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An RPA program for jellium spheres

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A FORTRAN 77 program is presented that calculates the electromagnetic response of small metal particles or atomic clusters. The program uses the random phase approximation and the local density approximation, and treats the clusters as jellium spheres. From the frequency-dependence response the polarizability, the plasmon resonance frequency, and the width of the resonance lines are directly extracted.

PROGRAM SUMMARY

Title of program: JELLYRPA

Catalogue number: ABTC

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue), and by electronic mail from bertsch@msunscl

Computer: Digital VAX 780; *Installation*: National Superconducting Cyclotron Laboratory, Michigan State University

Operating system: VAX/VMS

Programming language used: FORTRAN 77

High speed storage required: 350 kwords

No. of bits in a word: 8

No. of lines in combined program and test deck: 485

Keywords: random phase approximation (RPA), local density approximation (LDA), jellium spheres, polarization propagator, radial transition density, strength function, sum rules, polarizability, plasmon, Mie resonance.

Nature of physical problem
The electromagnetic response of small metal particles and atomic clusters is an object of current experimental interest. The electric polarizability and the plasmon resonance are measured, among other properties. The quantum-mechanical theory of the response in the many-electron system is still not fully developed, but the random phase approximation (RPA) in the local density approximation (LDA) is simple and accurate enough to serve as a theoretical baseline for more elaborate treatments. The program JELLYRPA computes the RPA/LDA response for small metal spheres, treating the atomic cores as a uniform positively charged background.

Method of solution
JELLYRPA uses the polarization propagator method in coordinate space to solve the equations for the response of the electrons to an external field. This method has the advantage that unbound excitations can be treated quite realistically, with the resonances automatically acquiring a width due to the ionization of the electrons. The method allows excitations to be calculated in very large spaces of configurations. The numerical difficulty in the evaluation of the polarization propagator is controlled by the mesh size in coordinate space, since the computation requires inversion of a matrix whose dimensionality is equal to the number of mesh points.

Restrictions on the complexity of the problem
The theory is best suited for closed-shell systems where a Hartree–Fock or some effective mean-field theory provides a good description of the ground state. Also, the polarization propagator method relies on a simple representation of the interaction, with very restricted possibilities for nonlocality. In particular, the exchange interaction can only be calculated approximately, in a zero-range approximation. The interaction

in the LDA is well suited to this method, because exchange and correlation effects are approximated by a local function of density.

Typical running time
250 s for input provided.

LONG WRITE-UP

1. Introduction

The electromagnetic response of small metal particles and atomic clusters is an object of current experimental interest. The electric polarizability and the plasmon resonance are measured [1,2], among other properties.

Plasma oscillations in a system of degenerate electrons are often treated theoretically using the random phase approximation (RPA), first discussed by Bohm and Pines [3]. The theory is equivalent to the time-dependent Hartree–Fock theory in the limit of small-amplitude oscillations. The program JELLYRPA uses the polarization propagator method in coordinate space, which is very efficient if the electronic potential is a local function of position. The exchange (or Fock) potential does not satisfy this, but local approximations to exchange and correlation energies have proven to be very successful, and one of these parameterizations is adopted in JELLYRPA. The JELLYRPA program is a modified version of the RPA program used in the theory of nuclear excitations [4]. The first applications of this method to electronic excitations in jellium spheres were by Ekardt [5] and by Beck [6]. An alternative method to compute the RPA response is by diagonalizing a matrix in the space of electron configurations [7].

Formally, the polarization propagator is a function of two spatial variables, $\boldsymbol{r}$ and $\boldsymbol{r}'$, giving the positions of a perturbing potential and the density response to it. It is also a function of the frequency ω of the perturbation. The RPA approximation to the polarization propagator is

$$\Pi^{\mathrm{RPA}} = \left[1 + \Pi^0 \frac{\delta V}{\delta \rho}\right]^{-1} \Pi^0. \tag{1}$$

Here Π^0 is the independent-particle polarization propagator, defined as

$$\Pi^0(\boldsymbol{r}, \boldsymbol{r}', \omega) = \sum_i \phi_i^{0*}(\boldsymbol{r})\big([T + V - \epsilon_i - \omega]^{-1}_{\boldsymbol{r},\boldsymbol{r}'} + [T + V - \epsilon_i + \omega)]^{-1}_{\boldsymbol{r},\boldsymbol{r}'}\big)\phi_i^0(\boldsymbol{r}'), \tag{2}$$

where T is the kinetic energy operator, V is the self-consistent potential, and ϵ_i and ϕ_i are the eigenenergies single-particle wave functions of the Hamiltonian $T + V$. The residual interaction between electrons is defined by the functional derivative, $\delta V/\delta\rho$, where ρ is the electron density.

