

## Contribution of the $E2$ transitions to the opacity of hot and dense plasmas of heavy elements by an average-atom approach

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The contribution of electric quadrupole ( $E2$ ) transitions to the opacity of hot and dense plasmas is taken into account by using an average-atom model. As an example, the increase of the opacity of Au due to the  $E2$  transition is shown to range from less than 1% to more than 10% depending on density and temperature. It reaches 15% when the density and temperature are, respectively, 100 g/cm<sup>3</sup> and 5000 eV. The most significant influence comes from the  $E2$  photoionization processes.

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Generally the magnitudes of the so-called higher order transitions, such as the magnetic dipole ( $M1$ ) and the electric quadrupole ( $E2$ ), are five to eight orders less than the electric dipole ( $E1$ ) transitions among the valence states of atoms or ions [1]. However, in a very hot and dense plasma, the inner-shell radiative transitions play an important role for the radiative transfer. For these kinds of inner-shell processes, transitions due to the higher order interactions than the  $E1$  term cannot be neglected. A detailed study on the multipole effects in photoionization cross sections of isolated atoms was carried out by Ron *et al.* [2] within the independent particle model. For photoionization processes caused by higher energy photons above keV, the cross sections due to the  $E2$  transition are comparable to, or even larger than those of the  $E1$  transitions. For many cases, the contributions of the bound-free processes to the total opacity of hot and dense matters are considerable [3]. In the present study, average-atom model is used to display the changes of the opacity caused by  $E2$  transitions. As the average-atom model is a one-electron approximation, there is no  $M1$  transition between different energy orbitals, though the  $M1$  transitions between the states of an actual atom within one electronic configuration can give comparable cross sections and interference effects with the  $E2$  processes. However, the neglect of the  $M1$  transitions would not induce loss in the radiative absorptions for high photon energies.

A widely used scheme of the average-atom calculation is to use a full self-consistent Dirac-Slater model to obtain the electron orbitals [4–7]. The same approach is used in the present study to include the  $E2$  transitions in the calculation of the frequency dependent as well as the Rosseland mean and Planck mean opacities [8]. The results will show that when the temperature is as high as a few thousands eV the changes of the opacity of heavy elements caused by  $E2$  transitions cannot be neglected.

The influence of the environment on the atom is assumed to have spherical symmetry in average. The movement of an electron under the interactions of nucleus and other electrons is approximated by a central field, which is determined with the standard self-consistent calculation. In the central field, the radial part of the Dirac equation has the form

$$\begin{aligned} \frac{dP_{n\kappa}(r)}{dr} + \frac{\kappa}{r}P_{n\kappa}(r) &= \frac{1}{c}[\epsilon_{n\kappa} + c^2 - V(r)]Q_{n\kappa}(r), \\ \frac{dQ_{n\kappa}(r)}{dr} - \frac{\kappa}{r}Q_{n\kappa}(r) &= -\frac{1}{c}[\epsilon_{n\kappa} - c^2 - V(r)]P_{n\kappa}(r). \end{aligned} \quad (1)$$

In the self-consistent potential  $V(r)$ , the static part is calculated from the charge distributions in the atom, and the exchange and correlation parts are approximated by Dharma-wardana and Taylor's [9] forms. For bound states, we have the boundary conditions satisfied by the radial wave functions

$$\begin{aligned} P_{n\kappa}(r) &\sim ar^{l+1}, \\ P_{n\kappa}(R_b) &= 0, \end{aligned} \quad (2)$$

where  $R_b$  is the radius of the atom sphere. The bound electron density is obtained according to

$$\rho_b(r) = \frac{1}{4\pi r^2} \sum_j b_j [P_j^2(r) + Q_j^2(r)] \quad (3)$$

where  $b_j$  is the occupation number of the state  $j$ . In average-atom model, the occupation number  $b_j$  is determined by the Fermi-Dirac distribution

$$b_j = \frac{2|\kappa_j|}{\exp[(\epsilon_j - \mu)/T] + 1}. \quad (4)$$

The free electron is considered much more simply with an assumption of the Thomas-Fermi treatment, and the local free electron density is calculated with a Fermi-Dirac distribution of the local free electrons in the plane wave momentum  $k$  space, which can be written as

