294	.2236E-01	-.2218E-01	-.4659E-03	.3156E-03	.5242E-05	-.2745E-05	-.4407E-07	.7278E-08
12	.2236E-01	-.2218E-01	.9878	.1467	.1394E-03	-.1025E-02	.4723E-07	-.3434E-05	.4911E-08	-.2791E-08
13	-.4659E-03	.3156E-03	.1394E-03	-.1025E-02	.9988	.4954E-01	-.1276E-04	.3967E-03	-.5048E-07	-.1695E-05
14	.5242E-05	-.2745E-05	.4723E-07	-.3434E-05	-.1276E-04	.3967E-03	.9998	.2149E-01	-.2304E-05	.2164E-03
15	-.4407E-07	.7279E-08	.4911E-08	-.2791E-08	-.5048E-07	-.1695E-05	-.2304E-05	.2164E-03	1.000	.9631E-02

TEST4/J503

ENERGY = 1.103
RMIN = .1000E-01
RMAX = 120.0

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.9872	.1469	-.4043E-01	.3519E-01	.2548E-02	-.4391E-02	-.3645E-03	.3052E-02	-.7317E-02	-.1542E-01
2	-.4043E-01	.3519E-01	.2454	.7186	.3997E-01	-.2976E-01	-.1370E-02	.1113E-02	-.2413	-.2733
3	.2548E-02	-.4391E-02	.3997E-01	-.2976E-01	.9875	.1445	.1921E-03	-.1281E-02	.7998E-02	.1648E-01
4	-.3645E-03	.3052E-02	-.1370E-02	.1113E-02	.1921E-03	-.1281E-02	.9989	.4842E-01	-.2080E-03	-.5511E-03
5	-.7317E-02	-.1542E-01	-.2413	-.2733	.7998E-02	.1648E-01	-.2080E-03	-.5511E-03	-.2603	.2677
6	.1873E-01	-.5751E-03	.3891	-.4978E-01	-.2451E-01	.1031E-01	.7065E-03	-.1558E-03	.1842	.1885
7	-.1461E-02	.7496E-04	-.3012E-01	.1268E-01	.2145E-02	-.3316E-02	-.5555E-04	.3597E-04	-.7640E-02	-.1477E-01
8	.2096E-04	.2724E-03	.9745E-03	-.6086E-03	-.2820E-03	.2572E-02	-.1142E-03	.2438E-02	.1747E-03	.4426E-03
9	.1842E-05	-.1028E-04	-.1928E-04	.2142E-04	-.9699E-06	.8665E-05	.4302E-04	-.1319E-02	-.3532E-05	-.8445E-05
10	.9300E-03	-.8189E-02	-.6230E-03	-.2041	-.1551E-02	.8274E-02	.4715E-04	-.2540E-03	-.3011	-.7233
11	-.1050E-01	-.3863E-02	-.2304	-.5973E-01	.1372E-01	.2569E-02	-.3914E-03	-.1134E-03	-.1430	-.1030
12	.9238E-03	.1627E-03	.1957E-01	.1949E-02	-.1221E-02	-.8753E-04	.3309E-04	.2300E-04	.7075E-02	.1179E-01
13	-.3194E-04	-.1174E-04	-.6935E-03	.2034E-03	.1809E-04	.2307E-03	.1250E-05	-.1184E-03	-.1626E-03	-.3761E-03
14	.2709E-06	.3717E-05	.1252E-04	-.1017E-04	.8870E-06	-.4762E-05	-.2230E-05	.1236E-03	.2725E-05	.6190E-05
15	.9405E-08	.7071E-06	-.1502E-06	.2222E-06	-.1680E-08	-.1324E-06	-.4043E-06	-.3037E-04	-.3694E-07	-.7396E-07
16	.7915E-02	.2390E-02	.1747	.2871E-01	-.9338E-02	-.2735E-02	.2777E-03	.9459E-04	.1030	-.3947E-01
17	-.5699E-03	-.2982E-03	-.1265E-01	-.5159E-02	.7536E-03	.2525E-03	-.2128E-04	-.1007E-04	-.6459E-02	-.7332E-02
18	.2121E-04	.3663E-05	.4514E-03	.7522E-04	-.2715E-04	-.1203E-04	.8886E-06	.3741E-05	.1505E-03	.2930E-03
19	-.4401E-06	-.1192E-06	-.8741E-05	.3329E-05	.2070E-06	.3138E-05	-.2140E-06	-.3852E-05	-.2400E-05	-.5015E-05
20	.8296E-08	.1452E-07	.9507E-07	-.9816E-07	.5160E-08	.1219E-06	.1129E-06	.1580E-05	.2691E-07	.5145E-07
21	-.3599E-11	.3617E-08	-.7602E-09	.1433E-08	.4030E-10	-.2576E-08	-.3104E-07	-.1719E-06	-.2827E-09	-.4334E-09

