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Scattering of X-ray emission lines by a hydrogen molecule

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ABSTRACT

As discussed by Sunyaev & Churazov (1996) and Vainshtein, Sunyaev & Churazov (1998) it is in principle possible to use distortions in the X–ray lines profiles after scattering by hydrogen and helium atoms to measure helium abundance in astrophysical objects. We briefly discuss below the differences of scattering X–ray photons by a hydrogen atom and a hydrogen molecule. The most significant and obvious difference is the enhanced elastic scattering cross section (by a factor of 2 per electron) for a hydrogen molecule. It is suggested that as a first approximation, reasonable for astrophysical conditions of interest, one can use known simple analytical expressions for a hydrogen atom (multiplying the elastic differential cross section by a factor of 2) when describing scattering by a hydrogen molecule.

1. Introduction

Progress in experimental X-ray astronomy and in particular in the energy resolution of the spectrometers made it possible to consider the use of weak spectral features for diagnostic of the chemical composition and ionization state of matter in the astrophysical objects. The energy resolution of the order of electron–volts is anticipated for two large X–ray missions – Constellation (White, Tananbaum & Kahn, 1997) and XEUS (Turner et al., 1997). As discussed by Sunyaev & Churazov (1996) and Vainshtein, Sunyaev & Churazov (1998) it might be possible to observe specific distortions in the X–ray lines profiles after scattering by hydrogen and helium atoms and to measure helium abundance in astrophysical objects using high resolution X–ray spectroscopy. Among the potential applications of this method are giant molecular clouds in the Galactic Center regions, distant AGNs and QSOs, surfaces of cold flaring star and our Sun. Practical application of this method demands very high energy resolution and very high sensitivity of the instruments.

One of the principle applications of interest is the determination of the helium abundance in the molecular clouds in the Galactic Center region. Forthcoming missions should be able to detect at high significance level and resolve a recoil spectra[1] formed due to the scattering of the X–ray emission lines by the matter of the molecular clouds. Scattering by a hydrogen atom (in the astrophysical context) was discussed in Sunyaev & Churazov (1996). Vainshtein, Sunyaev & Churazov (1998) made simple estimates for the scattering by a helium atom. It was shown that "recoil spectra" for hydrogen and helium atoms differ strongly enough to hope that this difference might be detected by future missions.

Most of the hydrogen in the clouds is in the form of molecules. It is therefore important to compare "recoil spectra" after scattering by hydrogen atoms, hydrogen molecules and helium atoms. Simple estimates given below show that for typical astrophysical application one need not use complex quantum mechanical calculations for a hydrogen molecule, but analytical formulae for scattering by a hydrogen atom with simple modification of the elastic scattering cross section. Of course the recoil spectra due to a hydrogen atom and molecule are different, but this difference is small compared to that due to the scattering by a helium atom.

The process of scattering of X–rays by atoms and molecules is well known and was studied in detail (see e.g. Heitler, 1960, Eisenberger & Platzman, 1970). Below we consider scattering by a hydrogen molecule from a point of view particularly relevant to the discussed astrophysical problems. Similar simplified consideration of the scattering by hydrogen and helium atoms is given in Sunyaev & Churazov (1996) and Vainshtein, Sunyaev & Churazov (1998).

We consider energies of the photons below ∼9 keV, since there are no bright X–ray emission lines above this energy in typical astrophysical conditions. In the discussion below we assume the initial energy of the photon of 6–7 keV unless stated otherwise.

2. Simple estimates

As is known, the differential cross section of the X–ray photon scattering by a light atom is defined by the following expression:

$$\frac{d\sigma}{d\Omega dh\nu_2} = 0.5r_e^2(1+cos^2\theta)\frac{\nu_2}{\nu_1}|\langle f|\sum_j e^{i\vec{q}\vec{r_j}}|i\rangle|^2 \times \delta(\Delta E_{if} - h\Delta\nu) \qquad (1)$$

[1]The term "recoil spectrum" is used since for free electron at rest change of photon energy during the scattering is caused by the recoil effect.