$$\rho_f(r) = \frac{1}{\pi^2} \int_{k_0(r)}^{\infty} \frac{k^2 dk}{e^{[\sqrt{k^2 c^2 + c^4 - c^2 - V(r) - \mu}/T] + 1}}, \quad (5)$$

where  $k_0(r) = [2V(r)c^2 + V(r)^2]^{1/2}/c$  and  $\mu$  is the so-called chemical potential. The total electron density is the sum of  $\rho_b(r)$  and  $\rho_f(r)$ ,

$$\rho_i(r) = \rho_b^i(r) + \rho_f^i(r). \quad (6)$$

The chemical potential  $\mu$  is determined so that the electrical neutrality is satisfied

$$\sum_i n_i \int_0^{R_b^i} 4\pi r^2 \rho_i(r) dr = \sum_i n_i Z_i, \quad (7)$$

where  $n_i$  is the number of the  $i$ th kind of atom and  $Z_i$  the nuclear charge. The summation runs over all kinds of atoms. In hot and dense plasmas, the size effects on the electronic structures of atoms and ions are considerable. For pure matter the average atomic size is taken to be

$$R_b = \left( \frac{3\Omega_0}{4\pi} \right)^{1/3}, \quad (8)$$

where  $\Omega_0$  is the average atomic volume. For the mixtures, a self-consistent approach was proposed to calculate the size of the atomic sphere for each kind of elements [10].

Contributions to the opacity consists of four parts

$$K_\nu = \frac{N_A}{A} [\sigma^{bb}(h\nu) + \sigma^{bf}(h\nu) + \sigma^{ff}(h\nu)] \times \left[ 1 - \exp\left(-\frac{h\nu}{k_B T}\right) \right] + K_{sc}, \quad (9)$$

where  $N_A$  is the Avogadro constant,  $A$  is the atomic weight, and  $k_B$  is the Boltzmann constant. The contributions of the bound-bound,  $\sigma^{bb}(h\nu)$ , and bound-free,  $\sigma^{bf}(h\nu)$ , transitions take both  $E1$  and  $E2$  terms. The free-free,  $\sigma^{ff}(h\nu)$ , contribution takes Kramers' [11] hydrogen like approximation. The scattering term,  $K_{sc}$ , is approximated by using Thompson scattering cross section. The detailed forms of these contributions for  $E1$  terms can be found elsewhere [12–14]. For  $E2$  transitions, we take the forms as

$$\sigma_{E2}^{bb}(h\nu) = \frac{2\pi^2}{c} \sum_{i,f} (2j_i + 1) p_i (1 - p_f) f_{i-f}(h\nu) \phi_{i-f}(h\nu) \quad (10)$$

and

$$f_{i-f}(h\nu) = \frac{1}{30c^2} (\epsilon_f - \epsilon_i)^3 [j_f][l_i, l_f] \times \left\{ \begin{matrix} l_i & \frac{1}{2} & j_i \\ j_f & 2 & l_f \end{matrix} \right\}^2 \begin{pmatrix} l_i & 2 & l_f \\ 0 & 0 & 0 \end{pmatrix}^2 \times \left\{ \int_0^{R_b} [P_i(r)P_f(r) + Q_i(r)Q_f(r)] r^2 dr \right\}^2 \quad (11)$$

for the bound-bound transitions and

$$\sigma_{E2}^{bf}(h\nu) = \frac{2\pi^2}{c} \sum_i (2j_i + 1) p_i \frac{df_{i-\epsilon}(h\nu)}{d(h\nu)} \quad (12)$$

