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Almost degenerate perturbation theory for scattering in a laser field

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Earlier derivations of approximations for electron-atom scattering in a low-frequency laser field are generalized to account for the effectively strong interaction of the field with groups of nearly degenerate states of the atomic target. The basis of the derivation is a reformulation of the scattering problem, obtained with the aid of a gauge transformation, which allows one to extract the strong-field effects explicitly in the form of dressed-atom and dressed-electron states. The effects of the weakened residual interaction can then be included in perturbation theory. The result obtained by working to first order in this modified perturbation theory has the simplifying feature that it involves as input the scattering operator in the *absence* of the field. This first-order approximation is studied in some detail in the dipole approximation, with the final target state taken to be one of a pair of nearly degenerate states.

I. INTRODUCTION

The analysis of electron-atom scattering in a laser field is simplified considerably in the low-frequency limit. It will be shown here that earlier versions of the low-frequency approximation[1-4] can be viewed as representing the leading terms in an expansion based on a perturbation theory modified to account for the appearance of near degeneracies. These will certainly be present at low frequencies since an electron incident with a given momentum $\vec{p}$ has available to it a sequence of energy levels with spacing $\hbar\omega$ where $\hbar\omega$ is the laser photon energy, assumed to be small compared to the kinetic energy $K=p^2/2\mu$. As will be seen, this approach can be extended in a natural way to take into account the effectively strong coupling between the laser field and states of the atomic target which are nearly degenerate. It is assumed that the field intensity is low enough so that ordinary perturbation theory suffices for those virtual transitions involving nondegenerate intermediate states. The basis for the theory is developed in Sec. II, below. The first two terms in the modified perturbation expansion are worked out in Sec. III and analyzed in greater detail, in the context of a particular model, in Sec. IV.[5] It will be clear from the discussion that higher-order corrections to this generalized low-frequency approximation can be obtained in a systematic manner.

As a guide in setting up an approximation scheme it will be useful to consider, in a qualitative way, the sizes of the various coupling strengths and physical parameters which will be relevant. A measure of the intrinsic strength of the field is provided by the ratio

$$\delta_1 = \left|\frac{e\vec{A}_c}{c}\right| \Big/ |\vec{p}|,$$

where $\vec{A}_c$ is the amplitude of the classical vector potential corresponding to a laser beam of intensity I and frequency ω, i.e.,

$$|\vec{A}_c| = \left(\frac{2\pi c I}{\omega^2}\right)^{1/2}.$$

Writing

$$\delta_1 = C\left(\frac{I}{I_0}\right)^{1/2}\left(\frac{K_0}{K}\right)^{1/2}\left(\frac{\omega_0}{\omega}\right)$$

and choosing $I_0 = 10^{12}\ \mathrm{W/cm^2}$, $K_0 = 10$ eV, and $\hbar\omega_0 = 0.1$ eV we find the constant C to be of order unity. One sees then that δ_1 will be a small parameter under a wide range of conditions of experimental interest. Other small parameters in the theory are $\delta_2 = \hbar\omega/K$ and $\delta_3 = p/\mu c$. Terms of second order in δ_3 should, for consistency, be neglected at the outset since the atomic system is treated nonrelativistically.

In the construction of the states describing the free electron in the laser field (this calculation is reviewed in Sec. II) one finds as the effective coupling strength the ratio of the interaction energy to the photon energy, a quantity of order δ_1/δ_2. This ratio is taken to be of zeroth order. That is, the electron-field interaction in asymptotic states is treated to all orders; this is the near-degeneracy effect mentioned above. The field also interacts with the target asymptotically. For the purpose of the present discussion we assume a classical electric field of amplitude $\vec{E}_c$ and treat the interaction in the electric-dipole approximation. Eigenstates of the isolated target satisfy

$$H_T|\chi_i\rangle = \epsilon_i|\chi_i\rangle.$$

The matrix element of the interaction, taken between states $|\chi_1\rangle$ and $|\chi_2\rangle$, is

$$-e\sum_j^{(T)} \langle\chi_2|\vec{r}_j\cdot\vec{E}_c|\chi_1\rangle,$$

the sum running over all target electrons. If one writes

$$\langle\chi_2|\vec{r}_j|\chi_1\rangle=(\epsilon_1-\epsilon_2)^{-1}\langle\chi_2|[\vec{r}_j,H_T]|\chi_1\rangle\,,$$

the matrix element of the interaction takes the form

$$-i\left(\frac{\hbar\omega}{\epsilon_1-\epsilon_2}\right)\sum_j^{(T)}\left\langle\chi_2\left|\frac{e\vec{p}_j\cdot\vec{A}_c}{\mu c}\right|\chi_1\right\rangle.$$