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.1873E-01	-.5751E-03	-.1461E-02	.7496E-04	.2096E-04	.2724E-03	.1842E-05	-.1028E-04	.9300E-03	-.8189E-02
2	.3891	-.4978E-01	-.3012E-01	.1268E-01	.9745E-03	-.6086E-03	-.1928E-04	.2142E-04	-.6231E-03	-.2041
3	-.2451E-01	.1031E-01	.2145E-02	-.3316E-02	-.2820E-03	.2572E-02	-.9699E-06	.8665E-05	-.1551E-02	.8274E-02
4	.7065E-03	-.1558E-03	-.5555E-04	.3597E-04	-.1142E-03	.2438E-02	.4302E-04	-.1319E-02	.4715E-04	-.2340E-03
5	.1842	.1885	-.7640E-02	-.1477E-01	.1747E-03	.4426E-03	-.3532E-05	-.8445E-05	-.3011	-.7233
6	.5032	.6015	.2941E-01	-.2368E-01	-.7257E-03	.4302E-03	.1092E-04	-.4861E-05	-.4838E-01	.1218
7	.2941E-01	-.2368E-01	.9877	.1454	.1751E-03	-.1315E-02	-.1833E-06	-.3743E-05	.2800E-02	-.6228E-02
8	-.7257E-03	.4302E-03	.1751E-03	-.1315E-02	.9987	.4976E-01	-.9712E-05	.3448E-03	-.6101E-04	.1799E-03
9	.1092E-04	-.4861E-05	-.1833E-06	-.3743E-05	-.9712E-05	.3448E-03	.9998	.1956E-01	.5621E-06	-.3682E-05
10	-.4838E-01	.1218	.2800E-02	-.6228E-02	-.6101E-04	.1799E-03	.5621E-06	-.3682E-05	-.4481	.6606E-01
11	.3147	-.7966E-01	-.1914E-01	.4611E-02	.4389E-03	-.2552E-04	-.6353E-05	-.8910E-06	.1321	-.3008E-01
12	-.2864E-01	.2361E-01	.1934E-02	-.2721E-02	-.4119E-04	.4008E-04	.4785E-06	.7699E-06	-.4836E-02	.2847E-02
13	.7701E-03	-.6080E-03	-.2937E-03	.2563E-02	-.1308E-03	.2694E-02	.8049E-06	-.4627E-04	.9104E-04	-.1129E-03
14	-.1004E-04	.9216E-05	-.1004E-05	.6180E-05	.3336E-04	-.9642E-03	-.2277E-04	.1134E-02	-.8354E-06	.2282E-05
15	.9301E-07	-.6217E-07	-.5634E-08	.3393E-07	.1955E-06	.9296E-05	.2705E-04	-.1862E-02	.3397E-08	-.3177E-07
16	-.1848	-.2674E-01	.1090E-01	.2591E-02	-.2676E-03	-.7920E-04	.4599E-05	.1197E-05	-.3001	-.1161
17	.1796E-01	-.1384E-02	-.1071E-02	-.6774E-04	.2316E-04	.1629E-04	-.3490E-06	-.1663E-06	.7722E-02	.2005E-02
18	-.6776E-03	.4741E-03	.1577E-04	.2217E-03	.1692E-05	-.1169E-03	.3823E-07	.2496E-03	-.1313E-03	.2535E-04
19	.9760E-05	-.1077E-04	.1135E-05	-.5209E-05	-.2876E-05	.1383E-03	-.6021E-06	-.1591E-04	.1277E-05	-.1249E-05
20	-.7768E-07	.9950E-07	-.5892E-08	-.1278E-06	-.1823E-06	-.2149E-04	.9298E-08	.3272E-04	-.6744E-08	.1825E-07
21	5242E-09	-.4484E-09	-.6079E-10	.8967E-09	.1142E-07	.6128E-07	-.1327E-05	-.1575E-04	.2501E-11	-.2008E-09

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.1050E-01	-.3863E-02	.9238E-03	.1627E-03	-.3194E-04	-.1174E-04	.2709E-06	.3717E-05	.9406E-08	.2071E-06
2	-.2304	-.5973E-01	.1957E-01	.1949E-02	-.6935E-03	.2034E-03	.1252E-04	-.1017E-04	-.1502E-06	.2222E-06
3	.1372E-01	.2569E-02	-.1221E-02	-.8753E-04	.1809E-04	.2307E-03	.8870E-06	-.4762E-05	-.1680E-08	-.1324E-06
4	-.3914E-03	-.1134E-03	.3309E-04	.2300E-04	.1250E-05	-.1184E-03	-.2230E-05	.1236E-03	-.4043E-06	-.3037E-04
5	-.1430	-.1030	.7075E-02	.1179E-01	-.1626E-03	-.3761E-03	.2725E-05	.6190E-05	-.3694E-07	-.7396E-07
6	.3147	-.7966E-01	-.2864E-01	.2361E-01	.7701E-03	-.6080E-03	-.1004E-04	.9216E-05	.9301E-07	-.6217E-07

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
7	-.1914E-01	.4611E-02	.1934E-02	-.2721E-02	-.2937E-03	.2565E-02	-.1004E-05	.6180E-05	-.9534E-08	.5593E-07
8	.4369E-03	-.2552E-04	-.4119E-04	.4008E-04	-.1508E-03	.2694E-02	.3536E-04	-.9642E-03	.1995E-06	.9296E-05
9	-.6353E-05	.8910E-05	.4785E-06	.7699E-06	.8049E-06	-.4627E-04	-.2277E-04	.1134E-02	.2703E-04	-.1862E-02
10	.1521	-.3008E-01	-.4856E-02	.2847E-02	.9104E-04	-.1129E-03	-.8554E-06	.2282E-05	.3598E-08	-.3176E-07
11	.4553	.7027	.2803E-01	-.2068E-01	-.5886E-03	.2752E-03	.6713E-05	-.2136E-05	-.5793E-07	-.5585E-10
12	.2803E-01	-.2068E-01	.9874	.1458	.1459E-03	-.1031E-02	.1614E-07	-.3233E-03	.2528E-08	-.2918E-08
13	-.5686E-03	.2750E-03	.1459E-03	-.1031E-02	.9988	.4955E-01	-.1188E-04	.3946E-03	-.5922E-07	-.1679E-05
14	.6713E-05	-.2136E-05	.1614E-07	-.3233E-03	-.1186E-04	.5946E-03	.9998	.2190E-01	-.1653E-05	.2156E-03
15	-.5793E-07	-.3560E-10	.2528E-08	-.2918E-08	-.5928E-07	-.1679E-05	-.1853E-05	.2156E-03	1.000	.8640E-02
16	.2863	-.5100E-01	-.1466E-01	-.5484E-03	.5179E-03	.5255E-04	-.4061E-05	-.7843E-06	.4026E-07	.7496E-08
17	-.3514E-01	.3739E-01	.1862E-02	-.2035E-02	-.3393E-04	.7883E-09	.5265E-06	.5716E-06	-.3421E-08	-.7174E-09
18	.7702E-03	-.6265E-03	-.5276E-03	.2902E-02	-.1148E-03	.2391E-02	.1015E-05	-.5255E-04	.9056E-08	.1495E-06
19	-.8577E-05	.6321E-05	-.9381E-06	.6270E-05	.3508E-04	-.9550E-03	-.3254E-04	.1524E-02	.2727E-07	-.1292E-04
20	.5726E-07	-.3193E-07	-.2621E-08	.5441E-07	.1739E-06	.1078E-04	.2582E-04	-.1627E-02	-.5097E-05	.5289E-03
21	-.3590E-09	.4743E-10	.4297E-10	-.1625E-09	-.2748E-08	-.1412E-07	.2414E-06	.2760E-03	.1206E-04	-.1630E-02