JELLYRPA computes the RPA response for spherical jellium clusters, with the potential given by the sum of three terms: a background potential from a uniform charge density (the "jellium"), the Coulomb interaction between electrons, and the exchange–correlation interaction from ref. [8]. JELLYRPA uses an angular-momentum representation of the functions appearing in the polarization propagator. This permits the RPA to be calculated from independent radial equations for each multipole, provided the static solution is spherically symmetric. We define the multipolar interaction v_L as follows,

$$\frac{\delta V(r)}{\delta \rho(r')} = \sum_{LM} v_L(r_1, r_2) Y^*_{LM}(\hat{r}_1) Y_{LM}(\hat{r}_2),$$

where Y_{LM} are the usual spherical harmonics. For the Coulomb interaction, the v_L is the usual Slater form,

$$v_L^{\mathrm{Coul}} = (2L+1)e^2 \frac{r_>^L}{r_<^{L+1}}.$$

The exchange–correlation interaction is of the form of a density-dependent contact interaction

with [8]

$$v_L^{\mathrm{exc}} = -\left(\frac{0.407}{r_s(r)} + \frac{0.253}{r_s(r)+11.4}\right)\frac{\delta(r-r')}{\rho(r)r^2}.$$

Here $r_s(r)$ is related to the local electron density by $r_s(r) = (4\pi\rho(r)/3)^{1/3}$ and is expressed in atomic length units; the v_L here has energy dimensions of rydbergs. The v_L are stored in the program in the two-dimensional array VRES(I, J). The angular-momentum decomposition of the response Π^0 is given by

$$\Pi(r_1, r_2) = \sum_{LM} \Pi_L(r_1, r_2) Y_{LM}^*(\hat{r}_1) Y_{LM}(\hat{r}_2)/(r_1 r_2)^2.$$

The single particle Green's function is similarly expanded in an angular-momentum basis labelled by l. Then the formula for the independent particle response is

$$\Pi_L^0(r, r', \omega) = \sum_{l,l'} \frac{(2l+1)(2l'+1)}{4\pi(2L+1)} (l'0l0 \mid L0)^2 \times u_l(r)^* u_l(r') \left([T+V-\epsilon_l-\omega]^{-1}_{l';r,r'} + [T+V-\epsilon_l+\omega]^{-1}_{l';r,r'}\right), \quad (3)$$

where the sum over single-particle states, l, l' is restricted to those with orbital angular momentum l and l' such that $L+l+l'$ is even. In this equation, the u_l are the radial wave functions of the occupied states, $\phi_l(\boldsymbol{r}) = u_l(r)Y_l(\hat{r})/r$.

The radial Green's function is evaluated in the coordinate representation by the usual Green's function formula for second-order linear differential equations,

$$[T+V-\epsilon]^{-1}_{r,r'} = \frac{u(r_<)w(r_>)}{W}.$$

Here u, w are solutions of the radial differential equation that have appropriate boundary conditions, i.e. u must be regular at the origin and w must be a pure outgoing wave at infinity, and W is the Wronskian.

The program computes the independent particle response Π^0 for each desired frequency, storing it in the array G(I, J). The matrix operations to evaluate the factor $(1 + \Pi\delta v/\delta\rho)^{-1}$ in eq. (1) are then performed and put in the array B(I, J).

The useful output is obtained from the radial transition densities associated with a given external field $V_{\mathrm{ext}}^L(r)$. These densities are defined as

$$\delta\rho_L^0(r) = \int_0^\infty dr' \Pi_L^0(r, r', \omega) V_{\mathrm{ext}}^L(r'),$$

$$\delta\rho_L^{\mathrm{RPA}}(r) = \int_0^\infty dr' \Pi_L^{\mathrm{RPA}}(r, r', \omega) V_{\mathrm{ext}}^L(r').$$