This interaction is of second order (i.e., of order $\delta_1\delta_2$), assuming the target states to be nondegenerate so that $\hbar\omega/(\epsilon_1-\epsilon_2)$ may be treated as a first-order quantity. A similar argument indicates that the interaction between the field and the electron-atom system in intermediate states of the scattering process is of second order. In this case one should introduce an average excitation energy in place of the level separation $\epsilon_1-\epsilon_2$.[6] It is assumed here that there are no scattering resonances in the energy range under consideration.

If the states $|\chi_1\rangle$ and $|\chi_2\rangle$ are nearly degenerate the preceding discussion breaks down and nonperturbative methods are required in general. For example, when $|\epsilon_1-\epsilon_2|\ll\hbar\omega$ it is the ratio of the interaction energy to the photon energy which provides a proper measure of the strength of the coupling (as shown explicitly in Sec. IV) and this ratio should be treated as a parameter of zeroth order. Approximation methods for solving such "dressed-atom" problems have been described previously[7] and further discussion in the context of the scattering problem will be found below.

As a final general remark it should be noted that in the preceding discussion the electron-field interaction was assumed to be of the "$\vec{p}\cdot\vec{A}$" form while the target-field interaction was taken to be of the "$\vec{r}\cdot\vec{E}$" form. This is justified formally, in Sec. II, with the aid of a gauge transformation. Such a transformation was employed previously in the derivation of a low-frequency approximation[8] and it provides a convenient starting point for the more general derivation given here.

II. GAUGE TRANSFORMATION

The Hamiltonian of the electron-atom system in the presence of a plane-wave laser field of propagation vector $\vec{k}$, frequency ω, and polarization $\vec{\lambda}$ is

$$H=\sum_j\left(\vec{p}_j-\frac{e}{c}\vec{A}(\vec{r}_j)\right)^2/2\mu+H_F+V\,. \tag{2.1}$$

Here V represents the sum of interparticle Coulomb potentials, $H_F=\hbar\omega a^\dagger a$ is the field Hamiltonian in the occupation number representation, and

$$\vec{A}(\vec{r})=\left(\frac{2\pi\hbar c^2}{\omega L^3}\right)^{1/2}(a\vec{\lambda}\,e^{i\vec{k}\cdot\vec{r}}+a^\dagger\vec{\lambda}^*e^{-i\vec{k}\cdot\vec{r}}) \tag{2.2}$$

is the vector potential appropriate to a quantization volume L^3. It will be convenient to treat the scattered electron as distinguishable from the target electrons with the understanding that antisymmetrization will ultimately be imposed by taking the proper linear combination of direct and exchange amplitudes. The asymptotic states satisfy

$$(H-E_\beta)|\Phi_\beta\rangle=V_\beta|\Phi_\beta\rangle\,, \tag{2.3}$$

where β is a channel index representing the set of observables which defines the state. These include the photon occupation number, the electron momentum, and the quantum numbers specifying the state of the target. (We are assuming here that the field interaction is switched on adiabatically before the scattering event and then switched off afterwards. The observables mentioned above are well defined in the absence of the field interaction and serve to label the states when the interaction in on.) The index β also distinguishes the projectile electron from the target electrons. In Eq. (2.3) V_β represents the net interaction between projectile and target. The transition amplitude takes the usual form

$$T_{\beta'\beta}=\langle\Phi_{\beta'}|[V_\beta+V_{\beta'}(E-H)^{-1}V_\beta]|\Phi_\beta\rangle\,, \tag{2.4}$$

with $E_{\beta'}=E_\beta$ and $E=E_\beta+i0$.

