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The Self-Consistent Calculation of Pseudomolecule Energy Levels, Construction of Energy Level Correlation Diagrams and an Automated Computational System for SCF–Xα–SW Calculations

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SUMMARY

This work is concerned with the self-consistent calculation of the electronic energy levels of noble gas pseudomolecules formed when a metal surface is bombarded by noble gas ions and with the construction of energy level correlation diagrams as a function of interatomic spacing. The self-consistent-field $x\alpha$ scattered wave (SCF-Xα-SW) method of Slater and Johnson is utilized. Preliminary results on the Ne-Mg system are given.

An interactive $x\alpha$ programming system, which has been implemented on the LeRC IBM 370 computer, is described in detail. This automated system makes use of special PROCDEFS (procedure definitions) to minimize the data to be entered manually at a remote terminal. Listings of the special PROCDEFS and of typical input data are given.

INTRODUCTION

Ferrante and Pepper (ref. 1) recently investigated Auger electron production by Ne^+ bombardment of Mg, Al, and Si surfaces. Ion energies in the range of 1-3 KeV were used. Auger electrons characteristic of both the target atoms and the incident Ne were observed. They attributed these observations to asymmetric Ne-surface atom collisions, and presented evidence that the Auger electrons resulted from autoionization of neutral, excited Ne. Their results on the variation in strength of Ne Auger signals with target in the sequence Mg, Al, Si appear to be in agreement with the predictions of the electron-promotion excitation mechanism of Barat and Lichten (ref. 2). Ferrante and Pepper (ref. 3) have also investigated the production of Auger electrons by bombardment of Mg and Al surfaces with other noble gas ions. To help elucidate the question of electron-promotion in the formation of collision-induced pseudomolecules, it is of great interest to obtain accurate energy level correlation diagrams for the pseudomolecules formed from various noble gas-metal pairs. In the present paper the results of a preliminary calculation of a Ne-Mg correlation diagram using the $x\alpha$ method are presented. In addition, a description of the $x\alpha$ program, which can be used for a wide variety of chemical and solid state calculation, is presented to facilitate its use by interested parties at LeRC.

Professor J. G. Norman, Jr., of the University of Washington, supplied basic $x\alpha$ programs and operating instructions.

SELF-CONSISTENT CALCULATION OF PSEUDOMOLECULE ENERGY LEVELS, CONSTRUCTION OF CORRELATION DIAGRAMS

This work is concerned with the self-consistent calculation of the energy levels of noble gas-metal pseudomolecules formed when a metal surface is bombarded by noble gas ions, and with the construction of energy level correlation diagrams. The theoretical method utilized in the molecular calculations is the self-consistent-field $x\alpha$ scattered-wave (SCF-$x\alpha$-SW) method of Slater and Johnson (ref. 4). The interactive $x\alpha$ programing system described in the following section was implemented on the LeRC IBM 370-3033 computer for this purpose. To construct a correlation diagram for a particular system, electronic energy levels must be calculated for a number of different interatomic spacings ranging from the separated atom to the united atom limits. The atomic calculations were performed using the modified Herman Skillman SCF program described below (ref. 5). Preliminary results on the Ne-Mg system are summarized in figure 1.

In the usual application of the $x\alpha$-SW method, the molecule is surrounded by a sphere, and the interior is partitioned into a number of spherical atomic regions and an interatomic region. The molecular potential is constructed to be spherically symmetric in the atomic and extra molecular regions and constant in the interatomic region. The Schrodinger equation is then solved self-consistently, subject to the boundary condition that the wave function and its first derivative are continuous across all boundaries, using the multiple scattering formalism combined with the $x\alpha$ density function formalism for treating the exchange and correlation. In general, the iterative self-consistent field computational scheme is reasonably rapidly convergent. In the earliest applications of the $x\alpha$-MS method, the atomic spheres were taken as non-overlapping. As larger and more "open" systems were investigated, the constant potential interatomic regions become an appreciable portion of the molecular volume, and convergence difficulties were found. This was remedied empirically by allowing the atomic spheres to overlap each other. Consequently, the theory was reformulated for the case of overlapping spheres. The major constraint on the use of overlapping atomic spheres is that the spheres may not overlap any adjacent atomic center. Thus, the largest allowable sphere for a given atomic center is slightly less than the nearest neighbor distance. In the present calculations, the use of overlapping spheres is essential, particularly for the small interatomic distances ($r < 2AU$) in the pseudomolecules formed at the projectile energies used in the experiments. The projectile energy range of interest in Ne-Mg (1-3 KeV) corresponds to interatomic distances in the range 0.47 AU to about 1.0 AU (ref. 6).

INTERACTIVE SCF-Xα-SW CALCULATIONS

The computer programs necessary to carry out SCF-xα-SW calculations in an interactive manner have been implemented on the LeRC IBM 370 computer using the TSS operating system. In order to facilitate use of the programs interactively from a terminal, and to minimize the amount of data to be entered from the terminal, a series of special PROCDEFS (procedure definitions) were created (appendix I). The use of these are demonstrated below. A complete xα calculation entails the following sequence of steps, each of which involves the use of a different program package:

(a) Generation of atomic potentials for each atom or ion in the molecule using a modified Herman Skillman SCF program

(b) Generation of a molecular potential by superposition of atomic potentials

(c) Generation of a contracted molecular potential for use in steps (e) and (f)

(d) Generation of symmetry input for use in steps (e) and (f)

(e) Calculation of the energy levels of the molecule

(f) SCF calculation starting with the results of step (e) plus subsequent interation

In addition, one may calculate the wave functions and charge densities corresponding to the SCF energy levels and also plot these quantities. (Thus far, these programs have not been implemented.) The output from each successive step is stored in a specified element on disk. The programs for each successive step are run under the control of an appropriate PROCDEF. The input data for a given step is automatically constructed by the PROCDEF by combining the previously stored elements with minimal input entered from the terminal.