and

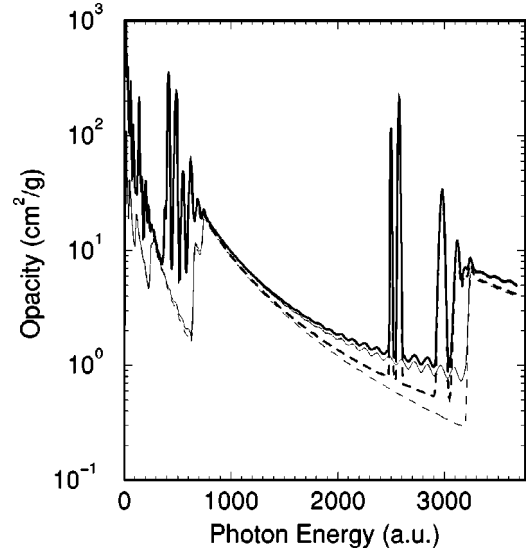


FIG. 1. The frequency dependent opacity of Au at 96.405 g/cm<sup>3</sup> and 5000 eV. The thick solid and dashed lines refer to the total opacities with and without the  $E2$  contribution, respectively; the thin solid and dashed lines refer to the bound-free opacities with and without the  $E2$  contribution, respectively.

$$\frac{df_{i-\epsilon}(h\nu)}{d(h\nu)} = \frac{1}{30c^2} (h\nu)^3 \sum_{l_\epsilon, j_\epsilon} [j_\epsilon][l_i, l_\epsilon] \times \left\{ \begin{matrix} l_i & \frac{1}{2} & j_i \\ j_\epsilon & 2 & l_\epsilon \end{matrix} \right\}^2 \begin{pmatrix} l_i & 2 & l_\epsilon \\ 0 & 0 & 0 \end{pmatrix}^2 \times \left\{ \int_0^{R_b} [P_i(r)P_\epsilon(r) + Q_i(r)Q_\epsilon(r)] r^2 dr \right\}^2 \quad (13)$$

for the bound-free transitions. In the above equations,  $l$  and  $j$  are, respectively, orbital and total angular momentum quantum numbers for the initial and final spin orbitals,  $p$  is the occupation probability, and  $\phi_{i-f}(h\nu)$  is the line profile for bound-bound transitions [13].

As an example, the influence of the  $E2$  transitions on the opacity of Au for different densities and temperatures is presented via the frequency dependent as well as the Rosseland mean opacities. In Fig. 1, the frequency dependent opacity of Au with a temperature of 5000 eV and a density of 96.405 g/cm<sup>3</sup> is plotted to show the difference with and without the  $E2$  terms. In the figure two sets of data are shown: one is the total opacity and the other one is the bound-free opacity. In Fig. 1, the bound-free processes determine the general photon energy dependent background of the absorptions and affect the Rosseland mean opacity significantly. One can find that the difference caused by the  $E2$  terms in both the total and the bound-free part of the opacity increases monotonously with the increase of the photon energy. This feature is easy to understand as the  $E1$  transition cross section contains a linear term of the photon energy while the  $E2$  contains a term of third power of the photon energy. The Rosseland mean opacities of with and without

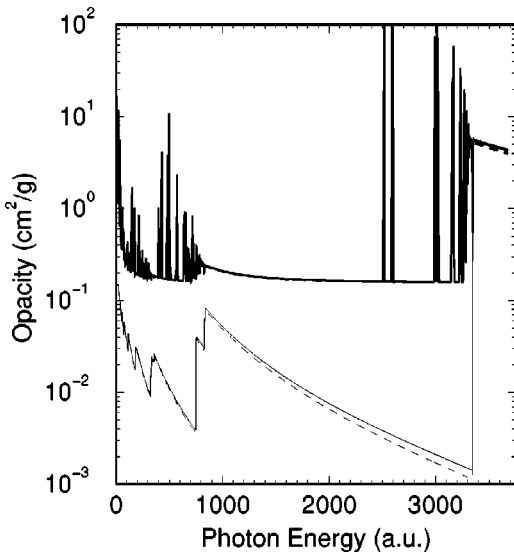


FIG. 2. The same as in Fig. 1 but for Au at  $0.19281 \text{ g/cm}^3$  and  $5000 \text{ eV}$ . However, one has to note that the thick solid and dashed lines are so close to each other that they cannot be resolved.

the  $E2$  contribution presented in Fig. 1 are, respectively,  $8.51$  and  $7.30 \text{ g/cm}^2$  corresponding to a relative difference of  $17\%$ . From Fig. 1, one can also find that up to  $E2$  terms the photoionization cross sections for high energies are far from converged results, which is beyond the present discussion.