An equivalent representation of the transition amplitude which is more convenient for our present purposes is obtained by introducing a unitary transformation represented by e^g, with

$$g=(ie/\hbar c)\sum_j\vec{A}(0)\cdot\vec{r}_j\,. \tag{2.5}$$

To determine its effect on the Hamiltonian we first observe that

$$\vec{p}_j-\frac{e}{c}\vec{A}(\vec{r}_j)=e^g\left(\vec{p}_j-\frac{e}{c}[\vec{A}(\vec{r}_j)-\vec{A}(0)]\right)e^{-g}\,. \tag{2.6}$$

The transformed field Hamiltonian may be expanded in multiple commutators as[9]

$$e^gH_Fe^{-g}=H_F+[g,H_F]+\frac{1}{2!}[g,[g,H_F]]+\cdots\,. \tag{2.7}$$

Since the double commutator is a c-number the terms shown explicitly are actually the only ones which contribute. We find that

$$[g,H_F]=e\sum_j\vec{E}(0)\cdot\vec{r}_j\,, \tag{2.8a}$$

where

$$\vec{E}(0)\equiv i\left(\frac{\omega}{c}\right)\left(\frac{2\pi\hbar c^2}{\omega L^3}\right)^{1/2}(a\vec{\lambda}-a^\dagger\vec{\lambda}^*) \tag{2.8b}$$

represents the electric field at the origin. Note that the operators a and $a^\dagger$ may be thought of as quantities of order $\sqrt{n}$ where n is the photon number of the incident beam. On the other hand, the double commutator

$$[g,[g,H_F]] = \left(\frac{4\pi e^2}{L^3}\right)\left|\sum_j \vec{\lambda}\cdot\vec{r}_j\right|^2, \tag{2.9}$$

which represents a level shift arising from spontaneous emission and absorption, is independent of the external field strength. Terms of this order will be consistently ignored in the following. We have then

$$e^g\Big(H_F - e\sum_j \vec{E}(0)\cdot\vec{r}_j\Big)e^{-g} = H_F. \tag{2.10}$$

This, along with Eq. (2.6), allows us to write

$$H = e^g \overline{H} e^{-g}, \tag{2.11}$$

where

$$\begin{aligned}\overline{H} = &\sum_j \frac{p_j^2}{2\mu} + H_F + V \\ &- \sum_j \frac{e}{\mu c}\vec{p}_j\cdot[\vec{A}(\vec{r}_j)-\vec{A}(0)] \\ &+ \sum_j \frac{e^2}{2\mu c^2}[\vec{A}(\vec{r}_j)-\vec{A}(0)]^2 - e\sum_j \vec{E}(0)\cdot\vec{r}_j.\end{aligned} \tag{2.12}$$

Returning to Eq. (2.3) we rewrite it as

$$(H_e + H_T + H_F + H')|\Phi_\beta\rangle = E_\beta|\Phi_\beta\rangle, \tag{2.13}$$

where H_e is the projectile kinetic-energy operator and $H' = H_e' + H_T'$ represents the interaction of the field with the projectile and with the target. (A channel label specifying which of the electrons is the projectile is omitted for notational simplicity.) Consider now the transformed state

$$|\overline{\Phi}_\beta\rangle = e^{-g_T}|\Phi_\beta\rangle, \tag{2.14}$$

where

$$g_T = (ie/\hbar c)\sum_j^{(T)} \vec{A}(0)\cdot\vec{r}_j, \tag{2.15}$$

the sum running over target electrons only. The Schrödinger equation satisfied by $|\overline{\Phi}_\beta\rangle$ is readily seen to be

$$(H_e + H_T + H_F + H_e' + \overline{H}_F')|\overline{\Phi}_\beta\rangle = E_\beta|\overline{\Phi}_\beta\rangle, \tag{2.16}$$

with

$$\begin{aligned}\overline{H}_T' = &-\sum_j^{(T)} \frac{e}{\mu c}\vec{p}_j\cdot[\vec{A}(\vec{r}_j)-\vec{A}(0)] \\ &+ \sum_j^{(T)} \frac{e^2}{2\mu c^2}[\vec{A}(\vec{r}_j)-\vec{A}(0)]^2 - e\sum_j^{(T)} \vec{E}(0)\cdot\vec{r}_j.\end{aligned} \tag{2.17}$$