These quantities are computed in the arrays DRHOF(I) and DRHORPA(I). In the program $V_{\mathrm{ext}}^L(r)$ is defined as pure multipole field, $V_{\mathrm{ext}}^L(r) = r^L$, stored in the array VEXT(I). The external field is integrated over the transition density to obtain the free and RPA response to the external perturbation of the system

$$\Pi_L^0(V_{\mathrm{ext}}, \omega) = \int_0^\infty dr \int_0^\infty dr' V_{\mathrm{ext}}^L(r) \times \Pi_L^0(r, r', \omega) V_{\mathrm{ext}}^L(r'), \quad (4)$$

$$\Pi_L^{\mathrm{RPA}}(V_{\mathrm{ext}}, \omega) = \int_0^\infty dr \int_0^\infty dr' V_{\mathrm{ext}}^L(r) \times \Pi_L^{\mathrm{RPA}}(r, r', \omega) V_{\mathrm{ext}}^L(r'). \quad (5)$$

The real and imaginary parts of these functions, PIFREE and PIRPA, are the primary output quantities printed by the program.

2. Physical quantities and sum rules

The units used in the program internally are atomic units for length, 1 a.u. = 0.053 nm, and rydbergs for energy, 1 Ry = 13.6 eV. In these units the electronic charge is $e^2 = 2$ and the electron's mass is $m_e = 1/2$. However, for input and output purposes energies and frequencies are expressed in units of eV.

Physical applications often require the properties of individual quantum transitions. The quantum mechanical response is defined in terms of the transition strengths between an initial state i and all final states f,

$$S(\omega) = \sum_f \langle i \mid V_{\mathrm{ext}} \mid f\rangle^2 \delta(E_f - E_i - \omega).$$

The relation to the polarization propagator is simply

$$S(\omega) = \frac{1}{\pi} \operatorname{Im} \Pi_L(V_{\text{ext}}, \omega). \tag{6}$$

The response function is often used in applications. For example, inelastic scattering in the continuum is conveniently calculated using eq. (4) with V_{ext} being the transition field of the projectile, or some approximation to the projectile interaction. The experimental strength function is often smoother than the RPA prediction, either because of experimental resolution or because of physical damping processes not described by the RPA. To facilitate comparison with smoothed strengths, it is convenient to add an imaginary part to the frequency. This is equivalent to convoluting the strength function with a Lorentzian. Otherwise, only the boundary condition on the single-particle Green's function, that continuum particles have outgoing asymptotic wave functions, provides an imaginary part to the response and a width to the resonances.

In the neighborhood of a resonance of the system, the response function may be expressed as

$$\Pi(\omega) \sim \langle i \,|\, V \,|\, R\rangle^2 \left(\frac{1}{E_{\text{R}} + \mathrm{i}\Gamma/2 - \omega} \right),$$

where E_{R} and $\Gamma/2$ are the real imaginary parts of the frequency of the mode. This connection is important for extracting the properties of individual resonances from the response. To find the squared matrix element for an individual resonance, one first calculates the response over a small frequency interval containing the mode in question. One may then either fit the imaginary part to the function $\operatorname{Im}(E_{\text{R}} + \mathrm{i}\Gamma/2 - \omega)^{-1} = (\Gamma/2)/((E_{\text{r}} - \omega)^2 + (\gamma/2)^2)$ or simply integrate over the interval,

$$\langle i \,|\, V_{\text{ext}} \,|\, R\rangle^2 \sim \int_{E_{\text{R}}-\Delta}^{E_{\text{R}}+\Delta} S(\omega)\, \mathrm{d}\omega.$$

The transition density associated with a resonance is defined in terms of the matrix element of the density operator as $\delta\rho_{\text{R}} = \langle \mathrm{i} \,|\, \hat{\rho} \,|\, R\rangle$. It may be calculated from the above quantities by the equation

$$\delta\rho_R(r) = \frac{-1}{\langle i \,|\, V_{\text{ext}} \,|\, R\rangle} \int_0^\infty \mathrm{d}r'\, \Pi_L^{\text{RPA}}(r, r') \times V_{\text{ext}}^L(r').$$

The integrated transition strengths obey sum rules which are respected by the RPA theory. It is an important check on calculations to see how well the sum rules are satisfied numerically. Also, it is convenient to express transition strengths as a fraction of the appropriate sum rule, which eliminates any possible ambiguity in the definition of the strength functions.

