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Energy dependence of the density of the generalized oscillator strength of atomic hydrogen

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The density of the generalized oscillator strength per unit energy range of excitation for transitions from the ground state to the continuum of atomic hydrogen is computed beyond the plane-wave Born approximation. We use the Coulomb-Born approximation to compute the density for a variety of energy transfers and impact energies as a function of the momentum transfer. Our results show that the density approaches the standard plane-wave Born approximation and depends only upon the momentum transfer at impact energies as low as 50 eV.

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The study of inelastic collisions of electrons with matter is of basic importance, mainly due to its relevance to such diverse fields as plasma physics, atmospheric physics, astrophysics, and electron microscopy [1]. Electron-impact ionization of atomic hydrogen plays an important role among these inelastic collisions for two reasons. On the one hand, the process involves the simultaneous escape of two electrons in the Coulomb field of the ion, thus its description is a focal point in the understanding of the fundamental problem of few particles interacting via Coulomb forces. On the other hand, electron-impact ionization of hydrogen tests basic concepts, since it contains the dynamics inherent in the ionization of a single electron, without the complications of multi-electron atoms.

The generalized oscillator strength (GOS) is the key quantity for characterizing the response of matter to the transient field of charged particles. An important characteristic of the generalized oscillator strength is the fact that, in the plane-wave Born approximation (PBA), it depends only upon the energy transfer and the momentum transfer of the projectile, and not on the impact energy. For most of the fields cited above, this is a very important property, since they require the GOS over wide ranges of parameters. Much is known about the GOS in PBA [1]. For transitions to bound states, calculations that go beyond PBA are also available [1]. However, it is recognized that the main fraction of the GOS density lies in the continuum, and no systematic calculations that go beyond PBA are available. Inokuti [1] recognized that a necessary, though not sufficient, condition for the validity of the Born approximation was that the measured generalized oscillator strength was independent of the impact kinetic energy. In this Brief Report we present the first calculation of generalized oscillator strengths for transitions to the continuum of atomic hydrogen beyond PBA. We use the Coulomb-Born approximation (CBA) [2,3] to compute the triple-differential cross section (TDCS) and then integrate numerically over the solid angle of the ejected electron. We compute the density of the generalized oscillator strength at different impact energies for different energy transfers as a function of the momentum transfer. We find that, as expected, the density depends strongly upon the impact energy at energies close to the energy transfer, where the PBA is known to be invalid, and, unexpectedly, that it becomes nearly independent of energy at energies as low as 50 eV for an energy transfer of $E=27.2$ eV, especially at the intermediate range of momentum transfer.

It is well known that the PBA does not give the correct angular distribution of the triple-differential cross section [4–6] for electron-impact ionization, the so-called $(e,2e)$ cross sections. Several theories have been used to improve the understanding of $(e,2e)$ cross sections beyond PBA, including different distorted-wave theories [2,3,7–9], second Born theories [10], and theories employing correlated three-body continuum wave functions [11], but none of these has been employed to compute the density of the generalized oscillator strength. The CBA used here was shown to give accurate $(e,2e)$ cross sections for He [2], inner shells of carbon [3], and atomic hydrogen [12]. In the next paragraphs, we review briefly the theory for the specific case of electron-impact ionization of hydrogen. Details of the derivation may be found in Refs. [2,3,12]. Atomic units are used throughout unless otherwise stated.

We use a perturbation theory [2] in which the ionization process is treated as an electron-electron collision in the Coulomb field of the proton, by using an expansion of the Coulomb T matrix in powers of the electron-electron interaction [2,3]. In first order, the CBA transition matrix element corresponding to ionization of a hydrogen atom by an electron is given by

$$T_{fi}^{(1)}=\langle \psi_{\mathbf{K}_f}^{-}(\mathbf{r}_2)\psi_{\mathbf{k}}^{-}(\mathbf{r}_1)|V_{\rm int}|\psi_{\mathbf{K}_i}^{+}(\mathbf{r}_2)\varphi_i(\mathbf{r}_1)\rangle \ , \tag{1}$$