Writing $g = g_T + g_e$ we have

$$e^{-g}|\Phi_\beta\rangle = e^{-g_e}|\overline{\Phi}_\beta\rangle. \tag{2.18}$$

An analogous relation is obtained for the final-state wave functions using the appropriate decomposition $g = g_T' + g_e'$. Now Eq. (2.11) implies that

$$(E-H)^{-1} = e^g(E-\overline{H})^{-1}e^{-g}. \tag{2.19}$$

It follows that Eq. (2.4) is equivalent to

$$T_{\beta'\beta} = \langle e^{-g_e'}\overline{\Phi}_{\beta'}|[V_\beta + V_{\beta'}(E-\overline{H})^{-1}V_\beta]|e^{-g_e}\overline{\Phi}_\beta\rangle. \tag{2.20}$$

A formal procedure for constructing solutions of equations of the type (2.16) has been described previously[10] and will now be very briefly reviewed. One first solves the projectile-field Schrödinger equation

$$(H_e + H_F + H_e')|\psi_{m\vec{p}}\rangle = E_{m\vec{p}}|\psi_{m\vec{p}}\rangle \tag{2.21}$$

corresponding to a state $|\psi_{m\vec{p}}\rangle$ which goes over into the unperturbed state $|m\rangle|\vec{p}\rangle$ containing m photons and an electron of momentum $\vec{p}$ when the field interaction is switched off adiabatically. The solution can be expressed in the form[3]

$$|\psi_{m\vec{p}}\rangle = \sum_{l=-\infty}^{\infty} \gamma_l(\vec{p})|m+l\rangle|\vec{p} - l\hbar\vec{k}\rangle. \tag{2.22}$$

The expansion coefficients are represented as

$$\gamma_l(\vec{p}) = \int_0^{2\pi}\frac{d\phi}{2\pi}e^{il\phi}f_{\vec{p}}(\phi), \tag{2.23a}$$

where

$$f_{\vec{p}}(\phi) = e^{iS_{\vec{p}}(\phi)} \tag{2.23b}$$

and

$$S_{\vec{p}}(\phi) = \rho_{\vec{p}}\sin(\phi+\theta) + \alpha\sin 2\phi. \tag{2.23c}$$

We have introduced the notation

$$\rho_{\vec{p}}e^{i\theta} = \frac{2}{\hbar\omega - \hbar\vec{k}\cdot\vec{p}/\mu}\left(\frac{2\pi\hbar e^2 n}{\mu^2\omega L^3}\right)^{1/2}\vec{p}\cdot\vec{\lambda}, \tag{2.23d}$$

$$\alpha = \frac{\Delta(\vec{\lambda}\cdot\vec{\lambda})}{2(\hbar\omega - \hbar\vec{k}\cdot\vec{p}/\mu)}, \tag{2.23e}$$

and

$$\Delta = \left(\frac{e^2}{2\mu c^2}\right)\frac{4\pi n\hbar c^2}{\omega L^3}. \tag{2.23f}$$

The energy is determined as

$$E_{m\vec{p}} = p^2/2\mu + m\hbar\omega + \Delta. \tag{2.24}$$

We also require the solution of the target-field eigenvalue equation

$$(H_T + H_F + \overline{H}_T')|D_{in}\rangle = E_{in}|D_{in}\rangle, \tag{2.25}$$

with $|D_{in}\rangle \to |n\rangle|\chi_i\rangle$ as the interaction is switched off adiabatically. The solution may be expanded in photon states as

$$|D_{in}\rangle=\sum_{m=-\infty}^{\infty}|D_m(i,n)\rangle|m\rangle\,, \tag{2.26}$$

where the D_m satisfy the coupled equations

$$(H_T+m\hbar\omega-E_{in})|D_m\rangle+\sum_{m'}\langle m|\overline{H}'_T|m'\rangle|D_{m'}\rangle=0\,. \tag{2.27}$$

The energy is $E_{in}=\epsilon_i+r_i+n\hbar\omega$, where r_i represents a level shift induced by the field. The solution to Eq. (2.16), in which the projectile and the target interact with the field, but not with each other, can be represented by the expansion[10]

$$|\overline{\Phi}_{in\vec{p}}\rangle=\sum_m|D_m(i,n)\rangle|\psi_{m\vec{p}}\rangle\,. \tag{2.28}$$

The energy of this state is $E_{in\vec{p}}=p^2/2\mu+E_{in}+\Delta$, so that the total level shift is $r_i+\Delta$, the sum of the target- and projectile-field level shifts. An index n has been omitted in our notation for these shifts to indicate that they depend only on the intensity of the incident beam and have negligible variation from one field state to another.[10] This is reasonable since photon depletion effects are negligible for the very high occupation numbers we are dealing with here.