To illustrate the use of the PROCDEFS referred to above, we shall consider the sequence of operations involved in carrying out an SCF calculation for a Mg-Ne pseudomolecule.

A. Generation of atomic potentials

The format of the input data cards necessary to generate atomic potentials using the modified Herman Skillman program are described in the unpublished operating instructions for the xα programs. A listing of the input cards for Ne, stored in element NEI, is given in appendix II(B). To generate the atomic potential for Ne and to store the card image output in element NEI, one enters

```
_HSRUN NEI, NE1
```

at the terminal. The terminal will respond with

```
DDNAME FT06F001 UNDEFINED ENTER Y. . . .
```

To print the condensed tabular output at the terminal, one enters D. The eigenvalues for each iteration, and the total charge density and core charge density for the final iteration are then printed at the terminal. Card image output is stored in element NE1.

B. Generation of molecular potential

The input data cards for a Ne-Mg pseudomolecule, stored in element NEMG, are listed in appendix II(C). The cards are for the case where the Ne atom has coordinates (2, 0, 0) AU and Mg (-2, 0, 0) AU. To run the program, one enters

_MRUN NEMG, VNM

at the terminal. The PROCDEF loads NEMG and goes into the edit mode now assuming that the Ne and Mg total and core charge densities are stored in Ne1 and MG1, respectively, one next types in

B; LOA NE1; B; LOA MG1

This loads NE1 and MG1. To reenter the PROCDEF and to continue the calculation, one types

_DEFAULT SYSINX=E

The output molecular potential is stored in element VNM. For this program tabular output is listed on the high-speed printer, rather than at the terminal, because the output is quite lengthy (2200 lines for NeMg).

C. Generation of contracted molecular potential

The next step is the generation of a contracted molecular potential assuming specific values of radii for the atomic and outer spheres in the molecule. If the input molecular potential is stored in element VNM, the contracted potential is to be stored in VVM and the radii of the outer, Ne, Mg spheres are 0.705, 0.4332, 0.470 AU, respectively, one enters at the terminal:

_CRUNT VNM, VVM

I .705 .4332 .47 0.0

_DEFAULT SYSINX = E

The terminal responds with

DDNAME FT06F001 UNDEFINED. . . .

Upon entry of D, the calculation proceeds and tabular output is printed at the terminal. The table of the output contracted molecular potential is listed in appendix II(E).

D. Generation of symmetry input

This program calculates spherical harmonic basis functions for a given set of l values, and writes out card images which are stored in a specified element. The calculation must be repeated for each unique group of equivalent atoms and each symmetry group. The output elements must then be edited to form the input for E and F. Suppose the required input cards, described in the $x\alpha$ operating instructions, have been placed in element PIN and the output element name is PIO. One would enter

_YLRUN PIN, PIO

at the terminal, which then responds with

DDNAME FT06001 UNDEFINED. . . .

Upon entry of D, the calculation proceeds and tabular output is printed at the terminal. The final edited versions of the symmetry output for the σ, π representations of the group of the heteronuclear diatomic molecule are given in appendix II(A).

E. Energy level calculation

Suppose that one wishes to search for energy levels in the energy range -0.5 AU to -10. AU in steps of 0.5 AU. One would enter

_FRUN VNM, PIZ

at the terminal. (The contracted potential is stored in element VNM, and the symmetry input is stored in PIZ.) The terminal will respond with

DDNAME FT06F001 UNDEFINED. . . .

and one enters D to print tabular output at the terminal. When the terminal indicated the editor is entered, one types in

I 3, 1, .5, -.5, -10., 0

DEFAULT SYSINX=E

and the calculation proceeds. The determinant value for each trial energy in the range specified is then calculated and printed. If the sign of the determinant changes in a

given energy range, the program automatically interpolates for the energy corresponding to zero determinant (that is, energy eigenvalue).

F. SCF calculation

The final step in the $x\alpha$ calculational procedure is the iterative SCF calculation. This is performed in two stages under control of two different PROCDEFs. In the first stage, the necessary input data for the second stage is constructed automatically by the PROCDEF. This is convenient because of the complexity of the input data and because similar input data is needed for the SCF calculations at different interatomic distances. The PROCDEF DIS constructs SCF input for NeMg in the case where there are 4 different sigma levels and 2 different pi levels occupied in the pseudomolecule. One must also specify the number of iterations to be performed and the energies of the frozen core levels. Suppose the number of iterations desired is 8, frozen core levels are found at -60.9204, -92.6720 AU, sigma states at -6.30841, -4.51048, -2.88924 -1.46411 AU, and pi states at -3.63858 and -1.601967. One enters at the terminal

DIG 8, -60.9204, -92.6720, -6.30841, -4.51048,

-2.88924, -1.46411, -3.63858, -1.601967

This generates the SCF input, placing it in element DIG. The SCF input generated for this case is listed in appendix II(F). Next, with input potential in VM and output in VM1, the SCF step is started by typing

_SCFR VM, DIG, VM1

The terminal responds with

DDNAME FT06F001 UNDEFINED. . . . .,

and one enters D to proceed. In each iteration the input levels and occupation numbers, the various components of potential energy, the total potential energy, kinetic energy, total energy and virial coefficient are printed. Also printed are the total charge in each region, the largest difference between the old and new potentials, calculated energy eigenvalues for the old potential, and predicted eigenvalues for the new potential. After the last iteration, charges are given as fractions of the total charge within the atomic spheres, and decomposed in their spherical-harmonic (s, p, d, f, etc.) components. Finally, the new potential is printed at the terminal.