The sum rules have the following form, valid whenever the potential depends only on density,

$$\int S(\omega)\omega\, \mathrm{d}\omega = \int \mathrm{d}^3r\, \frac{(\nabla V_{\text{ext}})^2}{2m_{\text{e}}} \rho_0. \tag{7}$$

The program computes the sum rule for a given angular momentum L from this formula, using

$$(\nabla V_{\text{ext}})^2 = (F'(r))^2 - \left(\frac{F(r)}{r} \right)^2 L(L+1).$$

With the pure multipole fields, the sum rule reduces to

$$\int S_L(\omega)\omega\, \mathrm{d}\omega = \frac{L(2L+1)}{8\pi m} \int \mathrm{d}r\, r^{2L} \rho_0 = \frac{L(2L+1)}{8\pi m} N \langle r^{2L-2} \rangle,$$

where N is the number of electrons. When $L = 1$, this is just the familiar f-sum rule, also known as the TRK sum rule,

$$\int S_1 \omega\, \mathrm{d}\omega = \frac{3N}{8\pi m_{\text{e}}}.$$

In the program, a loop allows the strength function to be computed over a range of energy, and the total strength in that interval is compared with the multipole sum rule.

The dipole sum rule may also be expressed in terms of the photon absorption cross section. The relationship is

$$\int \sigma\, \mathrm{d}\omega = \frac{2\pi^2 N e^2}{m_{\text{e}} c}.$$

This quantity is also printed when the $L = 1$ response is evaluated. The static polarizability of a system, defined as the ratio of the induced dipole moment and the electric field that induced it, is given by

$$\alpha = -\tfrac{4}{3}\pi \Pi_{L=1}(\omega = 0).$$

This quantity is printed if the $L = 1$ response is evaluated including the value at zero frequency. The polarizability is very useful in making the connection between the quantum and the classical responses. For a classical conduction sphere, $\alpha = R^3$. If one assumes that the polarizability is due to the plasmon alone, the plasmon frequency can be obtained from the ratio of f-sum rule to polarizability,

$$\omega_p \sim \frac{Ne^2}{m_e \alpha}.$$

3. Program structure

The program is quite straightforward with the computation of $\Pi^{(0)}$ requiring the most attention. The task of computing the self-consistent wave functions and eigenenergies is done in the subroutine STATIC, using the same elementary integration method as GREEN. In GREEN each function requires a single integration from one extreme in radius to the other, with the direction determined by the boundary condition. In STATIC, the eigenenergy is determined by the bisection method, looping over integrations of the wavefunction. If consistency in the integration methods between GREEN and STATIC is not maintained, transition strength may appear at frequencies corresponding to transitions between occupied states. These Pauli-forbidden transitions in principle cancel out in the two terms in eq. (2). The subroutine RESPONSE computes the physical quantities at a fixed frequency, using the arrays generated in STATIC and GREEN. The subroutine CLEBSCH which computes the Clebsch–Gordan coefficients for eq. (3) is a general-purpose routine; there are more efficient formulas to calculate the specific coefficients required by the present application.

The most time-consuming part of the calculation is the inversion of the polarization matrix, the first factor in eq. (1). Since the matrix is complex, most available library inversion routines cannot be used; a simple matrix-inversion subroutine, MATR, is included with the program. If execution time is a real consideration, matrix inversion should not be used. Only the product of the inverse matrix with the vector DRHOF is needed to obtain the vector DRHORPA. It is faster to obtain DRHORPA directly by solving the simultaneous equations.

The external field is determined in the subroutine EXTV. The spatial form of the field is a pure multipole, $V_{ext} = r^L Y_L$. The sum rule associated with the field, eq. (7), is calculated in the subroutine SUMRULE. Other fields besides multipole fields may be of interest. For example, electron scattering could be represented by a plane-wave field, which would have a Bessel function radial dependence in the multipole expansion. If the user substitutes another field, the corresponding sum rule is automatically calculated by SUMRULE.

4. Program input and test run

A detailed description of the format for the input parameters is given in table 1. The first line contains the parameters specifying the mesh in coordinate space. Different mesh sizes can be used for the wave-function integration and the matrix inversion. The length scale of the mesh is set by the radius of the jellium cluster, obtained from the input on the second line. The integrations take place over an interval equal to twice the radius of the jellium cluster. Regarding the choice of a suitable mesh interval, we note that a mesh spacing of 0.5 a.u. is quite adequate to obtain an accuracy of less than 0.01 eV for the single-particle energies. Another consideration in the choice of the mesh is to avoid a long integration into the forbidden region; the algorithm is not stable here. The mesh size for the matrix operations controls the execution time of the program. The strength functions can be computed to about 10% accuracy with a mesh as coarse as 1 a.u.; for most calculations we use 0.5 a.u.