where i and f denote initial and final states of the system, $\vec{q} = (\vec{k_1} - \vec{k_2})$, $\vec{k_1}$ and $\vec{k_2}$ are the initial and final momenta of the photon, ν_1 and ν_2 are the initial and final frequencies of the photon, ΔE_{if} is the change of energy of the atom or molecule, r_j is the coordinate of the j-th electron. We adopt below atomic units for q and r. Depending on the final state of the electron after scattering[2] the process of scattering is usually called as

- Rayleigh scattering ($f \equiv i$) – elastic scattering
- Raman scattering (f corresponds to one of the exited discrete states)
- Compton scattering (f corresponds to the continuum state, i.e. photon ionizes atom or molecule)

Since the process is essentially the same for each of the above channels, this division is purely artificial. Frequently the last two channels are called inelastic scattering, since the scattering changes the energy of the photon.

As discussed below the largest change (when we switch from a hydrogen atom to a hydrogen molecule) occurs for Rayleigh (elastic) scattering due to coherent scattering by two electrons. The other two processes (Raman and Compton) lead to the rather similar distortions both for a hydrogen atom and a molecule. All three processes are discussed below in more detail.

2.1. Rayleigh

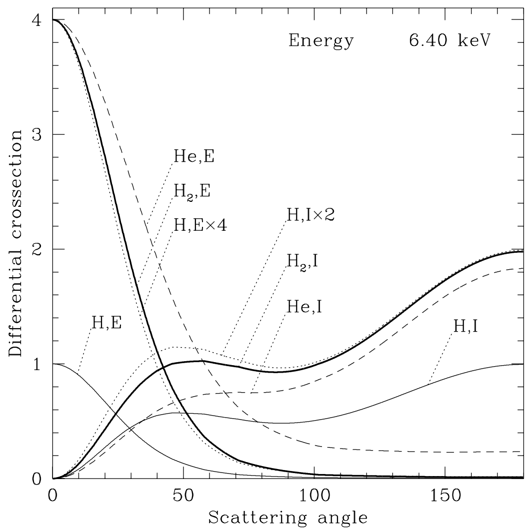
Rayleigh scattering is not accompanied by the change of the photon energy or the state of the atom or molecule. Only the direction of the photon changes. In the presence of several electrons in the atom or molecule they can coherently scatter the photon. As a result elastic scattering by zero angle will be proportional to N^2 (see equation (1)), where N is the total number of electrons in the atom or molecule. As is clear from eq. (1) the range of angles for which Rayleigh scattering is a dominant process is defined by the condition that the value $\vec{q}\vec{r_j}$ is small. For small scattering angles θ this condition can be rewritten as $\theta 2\pi \frac{R}{\lambda} \ll 1$, where λ is a wavelength of the photon and R is the characteristic size of the electron wave function. For the hydrogen atom the characteristic size $\sim a_0 \sim 0.5$Å and the photon wavelength $\lambda \approx 2$Å (for the 6.4 keV photon) are comparable resulting in appreciable Rayleigh scattering up to 30–50 degrees. For the helium atom the characteristic size of

[2] we assume that the initial state i is a ground state of the molecule

the electron distribution is smaller and as a result Rayleigh scattering dominates till larger angle and for larger photon energies. For the hydrogen molecule the characteristic size of the electrons distribution is comparable with that for the hydrogen atom. It is therefore expected that for the molecule, the major change associated with the Rayleigh scattering will be the increase of the cross section by a factor of 2 (per electron) due to the coherence effect. Shown in Fig.1a is an angular dependence of the elastic (Rayleigh) and inelastic cross sections for the hydrogen atom, helium atom and hydrogen molecule. The tabulated data of Hubbell et al. 1975 were used for this plot. The differential cross sections of the elastic and inelastic scatterings were calculated by Hubbell et al. 1975 using the electron wave function of the ground state. For a hydrogen molecule Hubbell et al. 1975 used the calculations of Bentley and Stewart 1973. Shown in Fig.1b is a total cross section of the elastic and inelastic scatterings as a function of energy (again using tabulated data from Hubbell et al. 1975).