APPENDIX I - PROCDEFS FOR RUNNING THE Xα PROGRAMS

A. HERMAN SKILLMAN ATOMIC POTENTIAL PROCDEF

```
LIST 0,1000
HSRUN    0000000 PROCDEF HSRUN
HSRUN    0000100 PARAM TN,OUT
HSRUN    0000150 DEFAULT SYSINX=E
HSRUN    0000200 IN
HSRUN    0000300 %E
HSRUN    0000400 REDIT TN
HSRUN    0000500 B;LOA INPU;VS INPU;Q
HSRUN    0000600 HRUN HSKK,OUT
HSRUN    0000700 ABEND
```

```
PROCDEF HRUN
LIST 100,2500
HRUN     0000100 PARAM JBLIB,CARD
HRUN     0000200 PPLI
HRUN     0000300 DDEF ASD,VP,JBLIB,OPTION=JOBLIB
HRUN     0000400 FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
HRUN     0000500 FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
HRUN     0000600 OSRUN MAIN
HRUN     0000700 PRINT CARD
HRUN     0000800 FILEREL FT05F001,FT07F001
HRUN     0000900 ERASE INPU
HRUN     0001000 RELEASE ASD
```

B. MOLECULAR POTENTIAL PROCDEF

```
PROCDEF MRUN
LIST 100,2500
MRUN     0000100 PARAM TNP,OUT
MRUN     0000200  DEFAULT SYSINX=E
MRUN     0000300 IN
MRUN     0000400 %E
MRUN     0000500 REDIT TNP
MRUN     0000600 PAUSE
MRUN     0000700  DEFAULT SYSINX=G
MRUN     0000800 CONEDIT
MRUN     0000900 B;LOA INPU;VS INPU
MRUN     0001000 Q
MRUN     0001100 SRUN MOLE,OUT
MRUN     0001200 ABEND
```

```
PROCDEF SRUN
LIST 100,2500
SRUN     0000100 PARAM JLIB,CARD
SRUN     0000200 PPLI
SRUN     0000300 FILEDEF FT06F001,VS,OUT,DCB=(RECFM=F,LRECL=136),RET=T
SRUN     0000400 HRUN JLIB,CARD
SRUN     0000500 PRINT OUT
SRUN     0000600 FILEREL FT06F001
-
```

```
PROCDEF HRUN
LIST 100,2500
HRUN     0000100 PARAM JBLIB,CARD
HRUN     0000200 PPLI
HRUN     0000300 DDEF ASD,VP,JBLIB,OPTION=JOBLIB
HRUN     0000400 FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
HRUN     0000500 FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
HRUN     0000600 OSRUN MAIN
HRUN     0000700 PRINT CARD
HRUN     0000800 FILEREL FT05F001,FT07F001
HRUN     0000900 ERASE INPU
HRUN     0001000 RELEASE ASD
-
```

C. CONTRAC PROCDEF

```
PROCDEF CRUNT
LIST 100,2500
CRUNT    0000100 PARAM TNP',OUT
CRUNT    0000200  DEFAULT SYSINX=E
CRUNT    0000300 IN
CRUNT    0000400 %E
CRUNT    0000500 REDIT TNP'
CRUNT    0000600 T;LOA RNEMG;T;N 2;D
CRUNT    0000700 PAUSE
CRUNT    0000800  DEFAULT SYSINX=G
CRUNT    0000900 CONEDIT
CRUNT    0001000 B;LOA INPU;VS INPU;Q
CRUNT    0001100 HRUN CONT,OUT
CRUNT    0001200 REDIT OUT
CRUNT    0001300 T;P 1000;Q
CRUNT    0001400 ABEND
```

```
PROCDEF HRUN
LIST 100,2500
HRUN     0000100 PARAM JBLIB,CARD
HRUN     0000200 PPLI
HRUN     0000300 DDEF ASD,VP,JBLIB,OPTION=JOBLIB
HRUN     0000400 FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
HRUN     0000500 FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
HRUN     0000600 OSRUN MAIN
HRUN     0000700 PRINT CARD
HRUN     0000800 FILEREL FT05F001,FT07F001
HRUN     0000900 ERASE INPU
HRUN     0001000 RELEASE ASD
```

D. SYMMETRIZATION PROGRAM PROCDEF

```
PROCDEF YLRUN
LIST 100,1500
YLRUN    0000100 PARAM YLIN,OUT
YLRUN    0000200 DEFAULT SYSINX=E
YLRUN    0000210 IN
YLRUN    0000220 %E
YLRUN    0000300 REDIT YLIN
YLRUN    0000400 B;LOA INPU;VS INPU;Q
YLRUN    0000500 PPLI
YLRUN    0000600 TTPE FT08F001,SCR
YLRUN    0000700 HRUN HAR,OUT
YLRUN    0000800 FILEREL FT08F001
YLRUN    0000900 REDIT OUT
YLRUN    0001000 T;P 300;Q
YLRUN    0001100 ABEND
```

```
PROCDEF HRUN
LIST 100,1900
HRUN     0000100 PARAM JBLIB,CARD
HRUN     0000200 PPLI
HRUN     0000300 DDEF ASD,VP,JBLIB,OPTION=JOBLIB
HRUN     0000400 FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
HRUN     0000500 FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
HRUN     0000600 OSRUN MAIN
HRUN     0000700 PRINT CARD
HRUN     0000800 FILEREL FT05F001,FT07F001
HRUN     0000900 ERASE INPU
HRUN     0001000 RELEASE ASD
```

```
PROCDEF TTPE
LIST 100,1300
TTPE     0000100 PARAM TAPE,SCRAT
TTPE     0000200 FILEDEF TAPE,VS,SCRAT,DCB=(RECFM=V,LRECL=800),OSRECFM=VS,RET=T
```