COL	16		17		18		19		20	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.7915E-02	.2590E-02	-.5699E-03	-.2982E-03	.2121E-04	.5663E-05	-.4401E-06	-.1192E-06	.8296E-08	.1452E-07
2	.1747	.2871E-01	-.1265E-01	-.5159E-02	.4514E-03	.7522E-04	-.8741E-05	.3529E-05	.9507E-07	-.9816E-07
3	-.9539E-02	-.2755E-02	.7536E-03	.2525E-03	-.2715E-04	-.1203E-04	.2070E-06	.3138E-05	.5160E-08	.1219E-05
4	.2777E-03	.9459E-04	-.2120E-04	-.1002E-04	.8686E-06	.5741E-05	-.2140E-06	-.5852E-05	.1129E-06	.1560E-05
5	.1030	-.3947E-01	-.6459E-02	-.7332E-02	.1505E-03	.7930E-03	-.2400E-05	-.5015E-05	.2691E-07	.5144E-07
6	-.1848	-.2674E-01	.1796E-01	-.1384E-02	-.6776E-03	.4741E-03	.9760E-05	-.1077E-04	-.9787E-07	-.9950E-07
7	.1090E-01	.2591E-02	-.1071E-02	-.6774E-04	.1577E-04	.2217E-03	.1135E-05	-.5209E-05	-.5892E-08	-.1278E-06
8	-.2676E-05	-.7920E-04	.2316E-04	.1629E-04	.1692E-05	-.1169E-03	-.2876E-05	.1383E-03	-.1825E-06	-.2149E-04
9	.4399E-05	.1197E-05	-.3490E-06	-.1663E-06	.5823E-07	.2496E-05	-.6021E-06	-.1591E-04	.9258E-06	.3272E-04
10	-.3001	-.1161	.7722E-02	.2005E-02	-.1313E-03	.2579E-04	.1277E-05	-.1249E-05	-.6745E-09	.1825E-07
11	.2863	-.5100E-01	-.3514E-01	.3739E-01	.7702E-03	-.6265E-03	-.8302E-05	.6521E-05	.9727E-07	-.3193E-07
12	-.1466E-01	-.5484E-03	.1862E-02	-.2035E-02	-.3276E-03	.2902E-12	-.9581E-06	.6270E-05	-.2620E-08	.5441E-07
13	.5179E-03	.5265E-04	-.3393E-04	.7883E-09	-.1148E-03	.2391E-.7	.3508E-04	-.9550E-03	.1739E-06	.1078E-04
14	-.4061E-05	-.7843E-06	.5265E-06	.5716E-06	.1015E-05	-.5255E-04	-.3254E-04	.1524E-02	.2582E-04	-.1627E-02
15	.4027E-07	.7496E-00	-.3421E-08	-.7177E-09	.9058E-08	.1498E-06	-.7277E-07	-.1202E-04	-.5057E-05	.5289E-03
16	.2251	.8272	.2383E-01	-.9222E-02	-.4265E-03	.3904E-04	.4705E-05	.8742E-07	-.5607E-07	-.5117E-08
17	.2383E-01	-.9222E-02	.9869	.1454	.1102E-03	-.6515E-03	-.1603E-06	-.2434E-05	.3913E-08	-.1609E-08
18	-.4265E-03	.3904E-04	.1102E-03	-.6515E-03	.9958	.4851E-01	-.1157E-04	.3637E-03	-.5235E-07	-.2011E-05
19	.4705E-05	.8741E-07	-.1603E-06	-.2434E-05	-.1157E-04	.3637E-03	.9998	.2162E-01	-.3606E-05	.3013E-03
20	-.3607E-07	-.3114E-08	.3914E-08	-.1609E-08	-.5235E-07	-.2011E-05	-.3606E-05	.3013E-03	.9999	.1062E-01
21	.2558E-09	.2227E-10	-.2539E-10	.1106E-10	.3579E-09	.1779E-08	-.2525E-07	-.5024E-06	-.4747E-06	.1147E-03

COL	21	
ROW	REAL	IMAG
1	-.3642E-11	.3617E-08
2	-.7610E-09	.1432E-06
3	.4038E-10	-.2579E-08
4	-.3104E-07	-.1719E-06
5	-.2835E-09	-.4504E-09
6	.9244E-09	-.4476E-09
7	-.6080E-10	.6967E-09
8	.1147E-07	.6128E-07
9	-.1327E-03	-.1575E-04
10	.4160E-11	-.2038E-09
11	-.3361E-09	.4340E-10
12	.4296E-10	-.1628E-09
13	-.2748E-08	-.1412E-07
14	.2414E-06	.2760E-05
15	.1206E-04	-.1630E-02
16	.2558E-09	.2005E-10
17	-.2336E-10	.1126E-10
18	.3579E-09	.1779E-08