From Fig.1 it is clear that simple multiplication of the Rayleigh cross section for the hydrogen atom by a factor of 4 (factor of 2 comes from the number of electrons in the molecule and an additional factor of 2 is due to coherence effects) produces a reasonable approximation of the elastic cross section for a hydrogen molecule. The differential cross section for inelastic scattering should be multiplied by a factor of 2 and also describes reasonably well the cross section for the hydrogen molecule.

Coherent scattering causes an increase of the total scattering cross section for the electrons bound in the hydrogen molecules compared to a similar number of electrons in the hydrogen atoms. However since coherent scattering is important only for relatively small scattering angles (e.g. below $\sim$30-40 degrees for the 6–7 keV photons) this increase should not strongly affect the observed spectra. Note that the photon does not change energy during coherent scattering and therefore unscattered and elastically scattered photons will be observed at the same energy. One can however imagine specific situations (e.g. when spatial or time–related effects allow one to observe only scattered photons) when the relative amplitude of the elastic and inelastic scatterings may be used for diagnostics of astrophysical plasma. At lower energies (e.g. for the $\sim$1–4 keV photons) the increase of the cross section due to coherent scattering is more important, since even for a large scattering angles differential cross section is larger than that for a free electron (or an electron bound in a hydrogen atom). Even although the energy of the photons does not change in the elastic scattering the intensity of the scattered component increases. E.g. the continuum intensity in the well known problem of an X–ray reflection from a semi–infinite slab of neutral matter will increase by a factor of two at low energies if the hydrogen is in the molecular form.



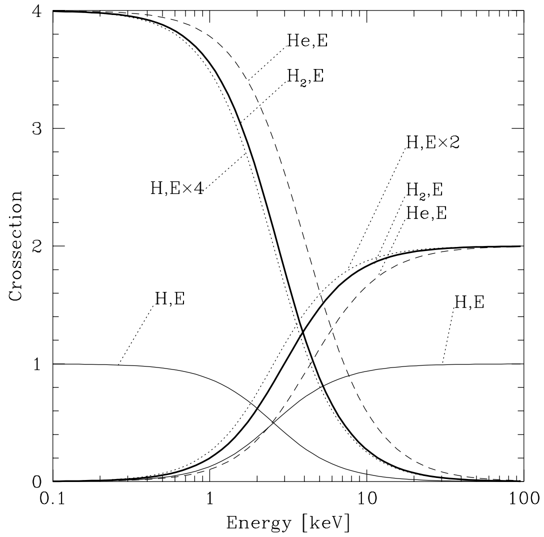


Fig. 1.— **(a)** Angular dependence of the differential cross sections (elastic and inelastic) for the hydrogen atom (thin solid line), helium atom (dashed line), hydrogen molecule (thick solid line). Symbols **"E"** and **"I"** denote elastic and inelastic scatterings respectively. The curves having maximum value at zero scattering angle and declining with angle correspond to the elastic scattering. The curves, representing inelastic scattering have zero value at zero scattering angle. Tabulated data of Hubbell et al. (1975) were used for this plot. The thin dotted line shows the elastic and inelastic curves for the hydrogen atom multiplied by a factor of 4 and 2 respectively (one factor of 2 simply accounts for two electrons per molecule; the additional factor of 2 for the elastic scattering is due to coherence effects). **(b)** The dependence of total elastic and inelastic cross sections (in units of Thomson cross section σ_T) on the energy of the photon (in the non-relativistic approximation). The notations are the same as in figure (a).