E. ENERGY CALCULATION PROCDEF

```
PROCDEF FRUN
LIST 100,1900
FRUN     0000100 PARAM NAME,DIA
FRUN     0000200  DEFAULT SYSINX=E
FRUN     0000300 IN
FRUN     0000400 %E
FRUN     0000500 REDIT NAME
FRUN     0000550 T;I ENERGY
FRUN     0000600 B;LOA DIA;B
FRUN     0000700 PAUSE
FRUN     0000800  DEFAULT SYSINX=G
FRUN     0000900 CONEDIT
FRUN     0001000 I 0,0,0,0,0,0
FRUN     0001100 B;LOA INPU;VS INPU;0
FRUN     0001200 YRUN ENER,ENEI
FRUN     0001300 ABEND
```

```
PROCDEF YRUN
LIST 100,1900
YRUN     0000100 PARAM JBLIB,CARD
YRUN     0000200 PPLI
YRUN     0000300 DDEF ASD,VP,JBLIB,OPTION=JOBLIB
YRUN     0000400 DDEF BSD,VP,NJLIB,OPTION=JOBLIB
YRUN     0000450 DDEF CSD,VP,TMA,OPTION=JOBLIB
YRUN     0000500 FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
YRUN     0000600 FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
YRUN     0000700 OSRUN MAIN
YRUN     0000800 PRINT CARD
YRUN     0000900 FILEREL FT05F001,FT07F001
YRUN     0001000 ERASE INPU
YRUN     0001100 RELEASE ASD
YRUN     0001200 RELEASE BSD
YRUN     0001300 RELEASE CSD
```

F. PROCDEF FOR GENERATING SCF PROGRAM INPUT

```
PROCDEF DIS
LIST 0,1000
DIS      0000000 PROCDEF DIS
DIS      0000100 PARAM NUM,N1,M1,A1,B1,C1,D1,E1,F1
DIS      0000200  DEFAULT SYSINX=E
DIS      0000250  ERASE RIG
DIS      0000300 REDIT DIG
DIS      0000400 PO 200;C /8/NUM/;N;DU 12/N1/;P;N;DU 12/M1/;P;N;DU 11/A1/;
                 P;PO 2300;DU 11/B1/;P;N;DU 11/C1/;P;N
DIS      0000500 DU 11/D1/;P;N;DU 11/E1/;P;B;DU 11/F1/;P;FIL RIG;0
DIS      0000600 ABEND
```

G. SELF-CONSISTENT FIELD CALCULATION

```
PROCDEF SCFR
LIST 100,3000
SCFR     0000100 PARAM NAME,DIA,SCFOT
SCFR     0000200  DEFAULT SYSINX=E
SCFR     0000250 ERASE INPU
SCFR     0000300 IN
SCFR     0000350 SCF
SCFR     0000400 %E
SCFR     0000500 REDIT DIA
SCFR     0000600 PO 100;LOA NAME;N;D;B
SCFR     0001000 I 0,0,0,0,0,0
SCFR     0001100 T;LOA INPU;VS INPU;Q
SCFR     0001200 XRUN SCFOT
SCFR     0001400 REDIT SCFOT
SCFR     0001450 T;I      1     1
SCFR     0001500 T;P 1000;FIL SCFOT
SCFR     0001600 PAUSE
SCFR     0001700  DEFAULT SYSINX=G
SCFR     0001750 CONEDIT
SCFR     0001800 FIL SCFOT;Q
SCFR     0001900 ABEND
```

```
PROCDEF XRUN
LIST 100,2500
XRUN     0000100 PARAM CARD
XRUN     0000200 PPLI
XRUN     0000300 DDEF ASD,VP,ENER,OPTION=JOBLIB
XRUN     0000310 DDEF BSD,VP,NJLIB,OPTION=JOBLIB
XRUN     0000320 DDEF DSD,VP,TMA,OPTION=JOBLIB
XRUN     0000355 DDEF CSD,VP,SCFL,OPTION=JOBLIB
XRUN     0000360 TTPE FT08F001,SC8
XRUN     0000365 TTPE FT10F001,SC0
XRUN     0000370 TTPE FT11F001,SC1
XRUN     0000375 TTPE FT12F001,SC2
XRUN     0000380 TTPE FT13F001,SC3
XRUN     0000500 FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
XRUN     0000600 FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
XRUN     0000700 OSRUN MAIN
XRUN     0000800 FILEREL FT
XRUN     0001000 ERASE INPU
XRUN     0001100 RELEASE ASD
XRUN     0001200 RELEASE BSD
XRUN     0001300 RELEASE CSD
XRUN     0001400 RELEASE DSD
```

```
PROCDEF TTPE
LIST 100,1200
TTPE     0000100 PARAM TAPE,SCRAT
TTPE     0000200 FILEDEF TAPE,VS,SCRAT,DCB=(RECFM=V,LRECL=800),OSRECFM=VS,RET=T
```

APPENDIX II - INPUT DATA FOR THE Xα PROGRAMS

A. DIATOMIC MOLECULE SYMMETRY INPUT FOR ENERGY, SCF CALCULATIONS

```
  REDIT PIZ
LOADING PIZ
EDIT

P;P 100;Q
        TOP RECORD
0000020    10    2   PI Z REP
0000200     1    1
0000300     0    1    1   1.00000000
0000400     2    1
0000500     1    1    1   1.00000000
0000600     3    1
0000700     0    1    1   1.00000000
0000800     3    1
0000900     2    1    1   1.00000000
0001000     4    1
0001100     1    1    1   1.00000000
0001200     4    1
0001300     3    1    1   1.00000000
0001500     1    1
0001600     0    1    2   1.00000000
0001700     2    1
0001800     1    1    2   1.00000000
0002000     1    1
0002100     0    1    3   1.00000000
0002200     2    1
0002300     1    1    3   1.00000000
EOF
```

```
REDIT SIGMB
LOADING SIGMA
EDIT

T;P 100;Q
        TOP RECORD
0000020     8    2   SIGMA REP
0000200     0    1
0000300     0    1    1   1.0000000
0000400     1    1
0000500     1    1    1   1.00000000
0000600     2    1
0000700     0    1    1   1.00000000
0000800     2    1
0000900     2    1    1   1.00000000
0002100     0    1
0002200     0    1    2   1.00000000
0002300     1    1
0002400     1    1    2   1.00000000
0003000     0    1
0003100     0    1    3   1.00000000
0003200     1    1
0003300     1    1    3   1.00000000
EOF
```