COL	21	
ROW	REAL	IMAG
19	-.2525E-07	-.5024E-06
20	-.4747E-06	.1147E-03
21	1.000	.5218E-02

TEST4/J5B4

ENERGY = 1.103
RMIN = .1000E-01
RMAX = 120.0

COL	1		2		3		4		5	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.9872	.1468	-.4162E-01	.5390E-01	.2612E-02	-.4309E-02	-.3664E-03	.3049E-02	-.4631E-02	-.1515E-01
2	-.4162E-01	.5390E-01	.2197	.6957	.4137E-01	-.2828E-01	-.1412E-02	.1066E-02	-.1888	-.2801
3	.2612E-02	-.4309E-02	.4157E-01	-.2878E-01	.9874	.1444	.1945E-03	-.1278E-02	.4943E-02	.1613E-01
4	-.3664E-03	.3049E-02	-.1412E-02	.1056E-02	.1943E-03	-.1278E-02	.9989	.4642E-01	-.1124E-03	-.5344E-03
5	-.4631E-02	-.1515E-01	-.1838	-.2801	.4945E-02	.1615E-01	-.1124E-03	-.5344E-03	-.4116	.1884
6	.1996E-01	.6988E-03	.4157	-.2735E-01	-.2595E-01	.8848E-02	.7496E-03	-.1087E-03	.1352	.1909
7	-.1532E-02	-.1450E-04	-.3171E-01	.1109E-01	.2229E-02	-.3213E-02	-.5804E-04	.3267E-04	-.4425E-02	-.1430E-01
8	.2275E-04	.2748E-03	.1014E-02	-.5656E-03	-.2841E-03	.2369E-02	-.1141E-03	.2438E-02	.8958E-04	.4262E-03
9	.1810E-05	-.1031E-04	-.1999E-04	.2073E-04	-.9322E-06	.8710E-05	.4302E-04	-.1519E-02	-.2029E-05	-.8246E-05
10	-.7479E-03	-.6655E-02	-.2460E-01	-.1666	.4331E-03	.6481E-02	-.1848E-04	-.2028E-03	-.1478	-.7628
11	-.1216E-01	-.5425E-02	-.2667	-.8660E-01	.1565E-01	.4373E-02	-.4495E-03	-.1716E-03	-.8621E-01	-.9806E-01
12	.1014E-02	.2644E-03	.2156E-01	.3736E-02	-.1326E-02	-.2045E-03	.3622E-04	.2676E-04	.3575E-02	.1111E-01
13	-.3401E-04	-.1427E-04	-.7396E-03	.1584E-03	.2050E-04	.2357E-03	.1178E-05	-.1185E-03	-.7557E-04	-.3569E-03
14	.3003E-06	.3750E-05	.1317E-04	-.9581E-05	.8526E-06	-.4800E-05	-.2229E-05	.1236E-03	.1473E-05	.6003E-05
15	.9084E-08	.2067E-06	-.1572E-06	.2166E-06	-.1305E-08	-.1320E-06	-.4043E-06	-.3037E-04	-.2331E-07	-.7317E-07
16	.1121E-01	.4857E-02	.2463	.6859E-01	-.1317E-01	-.5621E-02	.3927E-03	.1884E-03	.1298E-01	-.6611E-01
17	-.7084E-03	-.4244E-03	-.1571E-01	-.7303E-02	.9158E-03	.3973E-03	-.2611E-04	-.1477E-04	-.2437E-02	-.6235E-02
18	.2408E-04	.8521E-05	.5149E-03	.1247E-03	-.3051E-04	-.1526E-04	.9886E-06	.3845E-05	.5982E-04	.2700E-03
19	-.4762E-06	-.1527E-06	-.9530E-05	.2748E-05	.2493E-06	.3175E-05	-.2153E-06	-.3852E-05	-.1186E-05	-.4815E-05
20	.8596E-08	.1477E-07	.1015E-06	-.9373E-07	.4804E-08	.1217E-06	.1129E-06	.1580E-05	.1611E-07	.5071E-07
21	-.6052E-11	.5616E-08	-.8097E-09	.1405E-08	.4291E-10	-.2518E-08	-.3104E-07	-.1719E-06	-.1998E-09	-.4385E-09
22	.6761E-03	.4542E-03	.1527E-01	.7558E-02	-.7974E-03	-.5218E-03	.2354E-04	.1697E-04	.1217E-02	-.2087E-02
23	-.1724E-04	-.1159E-04	-.3849E-03	-.2035E-03	.2233E-04	.1133E-04	-.6446E-06	-.4577E-06	-.4372E-04	-.1515E-03
24	.3233E-06	.9889E-07	.6860E-05	.1373E-05	-.4267E-06	-.1762E-06	.2749E-07	.9366E-07	.9120E-06	.3348E-05
25	-.4295E-08	-.2645E-07	-.7501E-07	.2837E-07	.6968E-08	.1258E-07	-.8970E-08	-.4473E-07	-.1264E-07	-.3949E-07
26	.7292E-10	.1558E-10	.5395E-09	-.5874E-09	-.9536E-12	.1921E-08	.2285E-06	.9856E-08	.1369E-09	.2940E-09
27	.2520E-11	.1306E-10	-.1099E-11	.3409E-11	-.1642E-11	-.1048E-10	-.2787E-09	-.5315E-09	-.5692E-11	-.1395E-12