2.2. Raman

The Raman scattering is accompanied by an excitation of an atom or molecule. In the scattered spectra of the monochromatic line with an initial energy $h\nu$ the photons will be detected at the energies of $h\nu - E_i$, where E_i is an excitation energy of the $i-$th state. Since the excitation energies are specific for a given atom or molecule one can learn the chemical composition of the scattering medium by studying the scattered spectrum. This opens the possibility to distinguish helium and hydrogen and to determine helium abundance in the scattering medium. Note that energies of the features do not depend on the scattering angle. However some assumptions on the geometry of scattering are required in order to estimate relative fractions of the helium and hydrogen in the gas, since the probability of an excitation of a given level depends on the scattering angle. The principle feature is associated with the first excited level of the hydrogen and helium atoms, since it has the largest separation from the ground level. For atomic hydrogen these are the $2s$ and $2p$ levels with an excitation energy of $\sim$10.2 eV. Levels with higher principle quantum numbers all have close excitation energies ($E_i \sim$ 12.1–13.6 eV). As a result a gap ($\sim$10.2 eV wide) between the unshifted line (corresponding to the elastic scattering) and the first Raman satellite is formed. For a helium atom this gap (corresponding to excitation of $n = 2$ level) is $\sim$20 eV, i.e. twice as large. For a hydrogen molecule the lowest electron states, which can be excited during the scattering, have an excitation energy of $\sim$11–12 eV i.e. comparable with the gap for a hydrogen atom. The most important question is whether this $\sim$11-12 eV gap will be filled due to excitation of the vibrational and rotational states of the ground electron state of the molecule (see Fig.2a).

Therefore we should estimate the probability that the vibrational and rotational states of the ground electron term of a hydrogen molecule will be excited during the scattering. Taking for simplicity para–hydrogen (i.e. total nuclear spin is zero) we have to consider only the levels with even rotational numbers $J = 0, 2, 4, ...$ As is known vibrational levels in the ground state of the hydrogen molecule are separated by $\Delta E_v \sim 0.5$ eV while the two lowest rotational levels ($J = 0$ and $J = 2$) are separated by $\Delta E_r \sim 4.3 \times 10^{-2}$ eV ($E_J \sim 0.00736 J(J+1)$ eV). For the calculation of the matrix element of $e^{iqr_1} + e^{iqr_2}$ (see expression (1)), where r_1 and r_2 are the radius vectors of two electrons, the wave function of the molecule was written in the simplest Heitler-London's form:

$$F(R, r_1, r_2, \theta, \phi) = A\left[\psi(r_{1A}, R)\psi(r_{2B}, R) + \psi(r_{2A}, R)\psi(r_{1B}, R)\right]\Phi(R, v)Y_{JM}(\theta, \phi) \qquad (2)$$

where R is an internuclear distance, $r_{1(A,B)} = r_1 \pm R/2$, $r_{2(A,B)} = r_2 \pm R/2$ – radius vectors of two electrons with respect to the nuclei A and B, ψ – is Sleter's 1S function, $\Phi(R, v)$ describes the vibrational wave function with the vibrational number v, $Y_{JM}(\theta, \phi)$ – is a spherical harmonic, θ and ϕ are the angles in the spherical coordinate system with the z axis along the vector q, A – normalization coefficient. For $\Phi(R, v)$ we used the Kratzer potential (see e.g. Simons 1974).

For simple estimates of the expression $X =< F_2|e^{iqr_1} + e^{iqr_2}|F_1 >$ let us first retain only one–center matrix elements dropping "exchange"–type integrals (containing products like $\psi(r_{1A}, R) \times \psi^*(r_{1B}, R)$). The expression then reduces to a simple factorised form:

$$X \approx < \psi|e^{iqr}|\psi >< v_2 J_2 M_2|e^{iqR/2} + e^{-iqR/2}|v_1 J_1 M_1 > \qquad (3)$$

The first term is simply the elastic scattering by a hydrogen-like atom and the second term describes transitions between vibrational and rotational states of the molecule. Typical change of the rotational number should be simply related to the change of the photon momentum and corresponding gain of the molecule angular momentum: $\Delta J \sim q * R_e/2$, where R_e is the equilibrium internuclear distance. Since in atomic units $q \leq 3$ (for the scattering of a ~ 6 keV photon by 180°) and $R_e \sim 1.4$ then $\Delta J \leq 2$. And even for $J = 6$ the excitation energy is only 0.3 eV. Thus it is clear that excitation of the rotational levels of the ground state of the molecule should not strongly change the appearance of the scattered spectrum. The excitation of the vibrational levels (and their rotational substructure) also expected to be small for the considered range of q ($q < 2 - 3$). Indeed, from the second multiplicative term in the right hand side of equation (3) one can estimate that the probability of excitation of the first vibrational level ($v_1 = 0$, $v_2 = 1$) without change of the molecule angular momentum ($J_1 = J_2 = 0$) is proporional to the factor $\sim Aq^4 R_e^2/q_0^2 \ll 1$, where $q_0 = \sqrt{m_p/2E_v} \approx 4.1$ ($E_v \sim 0.5$ eV, m_p – proton mass), and A is a numeric coefficient of ~ 0.0139 (for $q < 2$). Account for rotational substructure and higher vibrational levels should not strongly affect this result.

