Electron-atom scattering in a resonant laser field

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Dressed states of an atom in a classical laser field of frequency close to an atomic transition frequency are obtained, which are a considerable improvement over the usual two-level rotating-wave approximation. These wave functions are used in a calculation of the cross section for elastic electron-atom scattering in a laser field. Numerical calculations for electron-hydrogen scattering demonstrate that scattering involving absorption or emission of photons can be strongly influenced by coupling to the nonresonant states, regardless of the field strength. Inclusion of the counter-rotating terms in the calculation is shown to be essential for extending the applicability of the theory to scattering in nonresonant fields, where a first-order perturbation-theoretic treatment of the atom-field interaction would be expected to be quite justified.

I. INTRODUCTION

Treatments of atom-field interaction in laser-assisted electron-atom scattering to date either involve the tacit assumption that the laser is nonresonant with any of the atomic transition frequencies[1-4] or refer to the near-resonance condition.[5-7] Though Dubois *et al.*[3] and Francken and Joachain[4] do not impose any limitation on the laser frequency, both treat the atom-field interaction by first-order perturbation theory, which, however, breaks down near resonances,[8] leading to spurious divergences.[3,4] On the other hand, the resonant case has so far been studied only in the two-level rotating-wave approximation (RWA), which ignores coupling to other states completely, and, of course, neglects the counter-rotating terms in the equations of motion of the two-level system. While, for moderate field strengths, one can define a range of frequencies where the nonresonance approximation (NRA) might be expected to hold, it is not certain whether the RWA will be adequate even close to resonance, especially for forward scattering, since the nonresonant states can contribute significantly to the dipole polarizability of the atom. In any event, there is hardly any overlap between the regions of validity of the two types of approximation. This work seeks to bridge this gap through a more refined calculation near a resonance, which (1) allows for the presence of the counter-rotating terms and (2) treats the coupling to the nonresonant levels by perturbation theory. Derivation of the dressed atomic states meeting these requirements is outlined in Sec. II, and explicit evaluation of the elastic scattering amplitudes and numerical calculations with atomic hydrogen as the target are described in Secs. III and IV, respectively. It will be seen that the cross sections thus obtained agree with the NRA in the appropriate limit, while remaining finite at exact resonance.

II. ATOMIC STATES IN A LASER FIELD NEAR A RESONANCE

In the following, we use atomic units with $e=-1$ for electrons. The laser field is taken to be linearly polarized and given in the dipole approximation by $\mathbf{E}(t)=\mathbf{E}_0\sin(\omega t)$. E_0 is assumed to be much less than an atomic unit, but large enough for the natural linewidth to be neglected. Expanding the wave function of an atom in this field in terms of its unperturbed eigenfunctions $\phi_n(\mathbf{r})e^{-i\omega_n t}$, we have the coupled differential equations for the time-dependent coefficients $a_k(t)$,

$$\dot{a}_k = i\sum_n M_{kn}a_n e^{i\omega_{kn}t}\sin(\omega t)\ , \tag{1}$$

where

$$M_{kn}=\left\langle k\left| e\sum_{j=1}^{z}\mathbf{r}_j\cdot\mathbf{E}_0\right| n\right\rangle$$

and $\omega_{kn}=\omega_k-\omega_n$. Let $n=0$ and $n=1$ denote the states which are strongly coupled by the field, i.e., ω is close to ω_{10}. As a first approximation, ignoring all other states, the dynamics of the two-level atom is governed by the pair of coupled equations

$$\dot{a}_0=\frac{M_{10}}{2}(e^{i\varepsilon t}-e^{-i(\omega_{10}+\omega)t})a_1\ , \tag{2a}$$

$$\dot{a}_1=\frac{M_{10}}{2}(e^{i(\omega+\omega_{10})t}-e^{-i\varepsilon t})a_0\ , \tag{2b}$$

$$\varepsilon=\omega-\omega_{10}\ .$$

The two pairs of RWA solutions to these equations, obtained by dropping the terms oscillating with frequencies $(\omega_{10}+\omega)$, are[8,9]

$$a_0^{\mathrm{RWA}}=i\alpha e^{-i\lambda t},\quad a_1^{\mathrm{RWA}}=-Ce^{-i\mu t}\ , \tag{3a}$$

and

$$a_0^{\mathrm{RWA}}=Ce^{i\mu t},\quad a_1^{\mathrm{RWA}}=-i\alpha e^{i\lambda t}\ , \tag{3b}$$