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.1996E-01	.6988E-03	-.1532E-02	-.1450E-04	.2275E-04	.2748E-03	.1810E-05	-.1031E-04	-.7479E-03	-.6655E-02
2	.4157	-.2735E-01	-.3171E-01	.1109E-01	.1014E-02	-.5656E-03	-.1999E-04	.2073E-04	-.2460E-01	-.1666
3	-.2595E-01	.8848E-02	.2229E-02	-.3213E-02	-.2841E-03	.2369E-02	-.9322E-06	.8710E-05	.4331E-03	.6481E-02
4	.7496E-03	-.1087E-03	-.5804E-04	.3267E-04	-.1141E-03	.2438E-02	.4302E-04	-.1519E-02	[illegible]	-.2028E-03
5	.1352	.1909	-.4425E-02	-.1430E-01	.8958E-04	.4262E-03	-.2029E-05	-.8246E-05	-.1478	-.7628
6	.4760	.5794	.3103E-01	-.2209E-01	-.7664E-03	.3875E-03	.1164E-04	-.4169E-05	-.2049E-01	.8355E-01
7	.3103E-01	-.2209E-01	.9876	.1453	.1774E-03	-.1312E-02	-.2257E-06	-.3792E-05	.5544E-03	-.4198E-02
8	-.7664E-03	.3875E-03	.1774E-03	-.1312E-02	.9987	.4976E-01	-.9711E-05	.3448E-03	.5340E-06	.1317E-03
9	.1164E-04	-.4169E-05	-.2257E-06	-.3792E-05	-.9711E-05	.3448E-03	.9998	.1956E-01	-.4434E-06	-.2832E-05
10	-.2049E-01	.8355E-01	.5544E-03	-.4198E-02	.5540E-06	.1317E-03	-.4434E-06	-.2832E-05	-.4697	.6928E-01
11	.3515	-.5266E-01	-.2133E-01	.2657E-02	.4936E-03	.2737E-04	-.7319E-05	-.1742E-05	.9548E-01	.2353E-01
12	-.3067E-01	.2184E-01	.2053E-02	-.2595E-02	-.4415E-04	.3670E-04	.5312E-06	.8253E-06	-.2269E-02	.2841E-03
13	.8169E-03	-.5635E-03	-.2964E-03	.2560E-02	-.1307E-03	.2694E-02	.8037E-06	-.4627E-04	.2465E-04	-.5786E-04
14	-.1069E-04	.8635E-05	-.9649E-06	.6221E-05	.3336E-04	-.9642E-03	-.2277E-04	.1134E-02	.4851E-07	.1518E-05
15	.1001E-06	-.5655E-07	-.6054E-08	.3353E-07	.1955E-06	.9296E-05	.2703E-04	-.1862E-02	-.5205E-08	-.2339E-07
16	-.2573	-.6961E-01	.1520E-01	.5798E-02	-.3753E-03	-.1660E-03	.6282E-05	.2559E-05	-.2638	-.2351
17	.2108E-01	.7198E-03	-.1255E-02	-.2203E-03	.2773E-04	.2045E-04	-.4289E-06	-.2345E-06	.5080E-02	.5916E-02
18	-.7425E-03	.4273E-03	.1961E-04	.2249E-03	.1593E-05	-.1169E-03	.4000E-07	.2497E-05	-.6192E-04	-.4555E-04
19	.1055E-04	-.1022E-04	.1084E-05	-.5237E-05	-.2871E-05	.1383E-05	-.6024E-06	-.1591E-04	.3797E-06	-.3971E-06
20	-.8428E-07	.9522E-07	-.5508E-08	-.1275E-06	-.1829E-06	-.2148E-04	.9300E-06	.3272E-04	.5560E-09	.1097E-07
21	.5713E-09	-.4148E-09	-.6329E-10	.8953E-09	.1143E-07	.6124E-07	-.1327E-05	-.1575E-04	-.4555E-10	-.1430E-09
22	-.1604E-01	-.7339E-02	.9323E-03	.5596E-03	-.2275E-04	-.1515E-04	.3823E-06	.2410E-06	-.1094E-01	-.1828E-01
23	.5167E-03	.4017E-04	-.2996E-04	-.1289E-04	.7635E-06	.2337E-05	-.1500E-07	-.5085E-07	.1160E-03	.1958E-03
24	-.9294E-05	.7009E-05	.2302E-06	.3206E-05	-.2101E-06	-.4028E-05	.2364E-07	.2206E-06	-.9366E-06	-.1007E-05

COL	6		7		8		9		10	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
25	.7907E-07	-.1019E-06	.6639E-08	.1294E-06	.1174E-06	.1748E-05	-.4739E-07	-.4186E-06	.3867E-08	-.1231E-08
26	-.4433E-09	.6380E-09	-.2376E-11	-.2287E-08	-.1994E-07	-.1129E-06	.3992E-07	.3276E-06	.4613E-11	.6561E-10
27	.2693E-11	-.4215E-11	.3878E-12	.4139E-11	.1091E-09	.2058E-09	-.1765E-07	-.7015E-07	.9514E-12	-.1564E-11

