Bandwidth-induced resonances in laser-assisted electron-atom scattering

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The theory of resonance effects in electron-atom scattering in a chaotic, nonresonant laser field with a bandwidth is reexamined. It is pointed out that, even though the laser is nonresonant with any of the atomic frequencies, use of the nonresonant dressed atomic states is not permissible for this purpose except for very weak fields. An ansatz for estimating the cross sections for these processes is presented, which is valid for higher field strengths.

In a recent study^{1,2} of electron-atom scattering in a chaotic, nonresonant laser field, intriguingly large cross sections were obtained for bandwidth-induced resonance scattering (BIRS), in which photons of energy corresponding to dipole-allowed atomic transition energies are exchanged. These calculations employed the exact dressed states for the incident electron in an arbitrary electromagnetic field, and approximate ones for a hydrogen atom, valid in the case of a nonresonant laser field of strength much less than that of the average atomic field. Furthermore, the stochastic averaging of the transition probability was carried out exactly. For electronhydrogen-atom scattering in the field of a laser with photon energy $\hbar \omega \simeq 1$ eV and intensity $\sim 10^{11}$ W/cm² (a numerical example considered in Refs. ¹ and 2, where this procedure would appear unexceptionable) the differential cross sections for BIRS corresponding to the 1s-2p transition turned out to be of comparable magnitude to those for scattering without any change in energy, for a bandwidth as small as $10^{-4}\omega$. To understand this curious result, we note that the laser is nonresonant only for exchange of photons of frequencies around the median frequency. On the other hand, the resonances owe their existence to the spectrum of photons around the atomic transition frequencies, which are mathematically introduced into the calculation by stochastic averaging, and therefore the nonresonant approximation cannot be expected to provide physically meaningful results unless the field-induced line broadening is much smaller than the natural linewidth. (In fact, the usual perturbation theory fails even when the intensity is small for a range of frequencies around the atomic transition frequencies, and can lead to divergent cross sections, as in Ref. 3.) In principle, if the dressed atomic states could be specified for all frequencies, stochastic averaging of the transition probability should give the correct cross sections for both types of scattering. However, in the absence of such a general solution, the only practicable approach is to treat the BIRS separately, as follows.

The resonant processes can be studied in isolation by following the recipe described in Ref. 1, which consists of letting the spectral distribution of the laser photons afFect only the atom, and assuming that the projectile electron is in the presence of a monochromatic field (insofar as BIRS is concerned). As shown in Ref. 1, this procedure

yields results in agreement with the exact results, for the (single) differential cross sections, for small bandwidths. (The calculation of the double differential cross section for BIRS without making questionable approximations seems an intractable problem at present.) Accordingly, we define the states of the incident electron in a singlemode laser field $E=E_0 sin\omega t$ (in Coulomb gauge and dipole approximation) by

$$
\chi_{\mathbf{k}} = \exp\left[i\mathbf{k}\cdot\mathbf{r}_1 + i\lambda\sin\omega t - \frac{k^2}{2}t\right], \quad \lambda = \frac{e\mathbf{E}_0\cdot\mathbf{k}}{\omega^2} \tag{1}
$$

k being the average momentum. (Atomic units are used throughout.) To calculate the transition probabilities involving energy changes around $\omega_{k0} = \omega_k - \omega_0$, ω_k being the energy of the kth atomic state (bare), the appropriate dressed states in the two-state rotating-wave approximation are given by $4,5$

$$
\Psi_{+} = C(\omega', E_0) \left[e^{i\omega' t/2} | 0 \rangle + \frac{F^*}{\epsilon + \Omega} e^{-i\omega' t/2} | k \rangle \right]
$$

$$
\times e^{-iW_{+} t/2} e^{i\epsilon A \cdot r_2/c}
$$
 (2)

and

$$
\Psi_{-} = C(\omega', E_0) \left[\frac{F}{\epsilon + \Omega} e^{i\omega' t/2} | 0 \rangle - e^{-i\omega' t/2} | k \rangle \right]
$$

× $e^{-iW_{-}t/2} e^{ieA \cdot r_2/c}$, (2a)

where

$$
\varepsilon = \omega' - \omega_{k0}, \quad \Omega = (\varepsilon^2 + |F|^{2})^{1/2}, \quad F = iE_0 M_{k0} ,
$$

$$
M_{k0} = \langle k | e\hat{\mathbf{E}}_0 \cdot \mathbf{r} | 0 \rangle, \quad W_{\pm} = \omega_k + \omega_0 \pm \Omega ,
$$

and

$$
C(\omega', E_0) = \frac{\epsilon + \Omega}{\left[(\epsilon + \Omega)^2 + |F|^2 \right]^{1/2}}.
$$