where

$$C=(\varepsilon+\Omega)/[(\varepsilon+\Omega)^2+|M_{10}|^2]^{1/2}\ ,$$

$$\Omega=(\varepsilon^2+|M_{10}|^2)^{1/2}\ ,$$

$$\alpha=CM_{10}/(\varepsilon+\Omega),\quad \lambda=-(\varepsilon+\Omega)/2\ ,$$

$$\mu=(\varepsilon-\Omega)/2 \ .$$

The constants here have been chosen so that the resulting wave functions are orthonormal. The first-order corrections to these coefficients from the counter-rotating terms may now be obtained by substituting these solutions back into Eqs. (2a) and (2b). In this way, a better approximation to the two pairs of solutions for a_0 and a_1 is obtained as

$$a_0^{(-)}=i\alpha e^{-i\lambda t}\left[1+\frac{\alpha_0}{\alpha}e^{-2i\omega t}\right] ,$$
$$a_1^{(-)}=-Ce^{-i\mu t}\left[1+\frac{\beta_1}{C}e^{2i\omega t}\right] , \tag{4a}$$

and

$$a_0^{(+)}=-a_1^{(-)*}, \quad a_1^{(+)}=a_0^{(-)*} , \tag{4b}$$

where

$$\alpha_0=\frac{CM_{10}}{2(\lambda+2\omega)} \text{ and } \beta_1=\frac{\alpha M_{10}}{2(\mu-2\omega)} \ .$$

As will be apparent later on, these correction terms ensure a smooth transition from the resonance to the nonresonance region.

We may now proceed to evaluate the coefficients a_k, $k\geq 2$ by first-order perturbation theory using $a_0^{\pm}$ and $a_1^{\pm}$ as given by Eqs. (4a) and (4b), together with the zeroth approximation $a_k^{(0)}=0$, $k\geq 2$. The required modification of the usual two-level RWA dressed states[9] is now effected by using these sets of coefficients in the expansion

$$\psi=\sum_n a_n(t)e^{-i\omega_n t}\phi_n(\mathbf{r})$$

to get, finally,

$$\psi^{\pm}=\sum_{k=0}^{1}a_k^{(\pm)}(t)e^{-i\omega_k t}\phi_k(\mathbf{r})-\alpha^{\pm}e^{-i(\lambda^{(\pm)}+\omega_0)t}\sum_{k=2}^{\infty}M_{k0}\frac{\lambda_k^{(\pm)}\sin(\omega t)-\omega\cos(\omega t)}{\lambda_k^{(\pm)2}-\omega^2}\phi_k(\mathbf{r})$$
$$-i\beta^{\pm}e^{-i(\mu^{(\pm)}+\omega_1)t}\sum_{k=2}^{\infty}M_{k1}\frac{\mu_k^{(\pm)}\sin(\omega t)-\omega\cos(\omega t)}{\mu_k^{(\pm)2}-\omega^2}\phi_k(\mathbf{r}) , \tag{5}$$

where

$$\lambda^{(-)}\equiv\lambda, \quad \mu^{(-)}\equiv\mu, \quad \lambda^{(+)}=-\mu, \quad \mu^{(+)}=-\lambda ,$$
$$\lambda_k^{(\pm)}=\lambda^{(\pm)}-\omega_{k0}, \quad \mu_k^{(\pm)}=\mu^{(\pm)}-\omega_{k1} ,$$
$$\alpha^-\equiv\alpha, \quad \alpha^+\equiv-\beta^-=C, \quad \beta^+=-\alpha \ .$$

In the spirit of first-order perturbation theory, terms of order higher than E_0 have not been retained in the above.

III. ELECTRON SCATTERING BY HYDROGEN ATOMS

To calculate scattering cross sections, it is preferable to work in the Coulomb gauge, in which the incident electron of momentum $\mathbf{k}$ is represented by

$$\chi_{\mathbf{k}}=\exp\left[i\left[\mathbf{k}\cdot\mathbf{r}+\delta\sin(\omega t)-\frac{k^2}{2}t\right]\right] , \tag{6}$$
$$\delta=e\mathbf{E}_0\cdot\mathbf{k}/\omega^2 \ .$$