III. FIRST-ORDER APPROXIMATION: GENERAL CASE

The expression (2.20) for the transition amplitude provides a convenient starting point for approximations. Thus, consider the resolvent $(E-\overline{H})^{-1}$ in Eq. (2.20), with $\overline{H}$ given by Eq. (2.12). In Sec. I we introduced a set of small parameters δ_i and have argued that the interaction between the field and the electron-atom system in intermediate states is of second order in these parameters. (Here and in the following by "second order" we shall mean a quantity of order $\delta_i\delta_j$.) We discussed only the electric-dipole interaction—the last term in Eq. (2.12)—but one readily sees that the remaining particle-field interaction terms are of the same order or smaller. To first order then,

$$(E-\overline{H})^{-1}\cong\left(E-\sum_j\frac{p_j^2}{2\mu}-V-H_F\right)^{-1}\equiv G(E-H_F)\,. \tag{3.1}$$

Since $G(E)$ is the resolvent for the isolated electron-atom system this suggests that when corrections of second order are ignored the transition amplitude can be expressed in terms of the amplitude for scattering in the absence of the field. Formal expressions for the higher-order corrections can be generated by expanding the resolvent in powers of the interaction. We shall confine our attention to the first-order approximation in the following.

In addition to the approximation (3.1) we have, to first order,

$$e^{-\mathcal{S}_e}\cong1-(ie/\hbar c)\vec{A}(0)\cdot\vec{r}=1+\frac{|e|}{c}\vec{A}(0)\cdot\vec{\nabla}_{\vec{p}}\,, \tag{3.2}$$

where the projectile coordinate $\vec{r}$ has been expressed as an operator in momentum space. With a similar form introduced for the final-state factor $e^{-\mathcal{S}'_e}$ we have

$$T_{\beta'\beta}\cong B_{\beta'\beta}+C_{\beta'\beta}\,, \tag{3.3}$$

with

$$B_{\beta'\beta}=\langle\overline{\Phi}_{\beta'}|[V_\beta+V_{\beta'}G(E-H_F)V_\beta]|\overline{\Phi}_\beta\rangle \tag{3.4}$$

and

$$C_{\beta'\beta}=\left(\frac{2\pi\hbar e^2}{\omega L^3}\right)^{1/2}\{(\vec{\nabla}_{\vec{p}}+\vec{\nabla}_{\vec{p}'})\langle\overline{\Phi}_{\beta'}|[V_\beta+V_{\beta'}G(E-H_F)V_\beta](a\vec{\lambda}+a^\dagger\vec{\lambda}^*)|\overline{\Phi}_\beta\rangle\}\,. \tag{3.5}$$

Let us first consider the contribution $B_{\beta'\beta}$. Since the asymptotic states are to be expanded in the form (2.28) it will be convenient to introduce the abbreviation

$$t_{m'm}(E;\vec{p}'\vec{p})=\langle\vec{p}'|\langle D_{m'}(i',n')|[V_\beta+V_{\beta'}G(E)V_\beta]|D_m(i,n)\rangle|\vec{p}\rangle\,. \tag{3.6}$$

(For simplicity channel indices β' and β have been suppressed in the notation for the t matrix.) Equation (3.4) then becomes

$$B_{\beta'\beta}=\sum_l\sum_{m'}\sum_m\gamma^*_{l+m-m'}(\vec{p}')\gamma_l(\vec{p})\times t_{m'm}[E-(m+l)\hbar\omega;\vec{p}'-(l+m-m')\hbar\vec{k},\vec{p}-l\hbar\vec{k}]\,. \tag{3.7}$$

We now write $t_{m'm}(e;\vec{q}',\vec{q})$ as $t_{m'm}(\nu,\tau,\xi',\xi)$ with the new scalar variables defined by

$$\nu=\tfrac{1}{2}(q'^2/2\mu+q^2/2\mu),\quad \tau=(\vec{q}'-\vec{q})^2,$$
$$\xi'=e-q'^2/2\mu-\epsilon_{i'}-r_{i'},\quad \xi=e-q^2/2\mu-\epsilon_i-r_i\,. \tag{3.8}$$