B. NEI: HERMAN SKILLMAN PROGRAM NE INPUT

```
0000100 CONT    PUNC
0000120         NEUTRAL NEON ATOMIC POTENTIAL ; 1S FROZEN
0000200     0 .001     .00001  441    1  50    1                                    .73081
0000300      1.00 .99205 .98387 .97552 .96705 .95850 .94990 .94128 .93266 .92407
0000400    .91553 .89862 .88202 .86578 .84994 .83451 .81947 .80484 .79058 .77670
0000500    .76316 .73706 .71215 .68835 .66558 .64381 .62303 .60322 .58438 .56648
0000600    .54948 .51795 .48923 .46280 .43822 .41523 .39363 .37332 .35422 .33627
0000700    .31941 .28880 .26198 .23853 .21805 .20015 .18447 .17068 .15851 .14773
0000800    .13812 .12180 .10847  .1     .1      .1      .1     .1      .1    .1
0000900     .1      .1     .1     .1     .1      .1     .1     .1      .1     .1
0001000     .1      .1     .1     .1     .1      .1     .1     .1      .1     .1
0001100     .1      .1     .1     .1     .1      .1     .1     .1      .1     .1
0001200     .1      .1     .1     .1     .1      .1     .1     .1      .1     .1
0001300     .1      .1     .1     .1     .1      .1     .1     .1      .1     .1
0001400    10   1   2
0001500   100 2.          -60.92
0001600   200 2.          -3.168
0001700   210 6.          -1.471
0001800
```

C. NEMG: INPUT FOR MOLEC PROGRAM (NE-MG)

```
0000100      1
0000200      3     3     1  PCH  PRT     1 .73
0000300   OUT      0     2     1 0.          0.          0.          .73
0000400      2     1     2     3     1     3
0000500   NE       0     1     2 2.          0.          0.          .73081
0000600      3     1     3
0000700   MG       0     1     3 -2.         0.          0.          .72913
0000800      2     1     2
```

D. RNEMG: CONTRAC INPUT FOR NE-MG

```
0000100      2    2
0000120  4.946          2.14942     2.946         0.
0000300 0.
0000400 0.
0000500 0.
```