Similar conclusions can be reached explicitly calculating the matrix element X and retaining all terms. Shown in Fig.2a are the values of $|X|^2$ as a function of q for the excitation of different vibrational and rotational levels of the hydrogen molecule ground state. The thick lines correspond to the hydrogen molecule (the solid line – true elastic scattering without change of rotational or vibrational numbers; the dash–dotted line – excitation of the rotational levels of the ground state without change of the vibrational level; the dashed line – excitation of the vibrational levels). For comparison the thin lines show the same matrix element for the elastic scattering by the hydrogen atom (solid line, multiplied by a factor of 4 for comparison with a molecule) and for the excitation of the $n = 2$ level in the hydrogen atom (dotted line, multiplied by 2). One can see that as long as we are not interested in the weak sub–eV features in the scattered spectra it is possible to neglect completely the excitation of the rotational and vibrational levels of the ground state of the molecule.

2.3. Compton

Compton scattering by an atom or molecule is accompanied by an ionization of the electron. If the energy transmitted to the electron is sufficiently larger than the binding energy of the electron, then the so–called "impulse approximation" is applicable (see e.g. Eisenberger & Platzman, 1970). For the free electron at rest scattering by a given angle corresponds to some definite change of energy (recoil effect). For bound electrons additional broadening of the photon energy takes place. This broadening is connected with the Doppler effect due to the motion of the electron in an atom or molecule. The width of the peak (corresponding to the Compton scattering by a give angle) is therefore solely determined by the distribution of the electron momentum in an atom or molecule. The momentum distributions are comparable for the hydrogen atom and molecule, but it is obviously broader (due to the larger binding energy) for helium. This is demonstrated in Fig.3. Shown in this figure are the expected profiles of the monochromatic 6.4 keV line after Compton scattering (by 180 degrees) by the hydrogen atom, hydrogen molecule and the helium atom. For the hydrogen and helium atom the tables of Briggs et al. 1975 were used. For the hydrogen molecule experimental results of Eisenberger 1970 were used (see also Smith et al. 1977 for accurate theoretical calculations of the Compton profile for the hydrogen molecule). Since in practice observed spectra contain contributions of various scattering angles it is difficult to use the shape of the Compton profiles for distinguishing contributions of various species in the scattered spectra. We just note here that the difference between the hydrogen molecule and the hydrogen atom is much smaller compared to the helium atom.

In principle the molecule need not initially be in a ground state. In the molecular clouds typical temperatures are below ∼100 K (i.e. ∼0.01 eV) and even if the rotational levels are populated according to this temperature it will not affect the scattered spectrum. Thermal motion of the atoms or molecules (in the molecular clouds) also has a negligible effect on the spectra since typical atom velocity at a temperature of 100 K is only $\sim 1\ km\ s^{-1}$. Turbulent motion with velocities of the order of 40 $km\ s^{-1}$ would cause smoothing of the spectral features on the scale of ∼1 eV (for 6 keV photons).