In Fig. 1, one can find some weak wiggles in the bound-free absorption with the  $E2$  transitions when the photon energy goes higher and higher. These kinds of wiggles arise from the environmental effect on the photoionization cross sections. Due to the screening of the free electrons, the wave functions of the bound states of an ion in hot and dense matter shift slightly away from the nucleus relative to the wave functions of the free ion. Although the very weak long tail of the wave functions is cutoff by the applied boundary condition for the bound orbitals, the major part of the orbitals extend over a larger space region than the free ion orbitals. The combination of the outward shift of the major part and the cutoff of the very weak long tail of the orbital makes the photoionization transition matrix element oscillating slightly with the photon energy. As the transition matrix of the  $E1$  photoionization contains a factor of  $r$  while the transition matrix of the  $E2$  photoionization contains a factor of  $r^2$ , this kind of oscillation is more strong for the  $E2$  photoionizations. Environmental modifications to the photoionization cross section were predicted by someone for an atom embedded in a cluster [15] due to a different mechanism.

In Fig. 2, the frequency dependent opacity of Au with a temperature of  $5000 \text{ eV}$  and a much lower density of  $0.192810 \text{ g/cm}^3$  is presented to show a quite different situation where the  $E2$  contribution seems not as significant as in the case we presented in Fig. 1. As we did in Fig. 1, both the total and the bound-free part of the opacity are displayed to find the reason why the influence of the  $E2$  transitions is so weak when the density is low even though the temperature is still quite high. The average ionization degree depends on both temperature and density. The loss of the bound electrons is mainly caused by the thermal collisions between the par-

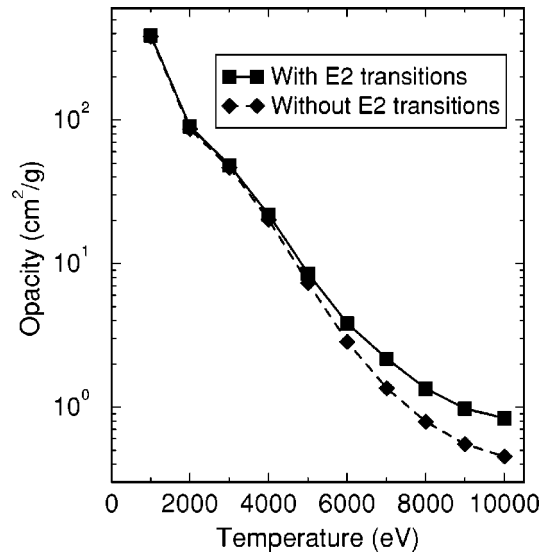


FIG. 3. The temperature dependence of the  $E2$  influence on the Rosseland mean opacity of Au with a density of  $96.405 \text{ g/cm}^3$ .

ticles (ions, electrons, and photons) in the plasma and is enhanced with the increasing of the temperature. The density dependence of the ionization is much more complex than the temperature. Generally with a high density of the material, the free electrons have more opportunity to attach the positive ions resulting in more electron bound. In most cases, the opacity is dominated by the bound-bound and bound-free absorption processes and, therefore, increases with the number of the bound electron and also with the increasing of the density. However, with the density going higher enough some bound orbitals will be moved to above the ionization threshold due to the size effects. This kind of so-called pressure induced ionization will reduce the number of the bound electrons resulting in the decrease of the opacity. In Figs. 1 and 2, the temperature is so high that the pressure induced ionization effect cannot be identified clearly. The average number of the bound electrons above the  $1s$  orbital is only  $0.063$  for the case in Fig. 2, which is much less than the corresponding value of  $4.949$  for the case in Fig. 1. From Fig. 2, one can find that the number of the bound electrons above  $1s$  orbital is so small that the bound-free opacity below the  $1s$  ionization threshold can only take a very insignificant role in the total opacity. For this reason, the  $E2$  transitions have little effects on both the total frequency dependent opacity and the Rosseland mean opacity, although the changes caused by the  $E2$  transitions in the bound-free opacity is apparent.