E. VVM: CONTRACTED MOLECULAR POTENTIAL

(INPUT FOR ENERGY, SCF PROGRAMS)

```
    1    1  0.0        0.0                                                          1
    3    3     1    2   0.73000     1     2                                         2
OUT  0 1 0  93   4     0.0          0.0          0.0          0.70500    0.73000    3
   22   42   62   82  102  122  142  162  182  202                                  4
 0.5843213E+00 0.6197348E+00 0.6551484E+00 0.6905621E+00 0.7259757E+00              5
 0.7613893E+00 0.7968029E+00 0.8322166E+00 0.8676302E+00 0.9030438E+00              6
 0.9384574E+00 0.9738711E+00 0.1009284E+01 0.1044696E+01 0.1080108E+01              7
 0.1115520E+01 0.1150931E+01 0.1186343E+01 0.1221755E+01 0.1257167E+01              8
 0.1292579E+01 0.1327991E+01 0.1398816E+01 0.1469642E+01 0.1540467E+01              9
 0.1611293E+01 0.1682118E+01 0.1752944E+01 0.1823770E+01 0.1894595E+01             10
 0.1965421E+01 0.2036246E+01 0.2107072E+01 0.2177897E+01 0.2248723E+01
```

```
 0.2319549E+01 0.2390374E+01 0.2461200E+01 0.2532025E+01 0.2602851E+01          11
 0.2673676E+01 0.2744502E+01 0.2886155E+01 0.3027808E+01 0.3169461E+01          12
 0.3311114E+01 0.3452767E+01 0.3594420E+01 0.3736073E+01 0.3877727E+01          13
 0.4019380E+01 0.4161033E+01 0.4302686E+01 0.4444339E+01 0.4585992E+01          14
 0.4727645E+01 0.4869298E+01 0.5010951E+01 0.5152604E+01 0.5294257E+01          15
 0.5435910E+01 0.5577563E+01 0.5860871E+01 0.6144179E+01 0.6427487E+01          16
 0.6710795E+01 0.6994103E+01 0.7277411E+01 0.7560719E+01 0.7844028E+01          17
 0.8127336E+01 0.8410644E+01 0.8693952E+01 0.8977260E+01 0.9260568E+01          18
 0.9543876E+01 0.9827184E+01 0.1011049E+02 0.1039380E+02 0.1067711E+02          19
 0.1096042E+02 0.1124372E+02 0.1181034E+02 0.1237696E+02 0.1294358E+02          20
 0.1351020E+02 0.1407681E+02 0.1464343E+02 0.1521005E+02 0.1577667E+02          21
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-0.2463831E+02-0.2177068E+02-0.1933852E+02-0.1725706E+02-0.1546275E+02          23
-0.1390690E+02-0.1255136E+02-0.1136551E+02-0.1032433E+02-0.9407094E+01          24
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-0.5702175E+01-0.5290941E+01-0.4920012E+01-0.4584542E+01-0.4280350E+01          26
-0.4003827E+01-0.3751849E+01-0.3311037E+01-0.2940171E+01-0.2625712E+01          27
-0.2357213E+01-0.2126528E+01-0.1927226E+01-0.1754170E+01-0.1603210E+01          28
-0.1470954E+01-0.1354603E+01-0.1251829E+01-0.1160684E+01-0.1079531E+01          29
-0.1006984E+01-0.9418747E+00-0.8832099E+00-0.8301487E+00-0.7819747E+00          30
-0.7380802E+00-0.6979455E+00-0.6272457E+00-0.5670267E+00-0.5151748E+00          31
-0.4700947E+00-0.4305671E+00-0.3956457E+00-0.3645864E+00-0.3367962E+00          32
-0.3117971E+00-0.2892004E+00-0.2686865E+00-0.2499905E+00-0.2328922E+00          33
-0.2172046E+00-0.2027718E+00-0.1894593E+00-0.1771549E+00-0.1657573E+00          34
-0.1551822E+00-0.1453576E+00-0.1276935E+00-0.1123301E+00-0.9892082E-01          35
-0.8718550E-01-0.7689518E-01-0.6785882E-01-0.5991211E-01-0.5291684E-01          36
-0.4675342E-01-0.4132001E-01-0.3653039E-01-0.3230766E-01-0.2858673E-01          37
-0.2529121E-01-0.2237942E-01-0.1980313E-01-0.1755022E-01-0.1554865E-01          38
-0.1377345E-01-0.1221491E-01-0.9601045E-02-0.7548936E-02-0.5935065E-02          39
-0.4675679E-02-0.3705234E-02-0.2968737E-02-0.2389941E-02-0.1862353E-02          40
-0.1335975E-02-0.6751183E-03-0.3205158E-03                                      41
NE    010 1  72  69     0.40000     0.0          0.0          0.43320     0.73081  42
   20    40    60   160   160   160   160   160   160   160                      43
 0.2054696E-02 0.4109390E-02 0.6164081E-02 0.8218773E-02 0.1027346E-01          44
 0.1232816E-01 0.1438285E-01 0.1643754E-01 0.1849223E-01 0.2054692E-01          45
 0.2260161E-01 0.2465630E-01 0.2671099E-01 0.2876569E-01 0.3082038E-01          46
 0.3287507E-01 0.3492976E-01 0.3698445E-01 0.3903914E-01 0.4109383E-01          47
 0.4520322E-01 0.4931261E-01 0.5342200E-01 0.5753139E-01 0.6164078E-01          48
 0.6575012E-01 0.6985950E-01 0.7396889E-01 0.7807827E-01 0.8218765E-01          49
 0.8629704E-01 0.9040642E-01 0.9451580E-01 0.9862518E-01 0.1027346E+00          50
 0.1068439E+00 0.1109533E+00 0.1150627E+00 0.1191721E+00 0.1232815E+00          51
 0.1315002E+00 0.1397190E+00 0.1479378E+00 0.1561565E+00 0.1643753E+00          52
 0.1725941E+00 0.1808128E+00 0.1890316E+00 0.1972504E+00 0.2054691E+00          53
 0.2136879E+00 0.2219067E+00 0.2301254E+00 0.2383442E+00 0.2465630E+00          54
 0.2547817E+00 0.2630005E+00 0.2712193E+00 0.2794380E+00 0.2876568E+00          55
 0.3040943E+00 0.3205318E+00 0.3369694E+00 0.3534069E+00 0.3698444E+00          56
 0.3862820E+00 0.4027195E+00 0.4191570E+00 0.4355946E+00 0.4520321E+00          57
 0.4684696E+00 0.4849072E+00                                                    58
-0.9694691E+04-0.4827574E+04-0.3205081E+04-0.2393760E+04-0.1906919E+04          59
-0.1582328E+04-0.1350458E+04-0.1176544E+04-0.1041272E+04-0.9330547E+03          60
-0.8445154E+03-0.7707383E+03-0.7083184E+03-0.6548245E+03-0.6084727E+03          61
-0.5679255E+03-0.5321599E+03-0.5003799E+03-0.4719570E+03-0.4463884E+03          62
-0.4022603E+03-0.3655332E+03-0.3345020E+03-0.3079480E+03-0.2849773E+03          63
-0.2649182E+03-0.2472579E+03-0.2315963E+03-0.2176178E+03-0.2050696E+03          64
-0.1937471E+03-0.1834826E+03-0.1741375E+03-0.1655964E+03-0.1577623E+03          65
-0.1505529E+03-0.1438982E+03-0.1377384E+03-0.1320216E+03-0.1267030E+03          66
-0.1171092E+03-0.1086993E+03-0.1012729E+03-0.9467226E+02-0.8877127E+02          67
-0.8346828E+02-0.7868033E+02-0.7433910E+02-0.7038782E+02-0.6677904E+02          68
-0.6347263E+02-0.6043454E+02-0.5763564E+02-0.5505083E+02-0.5265831E+02          69
-0.5043915E+02-0.4837672E+02-0.4645638E+02-0.4466516E+02-0.4299158E+02          70
-0.3995744E+02-0.3728436E+02-0.3491637E+02-0.3280814E+02-0.3092279E+02          71
-0.2923012E+02-0.2770522E+02-0.2632742E+02-0.2507945E+02-0.2394675E+02          72
-0.2291695E+02-0.2197952E+02                                                    73
 0.2975518E-01 0.1142313E+00 0.2466817E+00 0.4209120E+00 0.6312420E+00          74
 0.8724714E+00 0.1139846E+01 0.1429028E+01 0.1736062E+01 0.2057357E+01          75
 0.2389649E+01 0.2729987E+01 0.3075704E+01 0.3424397E+01 0.3773910E+01          76
 0.4122313E+01 0.4467883E+01 0.4809093E+01 0.5144590E+01 0.5473190E+01          77
 0.6105685E+01 0.6699875E+01 0.7250917E+01 0.7755533E+01 0.8211730E+01          78
 0.8618584E+01 0.8976037E+01 0.9284736E+01 0.9545879E+01 0.9761108E+01          79
 0.9932391E+01 0.1006194E+02 0.1015215E+02 0.1020552E+02 0.1022460E+02          80
 0.1021198E+02 0.1017021E+02 0.1010181E+02 0.1000925E+02 0.9894886E+01          81
 0.9609775E+01 0.9263420E+01 0.8870938E+01 0.8445575E+01 0.7998744E+01          82
 0.7540126E+01 0.7077803E+01 0.6618404E+01 0.6167270E+01 0.5728602E+01          83
 0.5305622E+01 0.4900701E+01 0.4515493E+01 0.4151058E+01 0.3807956E+01          84
 0.3486343E+01 0.3186051E+01 0.2906652E+01 0.2647525E+01 0.2407896E+01          85
 0.1983549E+01 0.1625896E+01 0.1326861E+01 0.1078561E+01 0.8736241E+00          86
 0.7053668E+00 0.5678670E+00 0.4559672E+00 0.3652385E+00 0.2919204E+00          87
 0.2328500E+00 0.1853884E+00                                                    88
```

```
MG   012 2  76  73   -0.40000     0.0          0.0          0.47000     0.72913      89
   20   40   60  160  160  160  160  160  160  160  160                              90
 0.1933543E-02 0.3867085E-02 0.5800623E-02 0.7734161E-02 0.9667698E-02               91
 0.1160124E-01 0.1353477E-01 0.1546831E-01 0.1740185E-01 0.1933539E-01               92
 0.2126892E-01 0.2320246E-01 0.2513600E-01 0.2706954E-01 0.2900307E-01               93
 0.3093661E-01 0.3287015E-01 0.3480368E-01 0.3673722E-01 0.3867076E-01               94
 0.4253784E-01 0.4640492E-01 0.5027201E-01 0.5413909E-01 0.5800617E-01               95
 0.6187325E-01 0.6574029E-01 0.6960732E-01 0.7347435E-01 0.7734138E-01               96
 0.8120841E-01 0.8507544E-01 0.8894247E-01 0.9280950E-01 0.9667653E-01               97
 0.1005436E+00 0.1044106E+00 0.1082776E+00 0.1121446E+00 0.1160117E+00               98
 0.1237457E+00 0.1314798E+00 0.1392139E+00 0.1469479E+00 0.1546820E+00               99
 0.1624160E+00 0.1701501E+00 0.1778842E+00 0.1856182E+00 0.1933523E+00              100
 0.2010863E+00 0.2088204E+00 0.2165545E+00 0.2242885E+00 0.2320226E+00              101
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 0.2861611E+00 0.3016294E+00 0.3170976E+00 0.3325658E+00 0.3480341E+00              103
 0.3635023E+00 0.3789706E+00 0.3944388E+00 0.4099070E+00 0.4253753E+00              104
 0.4408435E+00 0.4563118E+00 0.4717800E+00 0.4872482E+00 0.5027165E+00              105
 0.5181847E+00                                                                     106
-0.1235791E+05-0.6151395E+04-0.4082400E+04-0.3047810E+04-0.2427000E+04              107
-0.2013093E+04-0.1717426E+04-0.1495669E+04-0.1323191E+04-0.1185215E+04              108
-0.1072334E+04-0.9782803E+03-0.8987109E+03-0.8305254E+03-0.7714485E+03              109
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-0.2434111E+03-0.2303642E+03-0.2184866E+03-0.2076313E+03-0.1976746E+03              113
-0.1885119E+03-0.1800540E+03-0.1722247E+03-0.1649581E+03-0.1581972E+03              114
-0.1460006E+03-0.1353075E+03-0.1258639E+03-0.1174695E+03-0.1099650E+03              115
-0.1032213E+03-0.9713354E+02-0.9161501E+02-0.8659364E+02-0.8200900E+02              116
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-0.6126698E+02-0.5864844E+02-0.5620914E+02-0.5393243E+02-0.5180360E+02              118
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-0.3419826E+02-0.3223416E+02-0.3045724E+02-0.2884576E+02-0.2738127E+02              120
-0.2604794E+02-0.2483218E+02-0.2372220E+02-0.2270770E+02-0.2177972E+02              121
-0.2093042E+02                                                                     122
 0.4580327E-01 0.1749096E+00 0.3757172E+00 0.6376935E+00 0.9512933E+00              123
 0.1307882E+01 0.1699668E+01 0.2119631E+01 0.2561462E+01 0.3019513E+01              124
 0.3488731E+01 0.3964619E+01 0.4443184E+01 0.4920897E+01 0.5394655E+01              125
 0.5861739E+01 0.6319783E+01 0.6766746E+01 0.7200876E+01 0.7620689E+01              126
 0.8412610E+01 0.9135054E+01 0.9783422E+01 0.1035542E+02 0.1085061E+02              127
 0.1126999E+02 0.1161568E+02 0.1189066E+02 0.1209854E+02 0.1224336E+02              128
 0.1232944E+02 0.1236126E+02 0.1234337E+02 0.1228029E+02 0.1217645E+02              129
 0.1203616E+02 0.1186354E+02 0.1166253E+02 0.1143685E+02 0.1119000E+02              130
 0.1064555E+02 0.1005243E+02 0.9430264E+01 0.8795227E+01 0.8160419E+01              131
 0.7536180E+01 0.6930467E+01 0.6349185E+01 0.5796524E+01 0.5275245E+01              132
 0.4786945E+01 0.4332289E+01 0.3911202E+01 0.3523043E+01 0.3166745E+01              133
 0.2840932E+01 0.2544016E+01 0.2274278E+01 0.2029923E+01 0.1809141E+01              134
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 0.4158553E+00 0.3215727E+00 0.2480209E+00 0.1908406E+00 0.1465265E+00              136
 0.1122804E+00 0.8588272E-01 0.6558204E-01 0.5000329E-01 0.3807138E-01              137
 0.2894885E-01                                                                     138
-0.1598589E+02                                                                     139
```