projectile with the target ion,

$$V_{\rm int}=-\frac{1}{r_2}+\frac{1}{r_{12}} \ , \tag{2}$$

with $r_{1(2)}$ the coordinate of the bound (projectile) electron, $r_{12}=1/|r_1-r_2|$, $\varphi_i(\mathbf{r}_1)$ the initial target eigenstate, and $\psi_{\mathbf{k}}^{\pm}(\mathbf{r})$ are Coulomb waves, normalized per unit momentum, in the attractive potential of the proton [13]. The term $-1/r_2$ of Eq. (2) does not contribute to $T_{fi}^{(1)}$ due to the orthogonality of $\psi_{\mathbf{k}}^{-}$ and φ_i.

The TDCS corresponding to ejection of the bound electron with momentum $\mathbf{k}$ into the solid angle $d\Omega_k$, and to scattering of the incident electron in the direction (θ_f,ϕ_f) into the solid angle $d\Omega_f$ is then given by

$$\frac{d^5\sigma}{d\Omega_f d\Omega_k dE_k}=(2\pi)^4\frac{kK_f}{K_i}|T_{fi}|^2 \ . \tag{3}$$

The GOS density is then defined as

$$\frac{df}{dE}=K^2\frac{E}{2}\frac{K_i}{K_f}\int\frac{d^5\sigma}{d\Omega_f d\Omega_k dE}d\Omega_k \ , \tag{4}$$

where $E=E_i-E_f$ is the energy transfer and $\mathbf{K}=\mathbf{K}_i-\mathbf{K}_f$ is the momentum transfer. Expressions for T_{fi} of Eq. (1) are given in Refs. [2,3]. Generally, T_{fi} depends upon the incident energy E_i as well as K and E. In PBA, the GOS density is given in closed form [1] as a function of K and E,

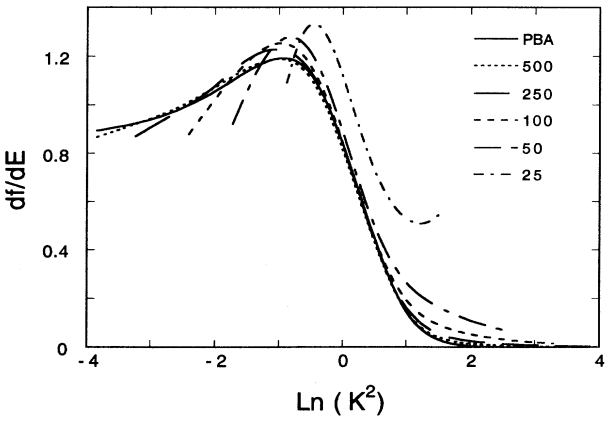

FIG. 1. GOS density per unit energy range of excitation for transitions from the ground state to the continuum for an energy transfer of 17 eV, and impact energies as shown (in eV). The full line, labeled PBA, is the plane-wave Born approximation.

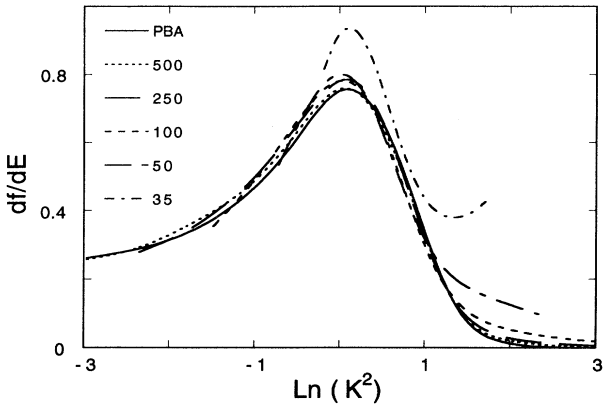

FIG. 2. As Fig. 1 but for an energy transfer of 27.2 eV.

$$\frac{df}{dE}=\frac{2^9E(K^2+2E/3)}{[(K+\sqrt{2E-1})^2+1]^3[(K-\sqrt{2E-1})^2+1]^3}\times[1-\exp(2\pi/\sqrt{2E-1})]\times\exp\left[-\frac{2}{\sqrt{2E-1}}\arctan\left[\frac{2\sqrt{2E-1}}{K^2-2E+2}\right]\right] \ . \tag{5}$$