COL	11		12		13		14		15	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.1216E-01	-.5425E-02	.1014E-02	.2644E-03	-.3401E-04	-.1427E-04	.3003E-06	.3750E-05	.9084E-08	.2067E-06
2	-.2667	-.8660E-01	.2156E-01	.3736E-02	-.7396E-03	.1584E-03	.1317E-04	-.9581E-05	-.1572E-06	.2166E-06
3	.1565E-01	.4373E-02	-.1326E-02	-.2045E-03	.2050E-04	.2357E-03	.8526E-06	-.4800E-05	-.1305E-08	-.1320E-06
4	-.4495E-03	-.1716E-03	.3622E-04	.2676E-04	.1178E-05	-.1185E-03	-.2229E-05	.1236E-03	-.4043E-06	-.3037E-04
5	-.8621E-01	-.9806E-01	.3575E-02	.1111E-01	-.7557E-04	-.3569E-03	.1473E-05	.6003E-05	-.2331E-07	-.7316E-07
6	.3515	-.5266E-01	-.3067E-01	.2184E-01	.8169E-03	-.5635E-03	-.1069E-04	.8635E-05	.1000E-06	-.5655E-07
7	-.2133E-01	.2657E-02	.2053E-02	-.2595E-02	-.2964E-03	.2560E-02	-.9649E-06	.6221E-05	-.6054E-08	.3353E-07
8	.4936E-03	.2737E-04	-.4415E-04	.3670E-04	-.1307E-03	.2694E-02	.3336E-04	-.9642E-03	.1955E-06	.9296E-05
9	-.7319E-05	-.1742E-05	.5312E-06	.8253E-06	.8037E-06	-.4627E-04	-.2277E-04	.1134E-02	.2703E-04	-.1862E-02
10	[illegible]	.2353E-01	-.2269E-02	.2841E-03	.2465E-04	-.5786E-04	.4851E-07	.1516E-05	-.5196E-08	-.2339E-07
11	1.056	.6691	.3075E-01	-.1850E-01	-.6511E-03	.2202E-03	.7582E-05	-.1421E-05	-.6725E-07	-.6928E-08
12	.3075E-01	-.1850E-01	.9873	.1466	.1473E-03	-.1027E-02	-.3214E-07	-.3316E-05	.6044E-08	-.2476E-08
13	-.6511E-03	.2202E-03	.1473E-03	-.1027E-02	.9988	.4955E-01	-.1188E-04	.3946E-03	-.5933E-07	-.1679E-05
14	.7582E-05	-.1421E-05	-.3214E-07	-.3316E-05	-.1188E-04	.3946E-03	.9998	.2150E-01	-.1853E-05	.2156E-03
15	-.6726E-07	-.6927E-08	.6044E-08	-.2476E-08	-.5933E-07	-.1679E-05	-.1853E-05	.2156E-03	1.000	.9640E-02
16	.3871	.2434E-01	-.2006E-01	-.4221E-02	.4402E-03	.1450E-03	-.5746E-05	-.1958E-05	.5819E-07	.1836E-07
17	-.3943E-01	.3498E-01	.2096E-02	-.1885E-02	-.3913E-04	.4179E-05	.3958E-06	.6200E-06	-.4182E-08	-.1246E-08
18	.8565E-03	-.5730E-03	-.3328E-03	.2900E-02	-.1145E-03	.2390E-02	.1001E-05	-.5231E-04	.9200E-08	.1494E-06
19	-.9533E-05	.5884E-05	-.8853E-06	.6269E-05	.3296E-04	-.9547E-03	-.5230E-04	.1524E-02	-.7497E-07	-.1211E-04
20	.6558E-07	-.2675E-07	-.3159E-08	.3432E-07	.1830E-06	.1076E-04	.2580E-04	-.1627E-02	-.5050E-05	.5289E-03
21	-.4215E-09	.9776E-11	.4632E-10	-.1614E-09	-.2794E-08	-.1409E-07	.2430E-06	.2757E-05	.1206E-04	-.1630E-02
22	.2507E-01	.4962E-02	-.1267E-02	-.5016E-03	.2696E-04	.1741E-04	-.3540E-06	-.2107E-06	.3610E-08	.1872E-08
23	-.9826E-03	.7895E-03	.2699E-04	.1891E-03	.5884E-06	-.7506E-04	.3080E-07	.2106E-05	-.6998E-09	-.5530E-08
24	.1130E-04	-.1113E-04	.1457E-05	-.6552E-05	-.2559E-05	.1280E-03	-.7153E-06	-.1972E-04	.1219E-07	.2289E-06
25	-.7525E-07	.6997E-07	-.4392E-08	-.1134E-06	-.1766E-06	-.2108E-04	.1169E-05	.4340E-04	-.1951E-06	-.2881E-05
26	.3818E-09	-.2230E-09	-.4091E-10	.8849E-09	.1260E-07	.6922E-07	-.1064E-05	-.1286E-04	.5424E-06	.1055E-04
27	-.1956E-11	-.4816E-12	.9765E-13	-.9053E-12	-.2925E-10	-.5555E-10	.3810E-08	.1503E-07	-.1041E-05	-.8479E-05