F. RIG: SCF INPUT (TRIAL EIGENVALUES AND SYMMETRY CARDS)

```
0000100     0    1
0000200 6,8,1,1,5,6,0,0,2,.05,1.
0000300   2.        -60.9204
0000400   2.        -92.6720
0000500  S1   2.  -6.30841   .005          1    1    0
0000600      8    2      SIGMA EP
0000700      0    1
0000800      0    1    1   1.00000000
0000900      1    1
0001000      1    1    1   1.00000000
0001100      2    1
0001200      0    1    1   1.00000000
0001300      2    1
0001400      2    1    1   1.00000000
0001500      0    1
0001600      0    1    2   1.00000000
0001700      1    1
```

```
0001800      1     1     2    1.00000000
0001900      0     1
0002000      0     1     3    1.00000000
0002100      1     1
0002200      1     1     3    1.00000000
0002300   S2    2.   -4.51048   .005           1     1     0
0002400   S3    2.   -2.88924   .005           1     1     0
0002420   S4    2.   -1.46411   .005           1     1     0
0002500    PI1 4.   -3.63858   .005           5     1     0
0002600     10     2    PI Z REP
0002700      1     1
0002800      0     1     1    1.00000000
0002900      2     1
0003000      1     1     1    1.00000000
0003100      3     1
0003200      0     1     1    1.00000000
0003300      3     1
0003400      2     1     1    1.00000000
0003500      4     1
0003600      1     1     1    1.00000000
0003700      4     1
0003800      3     1     1    1.00000000
0003900      1     1
0004000      0     1     2    1.00000000
0004100      2     1
0004200      1     1     2    1.00000000
0004300      1     1
0004400      0     1     3    1.00000000
0004500      2     1
0004600      1     1     3    1.00000000
0004700   PI2 4.   -1.601967 .005           5     1     0
```