3. Conclusions

It is shown that all basic features of the X–ray photons scattering by a hydrogen molecule resemble those for a hydrogen atom. The only apparent difference is an increased cross section of the elastic scattering in the molecule (due to coherence effects), which can be reasonably well accounted for by multiplying the differential cross section of the elastic scattering for a hydrogen atom by a factor of 4 (or 2 per electron). In particular the continuum intensity in the well known problem of the X–ray reflection from a semi–infinite slab of neutral matter will increase by a factor of two at low energies (below ∼4 keV) if the hydrogen is in the molecular form. The "energy gap" between the unshifted line and the first important Raman satellite is 10 and ∼11–12 eV for a hydrogen atom and a molecule respectively. This contrasts with the 20 eV gap for the helium atom. The contribution of rotational and vibrational levels of the molecule is not sufficient to fill this gap with scattered photons. Compton scattering both for a hydrogen atom and a molecule causes similar broadening. Therefore (i) one can use simple analytical results for a hydrogen atom when describing the scattering of X–ray photons by a hydrogen molecule and (ii) the possibility to identify spectral features due to the scattering by a helium atom does not depend on whether the hydrogen is in atomic or molecular form.

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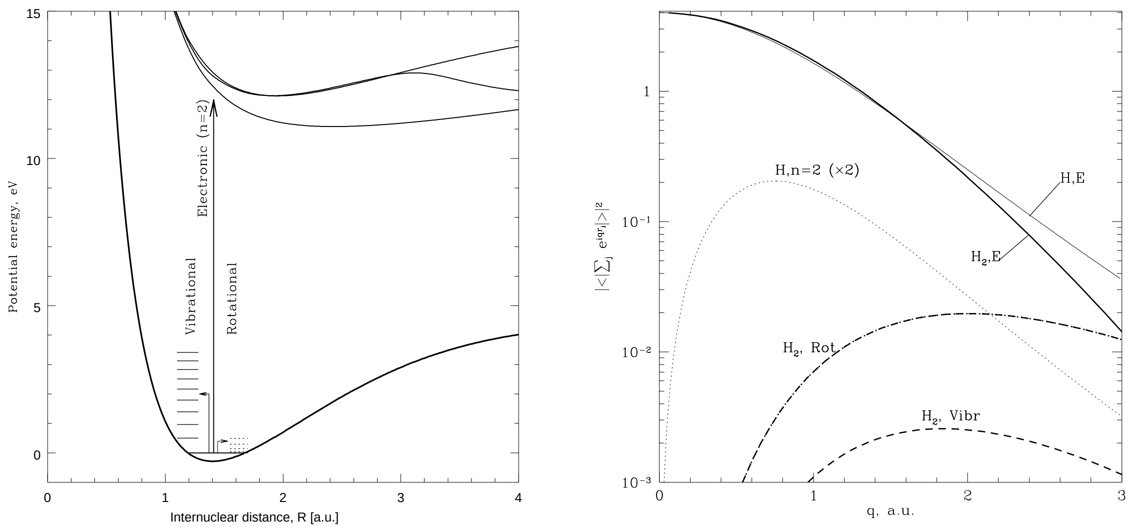

Fig. 2.— **(a)** Schematic structure of the energy levels of the hydrogen molecule. The thick line show the potential curves for ground state and singlet states with one electron excited to the $n = 2$ level. A few lowest vibrational levels are shown with thin solid horizontal lines. A few lowest rotational levels of the ground state are shown with dotted horizontal lines. Three arrows schematically show excitation of the electron states, vibrational and rotational levels. **(b)** The square of the matrix element $|X|^2 = | < | \sum_j e^{i\vec{q}\vec{r}_j} | > |^2$ as a function of q for the excitation of vibrational and rotational levels of the ground electronic term of the hydrogen molecule. The thick lines correspond to the hydrogen molecule (the solid line – true elastic scattering without change of rotational or vibrational numbers; the dash–dotted line – excitation of the rotational levels without change of the vibrational level; the dashed line – excitation of the vibrational levels). For comparison the thin lines show $|X|^2$ for elastic scattering in the hydrogen atom (the solid line, multiplied by a factor of 4 for comparison with a molecule) and $|X|^2$ for excitation of the $n = 2$ level in the hydrogen atom (the dotted line, multiplied by 2).