Note that we include only the direct term in Eq. (3). We therefore refer here to a hypothetical experiment, although achievable in principle, where the incident electron has spin down (up) and the hydrogen atom has spin up (down), and only spin-down (-up) electrons are detected. The exchange term could also be obtained experimentally by detecting the spin-up (-down) electrons. In the CBA, the exchange term is obtained by interchanging $\mathbf{K}_f$ and $\mathbf{k}$ in the T-matrix element of Eq. (1). The momentum transfer is then a function of the direction Ω_k, $\mathbf{K}=\mathbf{K}(\Omega_k)$, and it has to go inside the integral in Eq. (4). The GOS is therefore not an explicit function of $\mathbf{K}$, since it is actually integrated over $\mathbf{K}$ when integrating over Ω_k. The same holds for the GOS in the PBA.

Figures 1–4 show the GOS density per unit range of

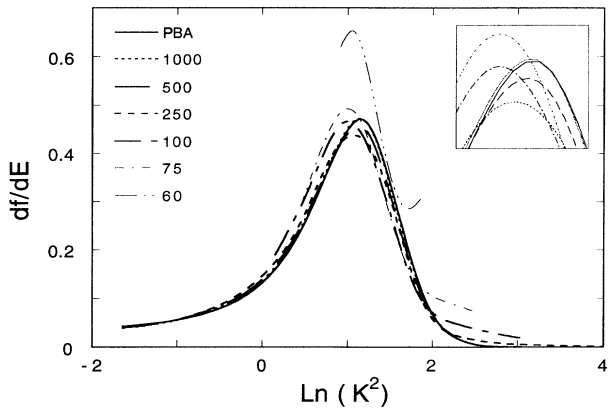

FIG. 3. As Fig. 1 but for an energy transfer of 54.4 eV. The inset shows how the PBA limit is approached by the CBA curve at high energies.

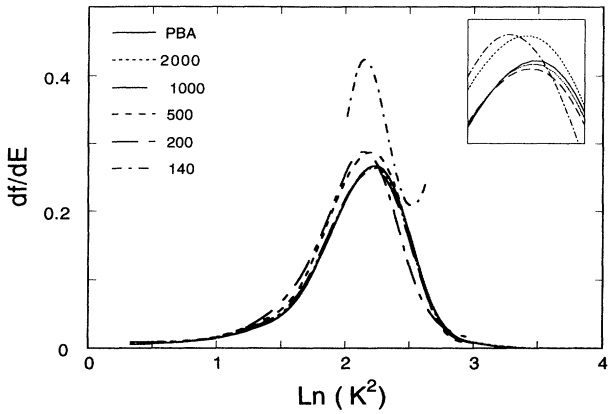

FIG. 4. As Fig. 1 but for an energy transfer of 132 eV. The inset shows how the PBA limit is reached by the CBA curve at high energies.

excitation energy as a function of the momentum transfer for different energy transfers and different impact energies for both the PBA, the full line in all figures, and the CBA. Notice that while the PBA curves are given at all K, the CBA curves always end at the minimum and at the maximum of the momentum transfer for a given impact energy and energy transfer. Figure 1 corresponds to an energy transfer of 17 eV. We see that at an impact energy of 25 eV, the density is quite different from the one given by the PBA and is strongly dependent on the impact energy. As the impact energy increases, the density approaches the PBA curve. The change of the density with impact energy is very small in the region of intermediate and large momentum transfer for $E_i > 50$ eV, while at small momentum transfer the dependence of the density on the impact energy is strong until the high-density limit, $E_i \sim 250$ eV, is reached. Figure 2 corresponds to an energy transfer of 27.2 eV. Again we see that at low energies the CBA density differs both in shape and magnitude from the PBA density. However, for this energy transfer, the PBA limit is reached at the remarkably low impact energy of 50 eV, in which case the CBA coincides with the PBA.