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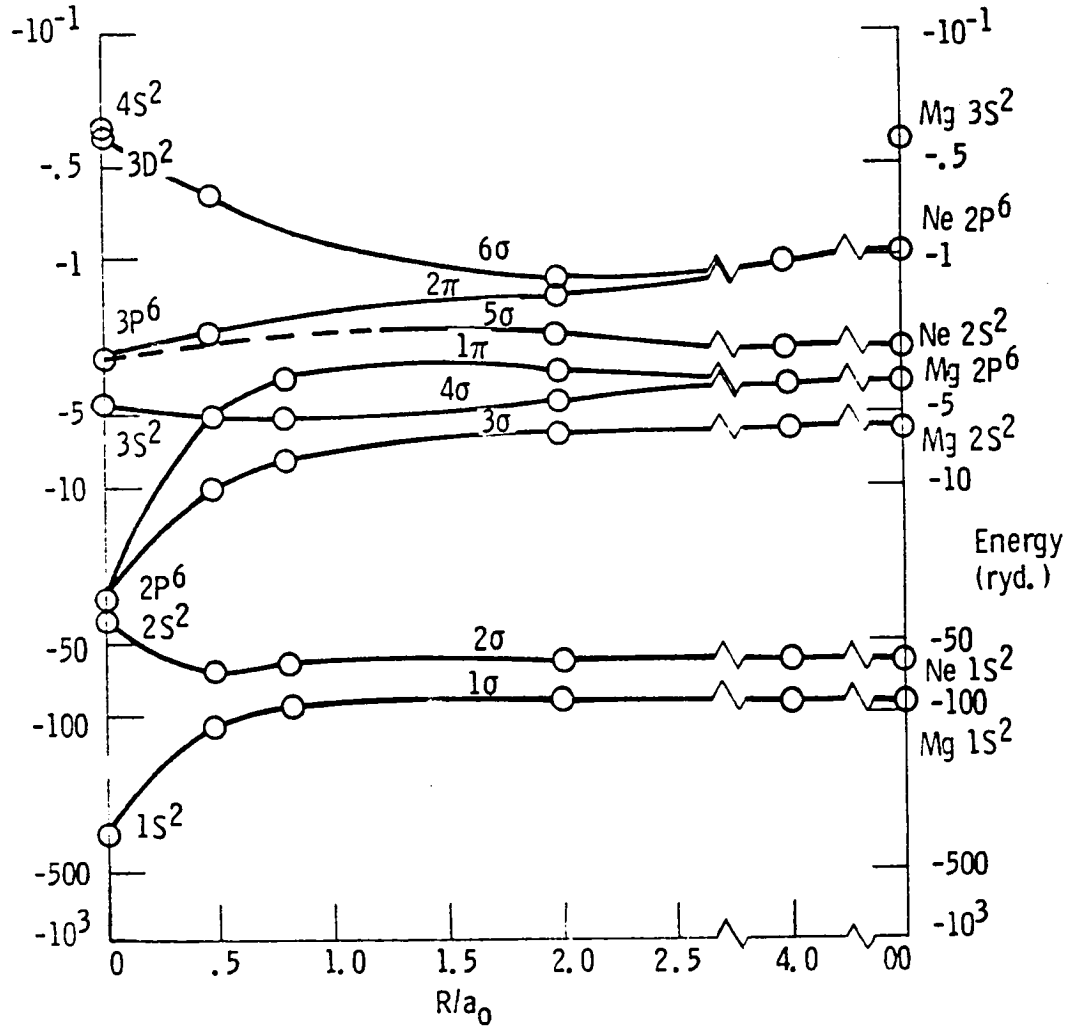

Figure 1. - Correlation diagram for Ne-Mg.

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16. Abstract

This work is concerned with the self-consistent calculation of the electronic energy levels of noble gas pseudomolecules formed when a metal surface is bombarded by noble gas ions and with the construction of energy level correlation diagrams as a function of interatomic spacing. The self-consistent-field xα scattered wave (SCF-Xα-SW) method of Slater and Johnson is utilized. Preliminary results on the Ne-Mg system are given. An interactive xα programming system, which has been implemented on the LeRC IBM 370 computer, is described in detail. This automated system makes use of special PROCDEFS (procedure definitions) to minimize the data to be entered manually at a remote terminal. Listings of the special PROCDEFS and of typical input data are given.

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