COL	16		17		18		19		20	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	.1121E-01	.4857E-02	-.7084E-03	-.4244E-03	.2408E-04	.8521E-05	-.4762E-06	-.1527E-06	.8595E-08	.1477E-07
2	.2463	.6859E-01	-.1571E-01	-.7303E-02	.5149E-03	.1247E-03	-.9530E-05	.2748E-05	.1015E-06	-.9372E-07
3	-.1317E-01	-.5621E-02	.9158E-03	.3973E-03	-.3051E-04	-.1526E-04	.2493E-06	.3175E-05	.4805E-08	.1217E-06
4	.3927E-03	.1884E-03	-.2611E-04	-.1477E-04	.9886E-06	.3845E-05	-.2153E-06	-.3852E-05	.1129E-06	.1580E-05
5	.1298E-01	-.6611E-01	-.2437E-02	-.6235E-02	.5982E-04	.2700E-03	-.1186E-05	-.4815E-05	.1611E-07	.5071E-07
6	-.2573	-.6961E-01	.2108E-01	.7198E-03	-.7425E-03	.4273E-03	.1055E-04	-.1022E-04	-.8427E-07	.9522E-07
7	.1520E-01	.5798E-02	-.1255E-02	-.2203E-03	.1961E-04	.2249E-03	.1084E-05	-.5237E-05	-.5508E-08	-.1275E-06
8	-.3753E-03	-.1660E-03	.2773E-04	.2045E-04	.1593E-05	-.1169E-03	-.2871E-05	.1383E-05	-.1829E-06	-.2148E-04
9	.6282E-05	.2559E-05	-.4289E-06	-.2345E-06	.4000E-07	.2497E-05	-.6024E-06	-.1591E-04	.9300E-06	.3272E-04
10	-.2638	-.2351	.5080E-02	.5916E-02	-.6192E-04	-.4555E-04	.3797E-06	-.3971E-06	.5330E-09	.1097E-07
11	.3871	.2434E-01	-.3943E-01	.3498E-01	.8565E-03	-.5730E-03	-.9533E-05	.5884E-05	.6558E-07	-.2675E-07
12	-.2006E-01	-.4221E-02	.2096E-02	-.1885E-02	-.3328E-03	.2900E-02	-.8853E-06	.6269E-05	-.3159E-08	.3432E-07
13	.4402E-03	.1450E-03	-.3913E-04	.4179E-05	-.1145E-03	.2390E-02	.3296E-04	-.9547E-03	.1430E-06	.1076E-04
14	-.5746E-05	-.1958E-05	.3558E-06	.6200E-06	.1001E-05	-.5231E-04	-.3230E-04	.1524E-02	[illegible]	-.1627E-02
15	.5820E-07	.1836E-07	-.4183E-08	-.1246E-08	.9200E-08	.1494E-06	-.7497E-07	-.1201E-04	[illegible]	.5289E-03
16	-.9441E-02	.7573	.3250E-01	-.5382E-02	-.5923E-03	-.5471E-04	.6661E-05	.1218E-05	-.5195E-07	-.1187E-07
17	.3250E-01	-.5382E-02	.9865	.1484	.1153E-03	-.6544E-05	-.2078E-06	-.2323E-05	.4441E-08	-.1789E-08
18	-.5923E-03	-.5471E-04	.1153E-03	-.6544E-05	.9988	.4852E-01	-.1071E-04	.3616E-03	-.6503E-07	-.1990E-05
19	.6661E-05	.1218E-05	-.2078E-06	-.2323E-05	-.1071E-04	.3616E-03	.9998	.2163E-01	-.2950E-05	.3002E-03
20	-.5194E-07	-.1187E-07	.4442E-08	-.1789E-08	-.6503E-07	-.1990E-05	-.2950E-05	.3002E-03	.9999	.1063E-01
21	.3754E-09	.7318E-10	-.2839E-10	.9010E-11	.5854E-09	.1751E-08	-.2867E-07	-.2000E-06	-.2655E-06	.1144E-03
22	-.7585E-01	.5036E-01	.2257E-02	-.5442E-03	-.3752E-04	-.1608E-04	.4072E-06	.3303E-06	-.3330E-08	-.1403E-08
23	.9312E-03	-.2460E-03	-.3770E-03	.3228E-02	-.8309E-04	.1787E-02	.6068E-06	-.3440E-04	.8030E-08	.1371E-06
24	-.8728E-05	.8406E-06	-.5959E-06	.6079E-05	.3604E-04	-.1054E-02	-.2953E-04	.1405E-02	-.8175E-07	-.1628E-04

COL	16		17		18		19		20	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
25	.5887E-07	.2510E-08	-.4051E-08	.2046E-07	.1708E-06	.1004E-04	.2565E-04	-.1605E-02	-.7961E-05	.7819E-03
26	-.3282E-09	-.3521E-10	.3492E-10	-.1298E-09	-.3244E-08	-.1702E-07	.3250E-06	.3762E-05	.1230E-04	-.1512E-02
27	.2785E-11	-.1118E-11	-.1376E-12	.1830E-12	.4518E-11	.7801E-11	-.5582E-09	-.2195E-08	.1207E-06	.9650E-06