The t matrix in Eq. (3.7) may be expanded about the values

$$\xi=\xi'=0,\quad \nu=\tfrac{1}{2}(p'^2/2\mu+p^2/2\mu),\quad \tau=(\vec{p}'-\vec{p})^2. \tag{3.9}$$

Taking into account the energy-conservation condition

$$E=p^2/2\mu+\epsilon_i+r_i+n\hbar\omega=p'^2/2\mu+\epsilon_{i'}+r_{i'}+n'\hbar\omega \tag{3.10}$$

(with the second order shift Δ ignored) we find, to first order,

$$\begin{aligned}t_{m'm}&[E-(m+l)\hbar\omega;\vec{p}'-(l+m-m')\hbar\vec{k},\vec{p}-l\hbar\vec{k}]\\&=t_{m'm}+\frac{1}{2\mu}\frac{\partial t_{m'm}}{\partial\nu}[(m'-m-l)\hbar\vec{k}\cdot\vec{p}'-l\hbar\vec{k}\cdot\vec{p}]\\&+\frac{\partial t_{m'm}}{\partial\xi}\left((n-m-l)\hbar\omega+l\hbar\vec{k}\cdot\frac{\vec{p}}{\mu}\right)\\&+\frac{\partial t_{m'm}}{\partial\xi'}\left((n'-m-l)\hbar\omega+(l+m-m')\hbar\vec{k}\cdot\frac{\vec{p}'}{\mu}\right)\\&+\frac{\partial t_{m'm}}{\partial\tau}[2(m'-m)\hbar\vec{k}\cdot(\vec{p}'-\vec{p})].\end{aligned} \tag{3.11}$$

The scalar variables in $t_{m'm}$ and its derivatives are understood to be fixed according to Eq. (3.9). When the expansion (3.11) is inserted in Eq. (3.7) we find an explicit dependence on the index l. The summation over this index can be performed using the formulas

$$\sum_l\gamma^*_{l+m-m'}(\vec{p}')\gamma_l(\vec{p})=\int_0^{2\pi}\frac{d\phi}{2\pi}e^{i(m'-m)\phi}f^*_{\vec{p}'}(\phi)f_{\vec{p}}(\phi), \tag{3.12}$$

$$\sum_l(-l)\gamma^*_{l+m-m'}(\vec{p}')\gamma_l(\vec{p})=\int_0^{2\pi}\frac{d\phi}{2\pi}e^{i(m'-m)\phi}f^*_{\vec{p}'}(\phi)f_{\vec{p}}(\phi)S'_{\vec{p}}(\phi), \tag{3.13}$$

and

$$\sum_l(m'-m-l)\gamma^*_{l+m-m'}(\vec{p}')\gamma_l(\vec{p})=\int_0^{2\pi}\frac{d\phi}{2\pi}e^{i(m'-m)\phi}f^*_{\vec{p}'}(\phi)f_{\vec{p}}(\phi)S'_{\vec{p}'}(\phi), \tag{3.14}$$

with $S'_{\vec{p}}(\phi)\equiv dS_{\vec{p}}/d\phi$. Equation (3.12) is derived directly from the integral representation (2.23) and the relation

$$\frac{1}{2\pi}\sum_l e^{il(\phi-\phi')}=\delta(\phi-\phi'). \tag{3.15}$$

A similar procedure is used to obtain Eq. (3.13), after performing an integration by parts to arrive at

$$(-l)\gamma_l(\vec{p})=\int_0^{2\pi}\frac{d\phi}{2\pi}e^{il\phi}f_{\vec{p}}(\phi)S'_{\vec{p}}(\phi); \tag{3.16}$$

Eq. (3.14) is derived in an analogous way. The result of the summation over l is

$$\begin{aligned}B_{\beta'\beta}=\sum_m\sum_{m'}\int_0^{2\pi}&\frac{d\phi}{2\pi}e^{i(m'-m)\phi}f^*_{\vec{p}'}(\phi)f_{\vec{p}}(\phi)\\&\times\left[t_{m'm}+\frac{1}{2}\frac{\partial t_{m'm}}{\partial\nu}\left(S'_{\vec{p}'}\hbar\vec{k}\cdot\frac{\vec{p}'}{\mu}+S'_{\vec{p}}\hbar\vec{k}\cdot\frac{\vec{p}}{\mu}\right)+\frac{\partial t_{m'm}}{\partial\xi}\left((n-m+S'_{\vec{p}})\hbar\omega-S'_{\vec{p}}\hbar\vec{k}\cdot\frac{\vec{p}}{\mu}\right)\right.\\&\left.+\frac{\partial t_{m'm}}{\partial\xi'}\left((n'-m'+S'_{\vec{p}'})\hbar\omega-S'_{\vec{p}'}\hbar\vec{k}\cdot\frac{\vec{p}'}{\mu}\right)+\frac{\partial t_{m'm}}{\partial\tau}[2(m'-m)\hbar\vec{k}\cdot(\vec{p}'-\vec{p})]\right].\end{aligned} \tag{3.17}$$