On the second line are input parameters having to do with the static mean-field calculation, as follows. The density parameter of the background positive charge, r_s, is given by RS. The total charge of the background is Z, in units of the elementary charge. Thus the radius of the jellium sphere is $r_s Z^{1/3}$. The number of iterations of a Hartree self-consistency loop is given by the parameter ITER. The test case has a value that produces convergence on all output quantities to less than a percent. Unfortunately, if extremely large clusters are calculated, the iteration process will not converge, and the user will have to change a numerical parameter in a formula in STATIC that updates the potential.

The next lines of input contain the quantum numbers of the occupied single-particle states, one line for each state. The table describes this in more detail. Finally, the last line of input contains the information about the multipolarity of the response and the frequency. The frequency may have a fixed imaginary part, given by half the parameter GAM. Frequencies are calculated on a mesh with the initial and final frequencies and the frequency interval specified.

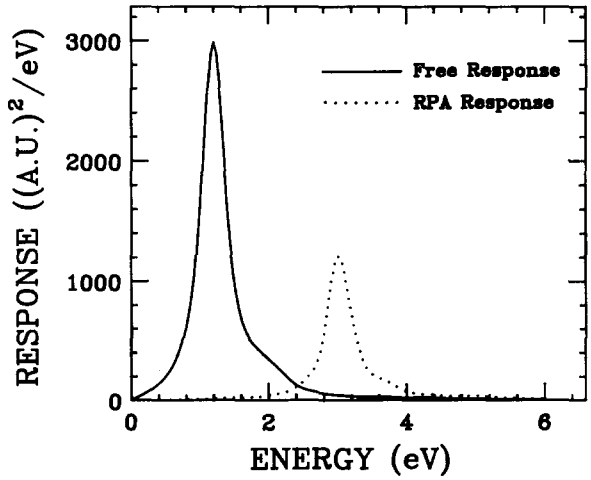

Fig. 1. The dipole response functions, defined in eqs. (4 and 5), are shown for the jellium cluster representing Na_{21}^+. The solid line and dashed lines show the independent particle response and the RPA response, respectively.

Table 1
Input to the RPA program. The numerical values are the data appropriate for the calculation of the dipole response of the singly-charged cluster Na_{21}^+

Line 1 NGRID, N, NX: NGRID = 50 is the number of mesh points in the spatial grid used to calculate the single-particle wave functions. N = 45 is the number of points in the matrix representation of the polarization propagator. NX = 1 is the spacing of these points in units of the wave function mesh.

Line 2 RS, Z, ITER: RS = 3.93 (a.u.) is the radius of a sphere of jellium containing a unit of charge. Z = 21 is the total positive charge of the jellium, so that the actual radius of the jellium is RS*$Z^{1/3}$. ITER = 15 is the number of iterations of the static solution to approach self-consistency.

Lines 3.1...3.*n* LH, NODE, NOCC: These are the quantum numbers for the occupied orbitals, with LH the orbital angular momentum, NODE the number of internal nodes in the radial wave function, and NOCC the occupancy of the orbital. If NOCC = −1, the filled-shell occupancy factor is used, NOCC = 2*(2*LH+1). Thus the filled p-orbital in Na_{21}^+ has LH = 1, NODE = 0, NOCC = −1 or 6 electrons. The orbital data is terminated by the line −1 0 0.

Line 4 L, EX, EXM, DEX, GAM: Here L = 1 is the multipolarity of the response. The response is calculated on a grid of energies starting from EX = 0 eV and ranging up to EXM = 15 eV in steps of DEX = 0.2 eV. GAM = 0.4 eV is an added imaginary part of the energy (actually i*GAM/2 is added) to smooth the strength function.

The test case shows the computation of the dipole response for the singly-charged cluster Na_{21}^+. The program first calculates the self-consistent particle states, and prints the eigenenergies of each state. Then the response is calculated, with the independent-particle and the RPA response printed as complex numbers for each frequency. Figure 1 shows a graph of the output. For the independent particle response, the imaginary part peaks at energies about 1 eV, corresponding to single-particle transitions such as 0d → 0f. Note that the interacting response is much weaker for low-energy transitions. This is the effect of the screening. In the interacting response, there is a dominant peak at 3.0–3.1 eV. This is the Mie plasmon. It is red-shifted from the classical value, $\omega_p = 27.2(r_s)^{-1/3} \sim 3.4$ eV, by about 13%.