As is well known,[10] in this gauge the wave function Eq. (5) acquires an additional factor $\exp(ie\mathbf{E}_0\cdot\mathbf{r}/\omega)$, which, however, drops out of the first-order matrix element for direct scattering, which alone we shall be considering in this work. For elastic scattering which leaves $\psi^{\pm}$ unaltered, we have

$$S^{\pm}=-i\int_{-\infty}^{\infty}\langle\psi^{\pm}\chi_{\mathbf{k}_f}\mid V\mid\psi^{\pm}\chi_{\mathbf{k}_i}\rangle dt , \tag{7}$$

where V is the interaction potential and $\mathbf{k}_i$ and $\mathbf{k}_f$ are the initial and final momenta of the incident electron. A straightforward calculation yields

$$S^{\pm}=4\pi^2 i\sum_n\delta(E_{if}-n\omega)f_{\pm}^n , \tag{8}$$

where $E_{if}=(k_i^2-k_f^2)/2$ and $f_{\pm}^n$, the amplitudes for scattering with a transfer of n photons, are given by

$$f_-^n=-\frac{1}{2\pi}[f_1^n(\alpha,c)+f_2^n+f_3^n(\alpha,c,\lambda_k^{(-)},\mu_k^{(-)})+f_4^n] , \tag{9a}$$

$$f_+^n=-\frac{1}{2\pi}[f_1^n(c,\alpha)-f_2^n+f_3^n(c,\alpha,\lambda_k^{(+)},\mu_k^{(+)})-f_4^n] , \tag{9b}$$

where

$$f_1^n(a,b)=(a^2\tilde{V}_{00}+b^2\tilde{V}_{11})J_n(\Delta) , \tag{9c}$$
$$f_2^n=2ic\alpha\tilde{V}_{01}J_n'(\Delta) , \tag{9d}$$
$$f_3^n(a,b,x,y)=2iJ_n'(\Delta)\sum_{k=2}^{\infty}\left[\frac{a^2xM_{k0}\tilde{V}_{0k}}{x^2-\omega^2}+\frac{b^2yM_{k1}\tilde{V}_{k1}}{y^2-\omega^2}\right] , \tag{9e}$$
$$f_4^n=2iJ_n'(\Delta)\tilde{V}_{01}(c\alpha_0+\alpha\beta_1) , \tag{9f}$$
$$\tilde{V}_{nk}=\frac{4\pi}{q^2}\langle n\mid(e^{i\mathbf{q}\cdot\mathbf{r}}-1)\mid k\rangle , \tag{9g}$$

$\mathbf{q}=\mathbf{k}_i-\mathbf{k}_f$, and $\Delta=e\mathbf{E}_0\cdot\mathbf{q}\mid\omega^2$. Here, the fact that, for hydrogen, $M_{nk}=M_{kn}=M_{nk}^*$ and $\tilde{V}_{nk}=\tilde{V}_{kn}=-V_{nk}^*$, has been made use of. Further, terms whose contribution to $\mid f_{\pm}\mid^2$ is of order higher than E_0^2 have been neglected. The various amplitudes f_i^n may be identified as follows.

f_1^n and f_2^n together correspond to the RWA, while f_4^n accounts for the counter-rotating terms. The effect of coupling to states $k \geq 2$ is represented by f_3^n.

As pointed out by Mittleman,[5] when the laser is switched on adiabatically, and the spontaneously radiated photons are not observed, the differential cross section for this scattering process will be a weighted average of the cross sections arising from f_+^n and f_-^n, the weighting factors being approximately given by

$$P_\pm = \left[1+\left|\frac{\alpha}{c}\right|^{\pm 4}\right]^{-1} \tag{10}$$

so that we finally get

$$\frac{d\sigma^{(n)}}{d\Omega} = \frac{k_f^{(n)}}{k_i}(P_+ |f_+^n|^2 + P_- |f_-^n|^2) , \tag{11}$$

where $k_f^{(n)} = (k_i^2 - 2n\omega)^{1/2}$.

At exact resonance, $P_+ = P_- = \frac{1}{2}$ and both f_+ and f_- contribute to the cross section. As ω decreases, P_+ decreases rapidly while P_- approaches 1, so that F_-^n dominates. The opposite is true for $\omega > \omega_{10}$. In either case, for $|M_{10}| \ll |\varepsilon|$, which is the condition for NRA to hold, $(d\sigma^{(n)}/d\Omega)$ approaches the NRA cross section, given by[4]

$$\left[\frac{d\sigma^{(n)}}{d\Omega}\right]_{\text{NRA}} = \frac{1}{4\pi^2}\frac{k_f^{(n)}}{k_i} \times \left| \left[V_{00} J_n(\Delta) + 2ieJ_n'(\Delta) \sum_k \frac{\omega_{k0} |M_{k0}| \tilde{V}_{k0}}{\omega_{k0}^2 - \omega^2} \right] \right|^2 , \tag{12}$$

thereby realizing one of the objectives of this work.