Turning now to the expression (3.5) for $C_{\beta'\beta}$ we write

$$a|l+m\rangle\cong\sqrt{n}\,|l+m-1\rangle, \tag{3.18a}$$

$$a^\dagger|l+m\rangle\cong\sqrt{n}\,|l+m+1\rangle, \tag{3.18b}$$

in the approximation in which photon depletion effects are ignored. This allows us to evaluate

$$\begin{aligned}\sum_l\sum_{l'}&\langle l'+m'|\gamma^*_{l'}(\vec{p}')(\vec{\lambda}a+\vec{\lambda}^*a^\dagger)\gamma_l(\vec{p})|l+m\rangle\\&=\sqrt{n}\sum_l[\vec{\lambda}\gamma^*_{l+m-m'}(\vec{p}')\gamma_{l+1}(\vec{p})+\vec{\lambda}^*\gamma_{l+m-m'}(\vec{p}')\gamma_{l-1}(\vec{p})]\\&=\sqrt{n}\int_0^{2\pi}\frac{d\phi}{2\pi}e^{i(m'-m)\phi}f^*_{\vec{p}'}(\phi)f_{\vec{p}}(\phi)(\vec{\lambda}e^{i\phi}+\vec{\lambda}^*e^{-i\phi}).\end{aligned}$$

The momentum derivatives appearing in Eq. (3.5) can be expressed in terms of the scalar variables as

$$\vec{\nabla}_{\vec{p}}=\frac{\vec{p}}{2\mu}\frac{\partial}{\partial\nu}\frac{\vec{p}}{\mu}\frac{\partial}{\partial\xi}-2(\vec{p}'-\vec{p})\frac{\partial}{\partial\tau}, \tag{3.19a}$$

$$\vec{\nabla}_{\vec{p}'}=\frac{\vec{p}'}{2\mu}\frac{\partial}{\partial\nu}-\frac{\vec{p}'}{\mu}\frac{\partial}{\partial\xi'}+2(\vec{p}'-\vec{p})\frac{\partial}{\partial\tau}. \tag{3.19b}$$

Note that according to the definitions (2.23) we have

$$\begin{aligned}\left(\frac{2\pi\hbar e^2}{\omega L^3}\right)^{1/2}&\sqrt{n}(\vec{p}\cdot\vec{\lambda}e^{i\phi}+\vec{p}\cdot\vec{\lambda}^*e^{-i\phi})/\mu\\&=(\hbar\omega-\hbar\vec{k}\cdot\vec{p}/\mu)\rho_{\vec{p}}\cos(\phi+\theta)\\&\cong(\hbar\omega-\hbar\vec{k}\cdot\vec{p}/\mu)S'_{\vec{p}}.\end{aligned} \tag{3.20}$$

The last version is obtained by recognizing that the term proportional to α in Eq. (2.23c) is of second order and hence may be neglected. We then find

$$C_{\beta'\beta}=\sum_m\sum_{m'}\int_0^{2\pi}\frac{d\phi}{2\pi}\,e^{i(m'-m)\phi}f^*_{\vec{p}'}(\phi)f_{\vec{p}}(\phi)\times\left[\left(\hbar\omega-\hbar\vec{k}\cdot\frac{\vec{p}}{\mu}\right)S'_{\vec{p}}\left(\frac{1}{2}\frac{\partial t_{m'm}}{\partial\nu}-\frac{\partial t_{m'm}}{\partial\xi}\right)+\left(\hbar\omega-\hbar\vec{k}\cdot\frac{\vec{p}'}{\mu}\right)S'_{\vec{p}'}\left(\frac{1}{2}\frac{\partial t_{m'm}}{\partial\nu}-\frac{\partial t_{m'm}}{\partial\xi'}\right)\right]. \tag{3.21}$$