In deriving Eqs. (2), we have chosen to specify the atomfield interaction in the electric field $(E \cdot r)$ gauge and the resulting wave function is transformed back to the Coulomb gauge. (A good discussion on the choice of gauge in the description of atoms in a radiation field may be found in Ref. 6.) The prime on ω in these equations

has the same function as before;¹ it permits averaging over the laser spectrum without disturbing the states of the incident electron. The first-order S-matrix element for direct elastic scattering which leaves the ψ_+ state unaltered, given by

$$
S_{+} = -i \int_{-\infty}^{\infty} \langle \Psi_{+} x_{f} | V | x_{i} \Psi_{+} \rangle dt
$$

where V is the electron-atom interaction potential in the absence of the field, is readily evaluated as

$$
S_{+} = -2\pi i \left| C \right|^{2} \left[\left| \tilde{V}_{00} + \frac{|F|^{2} \tilde{V}_{kk}}{(\epsilon + \Omega)^{2}} \right| \sum_{m} J_{m}(\lambda_{q}) \delta(E_{fi} + m\omega) + \frac{F^{*}}{\epsilon + \Omega} \tilde{V}_{0k} \sum_{n} J_{n}(\lambda_{q}) \delta(E_{fi} + n\omega - \omega') + \frac{F}{\epsilon + \Omega} \tilde{V}_{k0} \sum_{l} J_{l}(\lambda_{q}) \delta(E_{fi} + l\omega + \omega') \right], \tag{3}
$$

where $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$, $E_{fi} = (k_f^2 - k_i^2)/2$, $\lambda_{\mathbf{q}} = e\mathbf{E} \cdot \mathbf{q}/\omega^2$, and

$$
\widetilde{V}_{kn} = \int \langle k \mid V(\mathbf{r}_1, \mathbf{r}_2) e^{i\mathbf{q} \cdot \mathbf{r}_1} \mid n \rangle d\mathbf{r}_2 . \tag{4}
$$

The first term in Eq. (3) is clearly a nonresonant one and hence of no interest here. The other two terms represent scattering involving a gain or loss of a quantum of energy $\hbar \omega'$ (in addition to photons of energy $\hbar \omega$). For $E_{if} = -\omega' + n\omega$, the scattering amplitude is

$$
f_k^{(n)}(E_{if} = -\omega' + n\omega) = -\frac{|C|^2}{2\pi} \frac{F^*}{\epsilon + \Omega} \widetilde{V}_{0k} J_n(\lambda_q) . \tag{5}
$$

The effect of spontaneous decay of the state $|k\rangle$ may now be phenomenologically accounted for by means of the usual prescription⁷ $\omega_{k0} \rightarrow \omega_{k0} - i\gamma_k$, where $2\gamma_k$ is the probability of decay per unit time. We thus get

$$
|f_k^{(n)}|^2 = \frac{|F|^2 |\tilde{V}_{k0}|^2 J_n^2(\lambda_q)}{16\pi^2(\epsilon^2 + \gamma_k^2 + |F|^2)}.
$$
 (6)

Exactly the same squared amplitude is obtained for elastic scattering from the Ψ state. The observed cross section would be the weighted sum of these partial cross sections,⁸ the weighting factors being the probabilities of encountering the atom in the Ψ_+ and Ψ_- states. Since the partial cross sections are the same in the present case, there is no need for weighting, and the differential cross section is given by

$$
\frac{d\sigma_k^{(n)}}{d\Omega} = \frac{k_f^{(n)}}{k_i} |f_k^{(n)}|^2,
$$
\n(7)

$$
(k_f^{(n)})^2 = k_i^2 + 2(\omega' - n\omega) \tag{7a}
$$

This has to be averaged over the spectrum of laser photons. For comparison with previous work^{1,2} we assume this to be a Lorentzian of width $\Delta\omega$, so that the spectrum-averaged cross section is given by

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$$
\left\langle \frac{d\sigma_k^{(n)}}{d\Omega} \right\rangle = \int_{-\infty}^{\infty} \frac{d\sigma_k^{(n)}}{d\Omega} (\omega') \frac{\Delta\omega d\omega'}{\pi [(\omega'-\omega)^2 + \Delta\omega^2]}.
$$
(8)

The integrand has poles at $\omega' = \omega \pm i \Delta \omega$ and $\omega' = \omega_{k0} \pm i (|F|^2 + \gamma_k^2)^{1/2}$, the latter giving rise to the resonant scattering we are seeking. Assuming $|F|$, γ_{k} , and $\Delta\omega$ to be small, this contribution, with $k_f^2 = k_i^2$