Figure 3 corresponds to an energy transfer of 54.4 eV. At an impact energy of 60 eV, just above the minimum impact energy required for this energy transfer, the density is quite different from the PBA. Increasing the impact energy to 75 eV brings the CBA curve very close to the PBA. As the impact energy increases, the CBA approaches the PBA. The insert in Fig. 3 shows how the PBA limit is approached at high energies. Figure 4 corresponds to an energy transfer of 132 eV. The CBA density obtained at an impact energy of 140 eV is quite different from the PBA one, even though the impact energy is relatively high. This implies that the GOS density in CBA approaches the high-energy limit, given by the PBA, at impact energies that depend on the energy transfer: the higher the energy transfer, the higher the impact energy at which the PBA limit is reached. A higher energy transfer implies a higher velocity of the secondary electron, since energy conservation gives $k=\sqrt{2E-1}$. Therefore, a necessary condition for the CBA to reach the PBA limit is that the velocity of the incoming and scattered electrons be much greater than the velocity of the ejected electron.

There is a simple explanation for the shape of the PBA curves in Figs. 1–4 [1]. When the energy transfer is large, as in Figs. 3 and 4, the effects of the binding of the atomic electron are small, and, if neglected, conservation of energy and momentum require $K^2=E/2$. The fact that the atomic electron is truly bound spreads the peak giving a distribution around that value as shown in Figs. 3 and 4. When the energy transfer is of the same order of magnitude as the binding energy of the atomic electron, the effects of the binding of the electron are not negligible and this simple picture does not apply; instead, the generalized oscillator strength in the region of small momentum transfer remains comparable to its value at $\ln(K^2)=-1$, as shown in Fig. 1. This trend is characteristic of optically allowed (dipole) transitions. Within the CBA the picture is more complicated. At high impact energies, the Sommerfeld parameter $\gamma=i/k$ is very small, and therefore the Coulomb waves of Eq. (1) become plane waves and the CBA approaches the PBA. At small impact energies, the effects of the proton's potential on the incoming and scattered electrons are important, and therefore the GOS density in CBA differs from the one in PBA. It should be noted that the good agreement between the PBA and CBA holds where the GOS density is large, i.e., for $\ln(K)^2 < 1.5$. For larger values of $\ln(K)^2$, the ratio of CBA to PBA is quite large at all incident energies. This happens because PBA describes only electron-electron scattering, which does not favor large momentum transfers, while CBA includes, in the distorted waves, the scattering of the incident electron from the nucleus. This scattering gives a term in the GOS that decreases as K^{-2}, which is much slower than the K^{-10} of Eq. (5). This slower decrease of the GOS at large momentum transfer was observed experimentally in the K-shell ionization of neon [14].

The CBA and the PBA may be thought of as the two extremes in the distorted-wave Born picture, since the CBA uses the full Coulomb potential of the proton as the distorting potential at all distances from the target, while the PBA uses no distorting potential, e.g., it uses plane waves at all distances from the target. The CBA represents the lowest-order term of an expansion of the scattering amplitude in powers of the electron-electron interaction, while the PBA represents the lowest-order term in an expansion in powers of the incident-electron target-atom interaction. Since the electron-electron interaction tends to keep the electrons apart, it has a smaller effect on the incident electron in the region where the target electron is initially located than does the interaction of the incident electron with the target atom as a whole. Other distorted-wave theories try to treat the competing effects of the electron-electron and electron-atom interactions more accurately. Therefore, the fact that the GOS density given in CBA reaches the PBA at such low energies implies that the lower limit for the validity of the PBA for the GOS is probably lower than generally anticipated, although this conclusion does not necessarily apply to the phase of the ionization amplitude

which is relevant for the interference between direct and exchange scattering. Another important conclusion from our results is that this lower limit depends on the energy transfer of the projectile. These calculations of the GOS for the continuum using a distorted-wave approximation suggest that the impact energy at which the CBA approaches the PBA increases as the energy transfer increases. This corroborates the fact that the PBA is justified if the impact energy is much greater than the energy transfer. In the case of hydrogen, where the binding energy is small, this means that the velocity of the ejected electron must be much smaller than the velocity of both the incoming and the scattered electrons.

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