COL	21		22		23		24		25	
ROW	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG	REAL	IMAG
1	-.5999E-11	.3616E-08	.6761E-03	.4542E-03	-.1724E-04	-.1159E-04	.3233E-06	.9889E-07	-.4295E-08	-.2644E-09
2	-.8083E-09	.1402E-08	.1527E-01	.7358E-02	-.3849E-03	-.2035E-03	.6860E-05	.1375E-05	-.7501E-07	.2837E-07
3	.4280E-10	-.2577E-08	-.7974E-03	.4221E-03	.2235E-04	.1135E-04	-.4267E-06	-.1762E-06	.6968E-08	.1258E-07
4	-.2104E-07	-.1719E-06	.2356E-04	.1697E-04	-.6446E-06	-.4372E-06	.2749E-07	.9 586-07	-.8970E-08	-.6473E-07
5	-.2043E-09	-.6356E-09	.1217E-02	-.2087E-02	-.4373E-04	-.1515E-03	.9120E-06	.3548E-05	-.1264E-07	-.3949E-07
6	.5719E-09	-.4180E-09	-.1604E-01	-.7539E-02	.5168E-03	.4017E-04	-.9294E-05	.7009E-05	.7907E-07	-.1019E-06
7	-.6523E-10	.8947E-09	.9523E-03	-.2996E-04	-.1269E-04	.2302E-05	.3206E-05	-.6639E-08	.1294E-06	
8	.1193E-07	.6124E-07	-.2273E-04	-.1513E-04	.7635E-06	.2837E-05	-.2101E-06	-.4029E-05	.1174E-06	.1745E-05
9	-.1327E-05	-.1575E-04	.3823E-06	.2410E-06	-.1500E-07	-.5385E-07	.2364E-07	.2206E-06	-.4739E-07	-.4186E-06
10	-.4280E-10	-.1492E-09	-.1094E-01	-.1828E-01	.1113E-03	.1958E-03	-.9366E-06	-.1007E-05	.3866E-08	-.1231E-06
11	-.4204E-09	.7451E-11	.2507E-01	.4962E-02	-.9826E-03	.7895E-03	.1130E-04	-.1115E-04	-.7525E-07	.6997E-07
12	-.4627E-10	-.1610E-09	-.1267E-02	-.5016E-03	.2698E-04	.1891E-04	.1457E-05	-.6552E-05	-.4933E-03	-.1134E-04
13	-.2794E-08	-.1409E-07	.2696E-04	.1741E-04	.5684E-06	-.7506E-04	. 559E-05	.1280E-03	-.1766E-06	-.2108E-04
14	.2430E-06	.2757E-05	-.3540E-06	-.2107E-06	.3080E-07	.2106E-05	-.7265E-06	-.1972E-04	.1169E-05	.4540E-04
15	.1206E-04	-.1650E-02	.3610E-06	.1872E-08	-.6998E-09	-.9530E-08	.1219E-07	.2289E-08	-.1961E-06	-.2881E-05
16	.5741E-09	.7511E-10	-.7385E-01	.9036E-01	.9312E-03	-.2466E-03	-.8928E-05	.8486E-06	.5887E-07	.2509E-05
17	-.2830E-10	.9017E-11	.2257E-02	-.5442E-03	-.3770E-03	.3228E-02	-.9999E-08	.6079E-05	-.4031E-08	.2046E-07
18	.3854E-09	.1751E-03	-.3752E-04	-.1602E-04	-.8309E-04	.1787E-02	.3604E-04	-.1054E-02	.1708E-05	.1004E-04
19	-.2869E-07	-.5000E-06	.4072E-06	.3503E-06	.6068E-06	-.3440E-04	-.2953E-04	.1405E-02	.2965E-04	-.1602E-02
20	-.2655E-06	.1144E-03	-.3350E-08	-.1403E-08	.8090E-08	.1371E-06	-.8175E-07	-.1625E-04	-.7961E-05	.7819E-03
21	1.000	.5224E-02	.2388E-10	.8632E-11	-.2604E-10	-.9912E-10	.1753E-08	.1609E-07	-.4119E-07	-.3723E-05
22	.2576E-10	.8803E-11	.9857	.1926	.8709E-04	-.2399E-03	-.4600E-06	-.1088E-09	.4039E-09	.7936E-09
23	-.2604E-10	-.9914E-10	.8709E-04	-.2399E-03	.9989	.4691E-01	-.8637E-05	.2827E-03	-.3784E-07	-.1382E-05
24	.1732E-08	.1605E-07	-.4600E-06	-.1088E-03	-.8637E-05	.2827E-03	.9998	.2110E-01	-.3375E-05	.2634E-03
25	-.4119E-07	-.3723E-05	.4039E-08	.7950E-09	-.3784E-07	-.1382E-05	-.3375E-05	.2834E-03	.6999	.1078E-01
26	-.1593E-05	.2717E-03	-.2222E-10	-.1012E-11	.3344E-09	.1716E-08	-.3405E-07	-.4191E-06	-.6392E-06	.1735E-03
27	.5903E-05	-.1342E-02	.1701E-12	.2149E-12	-.3591E-12	-.5464E-12	.4251E-10	.1774E-09	-.7936E-08	-.7053E-07

COL	26		27	
ROW	REAL	IMAG	REAL	IMAG
1	.7276E-10	.1558E-10	.2448E-11	.1549E-10
2	.5303E-09	-.5645E-09	-.1706E-11	.5784E-11
3	-.8225E-12	.1922E-08	-.1632E-11	-.1051E-10
4	.2285E-08	.9696E-08	-.2787E-09	-.5515E-09
5	.1574E-09	.2570E-09	-.1418E-11	-.1498E-11
6	-.4414E-09	.6376E-09	.1879E-11	-.2286E-11
7	-.2528E-11	-.2287E-08	.3965E-12	.4229E-11
8	-.1994E-07	-.1129E-06	.1091E-09	.2037E-09
9	.3992E-07	.3276E-06	-.1765E-07	-.7015E-07
10	.3499E-11	.6594E-10	-.4220E-12	-.3495E-12
11	.3804E-09	-.2228E-07	-.1766E-11	.6162E-12
12	-.4079E-10	.8848E-09	.7574E-13	-.1007E-11
13	.1200E-07	.6922E-07	-.2923E-10	-.5352E-10
14	-.1064E-05	-.1266E-04	.3810E-08	.1503E-07
15	.5424E-06	.1055E-04	-.1041E-05	-.8429E-05
16	-.3268E-09	-.3539E-10	.1675E-11	-.2180E-12
17	.3481E-10	-.1296E-09	-.1177E-12	.1277E-12
18	-.3244E-08	-.1702E-07	.4517E-11	.7799E-11
19	.3250E-06	.3762E 5	-.5582E 9	-.2195E-08
20	.1230E-04	-.7512E-0	.1207 6	.9650E-06
21	-.1353E-05	.2717E-03	.5605E	-.1342E-02
22	-.2215E-10	-.9537E-12	.1128E-12	.7341E-15
23	.3344E-09	.1714E-08	-.3586E-12	-.5431E-12
24	-.3405E-07	-.4191E-06	.4251E-10	.1774E-09

COL	26		27	
ROW	REAL	IMAG	REAL	IMAG
25	-.8392E-06	.1735E-03	-.7936E-08	-.7053E-07
26	1.000	.3706E-02	-.9604E-07	.6376E-04
27	-.9604E-07	.6376E-04	1.000	.3001E-02

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