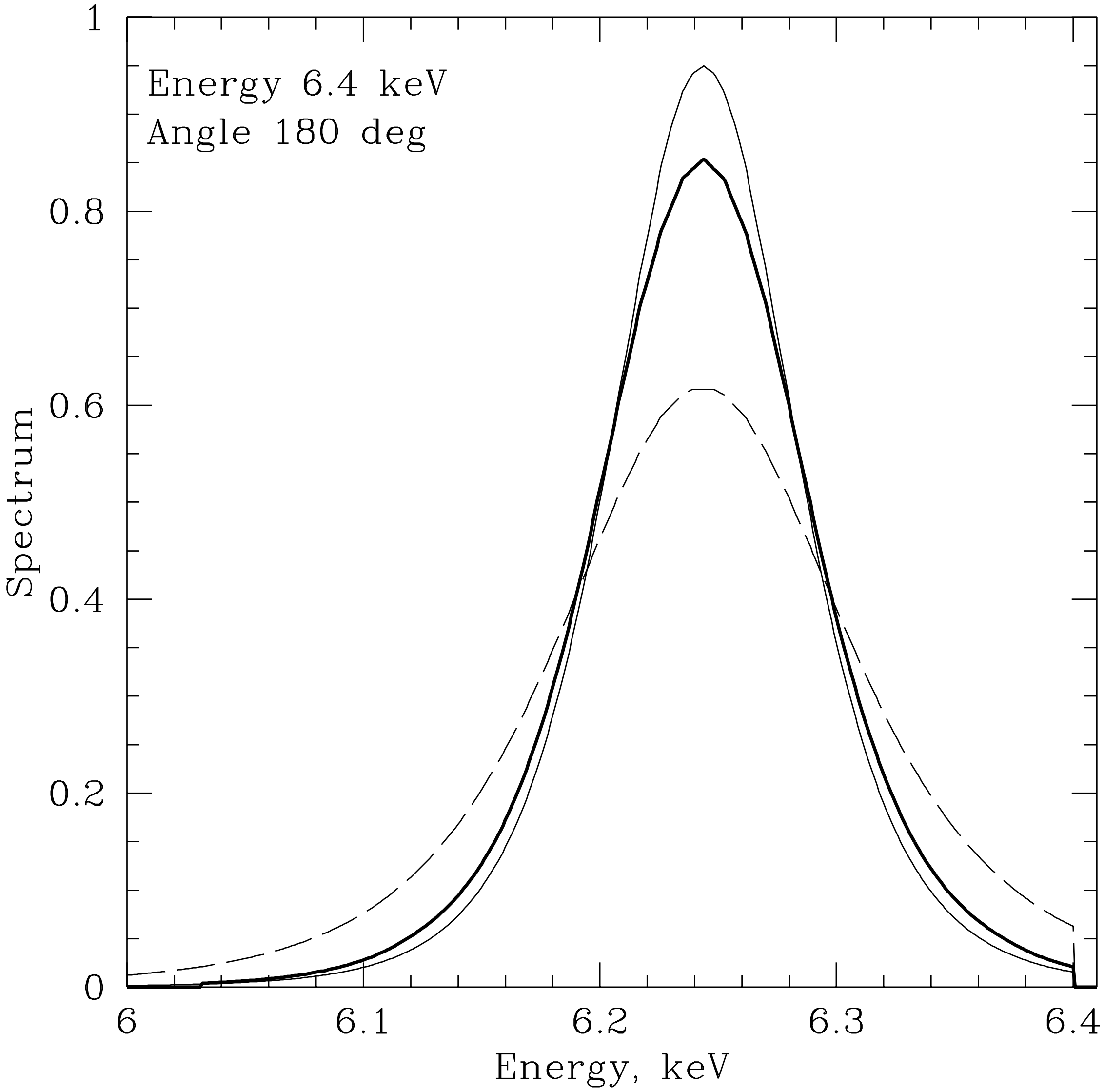

Fig. 3.— Comparison of the spectra of the 6.4 keV line scattered (by 180 degrees) by a hydrogen atom (thin solid line), hydrogen molecule (thick solid line) and helium atom (dashed line) in an "impulse approximation". The data from Briggs et al., 1975 and Eisenberger 1970 were used. See also Smith et al. 1977 for more accurate calculations of the Compton profile for a hydrogen molecule.

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