An important check on the reliability of the computation is the sum rule. It may be seen from the output that the *f*-sum rule is violated by 3%.

Acknowledgement

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TEST RUN OUTPUT

```
  50 grid points in wfn;   45 in matrix;  1 relative step size
RS,Z,ITER=  3.93 21.0 15
 R=    10.84246
          0           0   2.000000
          1           0   6.000000
          2           0   10.00000
          0           1   2.000000
         -1           0  0.0000000E+00
NET CHARGE =     1.000000
iteration number            15
L,NODE,E=  0  0  -7.52008eV
L,NODE,E=  1  0  -6.78580eV
L,NODE,E=  2  0  -5.79885eV
L,NODE,E=  0  1  -5.11664eV
 L=           1 GAM=   0.4000000
   Energy          Free response          RPA Response
    (eV)        Real       Imaginary     Real        Imaginary
Polarizability is   0.1506E+04 a.u.**3
   0.00000  0.1071E+04  0.0000E+00  0.1798E+03  0.0000E+00
   0.20000  0.1096E+04  0.5918E+02  0.1806E+03  0.1605E+01
   0.40000  0.1180E+04  0.1392E+03  0.1830E+03  0.3318E+01
   0.60000  0.1344E+04  0.2814E+03  0.1871E+03  0.5279E+01
   0.80000  0.1628E+04  0.6112E+03  0.1933E+03  0.7734E+01
   1.00000  0.1890E+04  0.1582E+04  0.2020E+03  0.1129E+02
   1.20000  0.2946E+03  0.2987E+04  0.2127E+03  0.1771E+02
   1.40000 -0.1162E+04  0.1600E+04  0.2207E+03  0.2370E+02
   1.60000 -0.8951E+03  0.6829E+03  0.2378E+03  0.2534E+02
   1.80000 -0.5775E+03  0.4550E+03  0.2638E+03  0.3257E+02
   2.00000 -0.5535E+03  0.4441E+03  0.2988E+03  0.4647E+02
   2.20000 -0.5381E+03  0.2330E+03  0.3474E+03  0.6931E+02
   2.40000 -0.4238E+03  0.1253E+03  0.4226E+03  0.1140E+03
   2.60000 -0.3374E+03  0.7964E+02  0.5399E+03  0.2202E+03
   2.80000 -0.2757E+03  0.5581E+02  0.6834E+03  0.5298E+03
   3.00000 -0.2299E+03  0.4164E+02  0.2746E+03  0.1217E+04
   3.20000 -0.1945E+03  0.3272E+02 -0.5361E+03  0.7460E+03
   3.40000 -0.1661E+03  0.2752E+02 -0.4390E+03  0.3082E+03
   3.60000 -0.1440E+03  0.2647E+02 -0.3092E+03  0.1959E+03
   3.80000 -0.1298E+03  0.2412E+02 -0.2769E+03  0.1421E+03
   4.00000 -0.1132E+03  0.2228E+02 -0.2268E+03  0.7609E+02
   4.20000 -0.1050E+03  0.2709E+02 -0.1765E+03  0.5822E+02
   4.40000 -0.1044E+03  0.2142E+02 -0.1503E+03  0.5472E+02
   4.60000 -0.9502E+02  0.1346E+02 -0.1340E+03  0.3695E+02
   4.80000 -0.8540E+02  0.1004E+02 -0.1102E+03  0.3542E+02
   5.00000 -0.7633E+02  0.9128E+01 -0.1127E+03  0.3998E+02
   5.20000 -0.7024E+02  0.8097E+01 -0.1047E+03  0.3111E+02
   5.40000 -0.6490E+02  0.7136E+01 -0.9624E+02  0.2363E+02
   5.60000 -0.6014E+02  0.6486E+01 -0.8755E+02  0.1731E+02
   5.80000 -0.5615E+02  0.6010E+01 -0.7912E+02  0.1253E+02
   6.00000 -0.5244E+02  0.5172E+01 -0.7181E+02  0.9894E+01
   6.20000 -0.4902E+02  0.4471E+01 -0.6543E+02  0.7697E+01
   6.40000 -0.4589E+02  0.3881E+01 -0.5960E+02  0.6193E+01
   6.60000 -0.4302E+02  0.3384E+01 -0.5468E+02  0.5130E+01
   6.80000 -0.4039E+02  0.2968E+01 -0.5037E+02  0.4326E+01
   7.00000 -0.3799E+02  0.2621E+01 -0.4659E+02  0.3709E+01
   7.20000 -0.3579E+02  0.2333E+01 -0.4325E+02  0.3227E+01
   7.40000 -0.3377E+02  0.2092E+01 -0.4028E+02  0.2844E+01
   7.60000 -0.3191E+02  0.1890E+01 -0.3764E+02  0.2533E+01
```