IV. NUMERICAL CALCULATIONS

In this section we present some illustrative numerical results for electron-hydrogen scattering in a laser field of frequency in the neighborhood of the $1s$-$2p$ resonance. The field polarization is taken to be parallel to the incident electron momentum. In these calculations, the amplitude f_3^n was evaluated as follows. The first term [cf. Eq. (9e)] was calculated exactly using the expression for matrix elements of the general form

$$\langle 0 | \exp(i\mathbf{q}\cdot\mathbf{r})(\Lambda - H)^{-1}\mathbf{r}\cdot\mathbf{E}_0 | 0 \rangle ,$$

given by Dubois *et al.*[3] The second sum involving transitions from the $2p$ state can in principle be reduced to a closed form by an extension of the technique used by Dubois *et al.*;[3] however, in this work we have followed the procedure of Holt and and Moiseiwitsch[11] to calculate exactly the matrix elements up to principal quantum number 3, and then approximate the remaining sum by means of the closure relation.

In Fig. 1 is presented the variation of the differential cross section for scattering in the forward direction ($\theta = 1°$) of electrons of energy 5 a.u., accompanied by the

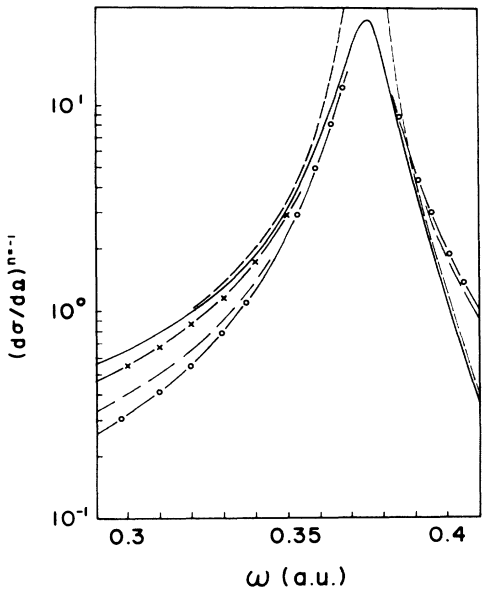

FIG. 1. Differential cross sections (a.u.) as a function of the laser frequency ω, for the scattering of electrons of energy 5 a.u., at an angle 1°, with an absorption of one photon. The field strength $E_0 = 0.01$ a.u. Solid line, full calculation; dashed line, nonresonance approximation (NRA); open circles, rotating-wave approximation (RWA); dashed-dotted line, resonance approximation (RA); dashed-crossed line, RWA with coupling to nonresonant states (RWA1).

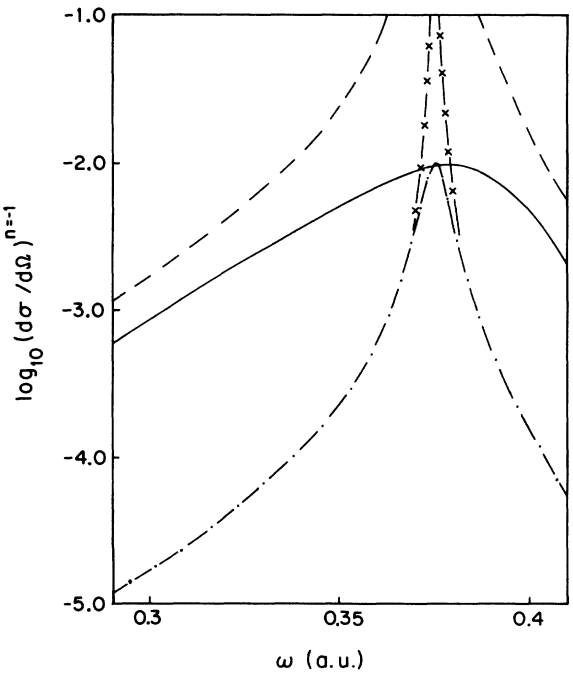

FIG. 2. Comparison of differential cross sections according to the present work and the NRA for two field strengths, at $\theta = 10°$ and $n = -1$. Solid curve, $E_0 = 0.05$, present work; dashed curve, $E_0 = 0.05$, NRA; dashed-dotted line, $E_0 = 0.005$, present work; dashed-crossed line, $E_0 = 0.005$, NRA.