+
$$
2(\omega_{k0} - n\omega)
$$
, may be calculated to be

$$
\left\langle \left(\frac{d \sigma_k^{(n)}}{d \Omega} \right)_{\text{BIRS}} \right\rangle
$$

=
$$
\frac{|F|^2 |\tilde{V}_{k0}|^2 J_n^2 (\lambda_q) \Delta \omega}{16\pi^2 (\omega_{k0} - \omega)^2 (|F|^2 + \gamma_k^2)^{1/2}} \frac{k_f}{k_i} .
$$
 (9)

Finally, for a chaotic field, whose amplitude fluctuations are described by the probability distribution

$$
P(E_0)dE_0 = e^{-E_0^2/\epsilon_0^2}d(E_0/\epsilon_0)^2,
$$
 (10)

where ε_0^2 is the variance of the field, the stochastic average (denoted by bold angular brackets) of Eq. (9) is given by

$$
\left\langle \left\langle \left(\frac{d\,\sigma_k^{(n)}}{d\,\Omega} \right)_{\text{BIRS}} \right\rangle \right\rangle = \int_0^\infty \left(\frac{d\,\sigma_k^n}{d\,\Omega} \right)_{\text{BIRS}} P(E_0) dE_0 \ . \tag{11}
$$

FIG. 1. Differential cross sections (a.u.) per unit bandwidth, for bandwidth-induced resonance scattering of 100-eV electrons from hydrogen in a chaotic laser field, with $\varepsilon_0 = 0.02$, $\omega = 0.0735$, and polarization parallel to the change in momentum. Solid curve, $E_{fi} = \frac{3}{8}$; dashed curve, $E_{fi} = \frac{3}{8} + \omega$; dot-dashed curve, $E_{fi} = \frac{3}{8} - \omega.$

Case 1: $|M_{k0}| \ll \gamma_k/\epsilon_0$. In this case, carrying out the integration in Eq. (11), neglecting $|F|^2$ in comparison with γ_k^2 in the denominator, we recover⁹ Eq. (13) of Ref. 1, viz.,

$$
\left\langle \left\langle \left(\frac{d\sigma_k^{(n)}}{d\Omega} \right)_{\text{BIRS}} \right\rangle \right\rangle
$$
\n
$$
= \frac{\varepsilon_0^2 \Delta \omega}{16\pi^2} \frac{k_f}{k_i} \frac{|V_{0k} M_{k0}|^2}{\gamma_k (\omega_{k0} - \omega)^2} e^{-\lambda_0^2/2} I_n(\lambda_0^2/2) , \quad (12)
$$

where $\lambda_0 = (q \cdot \mathbf{E}_0) \varepsilon_0 / \omega^2$. However, this is by far the less interesting case, being applicable to fields so weak as to be of no consequence in practice. For BIRS corresponding to the $1s \rightarrow 2p$ transition, this condition can be met only for $\varepsilon_0 \ll 10^{-8}$ a.u. It is therefore inappropriate to use Eq. (13), or its precursor, Eq. (10), of Ref. ¹ to the example considered there, where $E_0 \approx 0.2$ a.u.

Case 2: $|M_{k0}| \gg \gamma_k/\epsilon_0$. In this case, we may neglec γ_k^2 in the denominator and perform the integration in Eq. (11) to obtain

$$
\left\langle \left\langle \left(\frac{d\,\sigma_k^{(n)}}{d\,\Omega} \right)_{\text{BIRS}} \right\rangle \right\rangle = \frac{k_f}{k_i} \frac{M_{k0} \left| \tilde{V}_{k0} \right|^2 \varepsilon_0 \Delta \omega}{16\pi^2 (\omega_{k0} - \omega)^2} S_{\nu}(\lambda_0) \right\rangle, \quad (13)
$$

where

$$
S_{\nu}(\lambda_0) = \left(\frac{\lambda_0}{2}\right)^{2\nu} \frac{\Gamma(\nu + \frac{3}{2})}{\nu! \nu!}
$$

$$
\times {}_2F_2(\nu + \frac{1}{2}, \nu + \frac{3}{2}, \nu + 1, 2\nu + 1; -\lambda_0^2),
$$

and $v = |n|$. This equation may now be used to recalcu late the BIRS cross section per unit bandwidth, for the case considered in Ref. 2, namely, with $\varepsilon_0 = 0.02$, ω =0.0735, E_i =100 eV, and $E_0||q$. The results for $n = 0, \pm 1$ are presented in Fig. 1. As one would expect from qualitative considerations, the cross sections are indeed small. To conclude, the distinguishing characteristic of BIRS is its linear dependence on the bandwidth (for small bandwidths and a Lorentzian laser spectrum), and this process can be significant only for targets with large dipole polarizability and not too large a detuning of the laser.

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