7.80000	-0.3021E+02	0.1718E+01	-0.3527E+02	0.2276E+01
8.00000	-0.2864E+02	0.1571E+01	-0.3313E+02	0.2061E+01
8.20000	-0.2720E+02	0.1443E+01	-0.3120E+02	0.1878E+01
8.40000	-0.2586E+02	0.1331E+01	-0.2944E+02	0.1722E+01
8.60000	-0.2462E+02	0.1232E+01	-0.2784E+02	0.1587E+01
8.80000	-0.2347E+02	0.1145E+01	-0.2638E+02	0.1470E+01
9.00000	-0.2241E+02	0.1066E+01	-0.2503E+02	0.1366E+01
9.20000	-0.2141E+02	0.9948E+00	-0.2380E+02	0.1273E+01
9.40000	-0.2048E+02	0.9304E+00	-0.2266E+02	0.1189E+01
9.60000	-0.1961E+02	0.8717E+00	-0.2161E+02	0.1113E+01
9.80000	-0.1880E+02	0.8178E+00	-0.2063E+02	0.1041E+01
10.00000	-0.1804E+02	0.7682E+00	-0.1973E+02	0.9739E+00
10.20000	-0.1732E+02	0.7222E+00	-0.1888E+02	0.9107E+00
10.39999	-0.1664E+02	0.6795E+00	-0.1809E+02	0.8509E+00
10.59999	-0.1601E+02	0.6398E+00	-0.1735E+02	0.7944E+00
10.79999	-0.1541E+02	0.6028E+00	-0.1665E+02	0.7411E+00
10.99999	-0.1484E+02	0.5684E+00	-0.1600E+02	0.6911E+00
11.19999	-0.1431E+02	0.5366E+00	-0.1538E+02	0.6445E+00
11.39999	-0.1380E+02	0.5072E+00	-0.1480E+02	0.6013E+00
11.59999	-0.1332E+02	0.4801E+00	-0.1425E+02	0.5615E+00
11.79999	-0.1286E+02	0.4554E+00	-0.1373E+02	0.5253E+00
11.99999	-0.1242E+02	0.4330E+00	-0.1324E+02	0.4926E+00
12.19999	-0.1201E+02	0.4126E+00	-0.1277E+02	0.4632E+00
12.39999	-0.1162E+02	0.3941E+00	-0.1233E+02	0.4370E+00
12.59999	-0.1125E+02	0.3775E+00	-0.1191E+02	0.4138E+00
12.79999	-0.1089E+02	0.3624E+00	-0.1151E+02	0.3932E+00
12.99999	-0.1055E+02	0.3485E+00	-0.1113E+02	0.3749E+00
13.19999	-0.1023E+02	0.3357E+00	-0.1077E+02	0.3585E+00
13.39999	-0.9927E+01	0.3238E+00	-0.1043E+02	0.3436E+00
13.59999	-0.9635E+01	0.3123E+00	-0.1011E+02	0.3298E+00
13.79999	-0.9356E+01	0.3013E+00	-0.9800E+01	0.3169E+00
13.99999	-0.9090E+01	0.2905E+00	-0.9506E+01	0.3046E+00
14.19999	-0.8835E+01	0.2799E+00	-0.9227E+01	0.2927E+00
14.39999	-0.8592E+01	0.2693E+00	-0.8960E+01	0.2811E+00
14.59999	-0.8358E+01	0.2587E+00	-0.8706E+01	0.2697E+00
14.79999	-0.8134E+01	0.2482E+00	-0.8462E+01	0.2584E+00
14.99999	-0.7919E+01	0.2377E+00	-0.8228E+01	0.2473E+00

TOTAL STRENGTH IN FREE RESPONSE,	RPA RESPONSE,	AND SUM RULE
0.8696E+03	0.8575E+03	0.8831E+03
energy-integrated photon cross section, (ev-A^2)		0.4260E+02