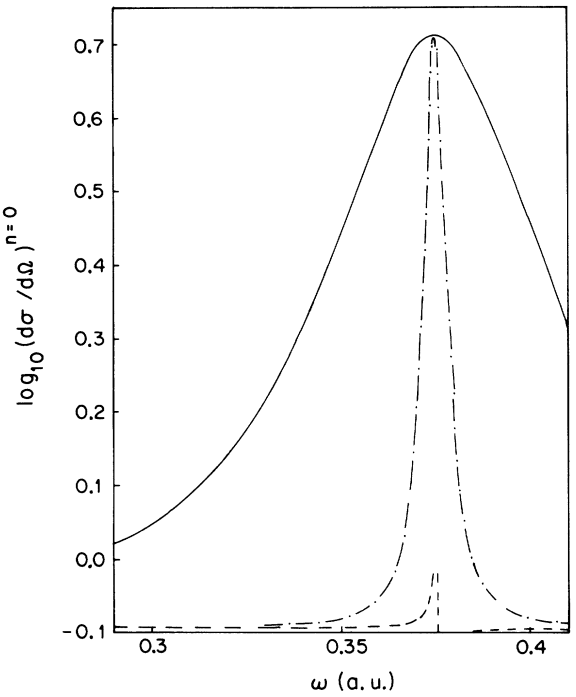

FIG. 3. Same as Fig. 2 but for $n=0$. The dashed line represents the NRA for both $E_0=0.05$ and 0.005.

absorption of a photon ($n=-1$). The solid curve represents the full calculation including all the amplitudes in Eq. (9), while the others reflect the consequences of retaining only certain terms, corresponding to a particular approximation. Thus the RWA keeps only f_1^n and f_2^n, whereas the resonance approximation (RA) also includes f_4^n, arising from the counter-rotating terms. An improved rotating-wave approximation, which takes cognizance of the coupling to other states, is represented by RWA1, formed from f_1^n, f_2^n, and f_3^n. Finally, the NRA refers to Eq. (12), which exhibits the characteristic divergence at exact resonance ($\omega=0.375$). The full calculation is seen to be free from this anomaly, while, at the same time, joining on smoothly to the NRA cross section, away from resonance. Near resonance, RWA1 also agrees with the full calculation, since there the effect of counter-rotating terms is negligible. However, the RWA is seen to be inadequate except at resonance because it ignores couplings to other states, which are important for the $n=\pm 1$ forward scattering process, whatever the field strength. It is clear from Eqs. (9a)–(9f) that for small Δ, f_2^1 and f_3^1 are the leading terms because of the presence of $J_0(\Delta)$. (This is not true at large angles; e.g., at $\theta=180°$, the RWA agrees very well with the full calculation near resonance.) For similar reasons, the RWA and

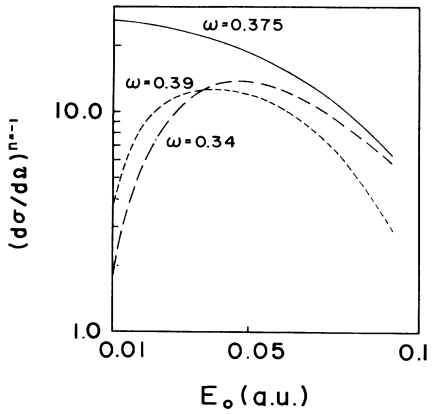

FIG. 4. Variation of $(d\sigma/d\Omega)^{(n=-1)}$ with field strength E_0, at $\theta=1°$.

the RA agree close to resonance. It is evident from these results that interference among the various terms in Eq. (9) plays a prominent role in determining the cross section.

The effect of field strength on the range of validity of the NRA is illustrated in Figs. 2 and 3, for $n=-1$ and 0, respectively. As expected, in both cases, the frequency range where resonance effects are important shrinks as the field strength is reduced. For the $n=-1$ process, the higher field is seen to introduce a small shift in the peak position. For the $n=0$ process, the RWA, RWA1, and the RA all yield essentially the same results as the full calculation, since, in this case, f_1^0 is the dominant term, being proportional to $J_0(\Delta)$.

Finally, the variation of $(d\sigma/d\Omega)^{n=-1}$ with the field strength at and around exact resonance is presented in Fig. 4. At sufficiently low fields, all cross sections increase with field strength as E_0^2, in accordance with the first-order theory;[3] in the frequency range shown in Fig. 4, this trend is apparent on either side of exact resonance.

In conclusion, it is rather surprising that the validity of the present formalism appears to extend far into the nonresonance region, though the starting point was the RWA. Numerical calculations confirmed that, provided the narrow pseudoresonances due to the dynamic Stark splitting of the coupled levels are smoothed over, agreement between the present theory and the NRA remains excellent, in the region of frequencies where the latter would be expected to be valid.

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