In Fig. 3, changes of the Rosseland mean opacities of Au with a density of  $96.405 \text{ g/cm}^3$  are presented along different temperatures. The Rosseland mean opacity is a weighted integration over the inverse of the spectrally resolved opacity as shown in Fig. 1. The integration is very sensitive to the positions and values of the minimum structures in the frequency dependent opacity. As we have seen in Fig. 1, in some cases the  $E2$  transitions change the bottom of the minimum structure considerably. The weight factor is a function of both photon energy and temperature and reaches its maximum value around the photon energy of about  $3.83$  times of

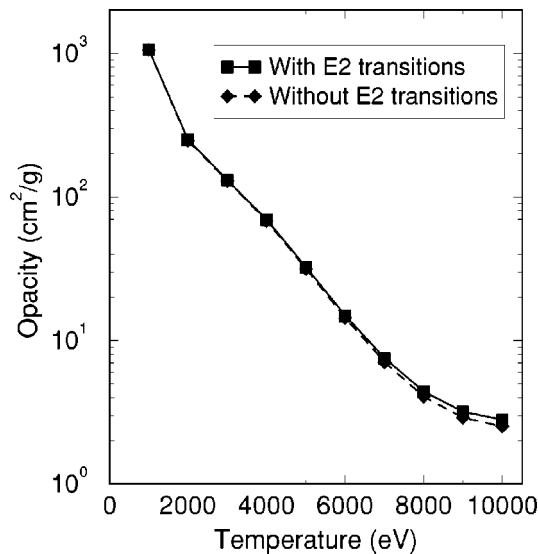


FIG. 4. The temperature dependence of the  $E2$  influence on the Planck mean opacity of Au with a density of  $96.405 \text{ g/cm}^3$ .

the temperature. Therefore, the temperature influence on the Rosseland mean opacity takes place via the frequency dependent opacity, which depends strongly on the ionization degree of the matter, as well as the average weight function. For lower temperatures, the opacities at lower photon energies take more significant actions. At the 1000 eV point in Fig. 3, as the number of the bound electrons is larger compared with other points the  $E2$  transitions should contribute more significantly to the frequency dependent opacity, however, as the weight function has its major part at lower photon energies the effects of the  $E2$  transition have not been reflected in the Rosseland mean value of the opacity for this point. The absolute changes of the Rosseland mean opacity at 1000 eV is  $6.6 \text{ cm}^2/\text{g}$  corresponding to a relative difference of only 1.7%, while for 10000 eV the absolute and relative changes are, respectively,  $0.38 \text{ cm}^2/\text{g}$  and 85%.

In Fig. 4, changes of the Planck mean opacities of Au

with a density of  $96.405 \text{ g/cm}^3$  are presented along different temperatures. The Planck mean opacity is a linear weighted average of the spectrally resolved opacity. The weight factor is also a function of both photon energy and temperature and reaches its maximum value around the photon energy of about 2.94 times of the temperature. As a linear weighted average, the Planck mean opacity is dominated by the positions and magnitudes of the maximum peaks, which are mainly related to the bound-bound transitions and near threshold photoionization structures. From the frequency dependent opacity in Figs. 1 and 2, we know that for these kinds of maximum structures the influences of the  $E2$  transitions are far from significant resulting in much less changes in the Planck mean opacity compared with the changes in the Rosseland mean opacity we have seen in Fig. 3. The largest relative changes in Fig. 4 is 11% observed at 10000 eV much less than the 85% of the corresponding Rosseland mean data.

In conclusion, a simple self-consistent field average-atom approach is used to show that for hot and dense plasmas of heavy elements when the temperature is above a few thousands of eV, the contributions by the  $E2$  transitions to the opacity can reach as large as a few tens of percent depending on the temperature and density. Combining with the so-called environmental influences, the cross section of the  $E2$  transition could be modified considerably. The results also indicate that contributions from the higher orders above the  $E2$  term must also be included in order to arrive to converged numerical results. The present treatment for the environmental effects takes the screening effect of the free electrons into account, and is however far from satisfactory for the boundary conditions of the electron wave functions.

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