Combining Eqs. (3.17) and (3.21) for the first-order approximation (3.3) we obtain

$$T_{\beta'\beta}\cong\sum_m\sum_{m'}\int_0^{2\pi}\frac{d\phi}{2\pi}e^{i(m'-m)\phi}f^*_{\vec{p}'}(\phi)f_{\vec{p}}(\phi)\left(t_{m'm}+\frac{1}{2}\hbar\omega\,\frac{\partial t_{m'm}}{\partial\nu}\,(S'_{\vec{p}}+S'_{\vec{p}'})+(n-m)\hbar\omega\,\frac{\partial t_{m'm}}{\partial\xi}+(n'-m')\hbar\omega\frac{\partial t_{m'm}}{\partial\xi'}+2(m'-m)\hbar\vec{k}\cdot(\vec{p}'-\vec{p})\frac{\partial t_{m'm}}{\partial\tau}\right). \tag{3.22}$$

It was noted earlier that the target-field interaction $\bar{H}'_T$ may be taken to be of second order in the absence of any near degeneracies in the spectrum of target states. Thus, in the nondegenerate case $|D_{in}\rangle$ may be replaced by $|\chi_i\rangle|n\rangle$ to first order. The t matrix then simplifies to

$$t_{m'm}(E;\vec{p}',\vec{p})=\delta_{mn'}\delta_{mn}\langle\vec{p}'|\langle\chi_{i'}|[V_\beta+V_{\beta'}G(E)V_\beta]|\chi_i\rangle|\vec{p}\rangle;$$

the matrix element on the right is just the scattering amplitude in the absence of the field. The derivatives with respect to ξ and ξ', for whose evaluation one requires knowledge of the scattering amplitude off the energy shell, make no contribution in Eq. (3.22) for $n=m$ and $n'=m'$. One sees, in fact, that the first-order approximation (3.22) reduces, as it should, to the approximation derived previously[2,8] for the case of nondegenerate target states. Note that while the result obtained in the nondegenerate case appears not to involve the target-field interaction at all, that interaction has in fact been included—its effect cancels in first order. This cancellation can be seen directly by explicit calculation.[2] A useful feature of the transformed expression (2.20) for the transition amplitude is that the cancellation becomes manifest at the outset (although a physical understanding of this somewhat surprising effect is still lacking). The off-shell contributions and infinite sums which appear in the more general result (3.22) account for the absorption and emission of photons by the target as it makes transitions within a group of nearly degenerate states. The essential simplifying feature of Eq. (3.22) to be recognized is that the dynamics of the interactions between the field and the projectile, the field and the target, and the projectile and target are to be computed *separately*; this decoupling of the interactions is not found in higher orders. To develop further insight into the structure of Eq. (3.22) we introduce, in Sec. IV, additional simplifying assumptions which enable one to put the result in more explicit form.

IV. EXPLICIT RESULTS FOR TWO NEARLY DEGENERATE TARGET STATES

Let us suppose that the initial state of the target is nondegenerate and, that of the excited final states of the target to which transitions can take place in the absence of the field, two of them, call them $|\chi_1\rangle$ and $|\chi_2\rangle$, are nearly degenerate. The effect of the field on these two states can be determined using almost degenerate perturbation theory. An additional small parameter $\delta_4=(\epsilon_1-\epsilon_2)/\hbar\omega$ is introduced and the calculation is carried out to first order only. The dressed-target states obtained in this way are used to construct the matrix elements $t_{m'm}$ in Eq. (3.22). We shall find that the sums over the indices m and m' which appear there can then be performed, leading to a more explicit representation of the transition amplitude $T_{\beta'\beta}$.

A. Dressed-target states

In the two-dimensional subspace of target states spanned by $|\chi_1\rangle$ and $|\chi_2\rangle$ the target Hamiltonian can be represented as $H_T=h_T+\delta h_T$, where

$$h_T=(\epsilon_1+\epsilon_2)/2(|\chi_1\rangle\langle\chi_1|+|\chi_2\rangle\langle\chi_2|),$$
$$\delta h_T=(\epsilon_1-\epsilon_2)/2(|\chi_1\rangle\langle\chi_1|-|\chi_2\rangle\langle\chi_2|); \tag{4.1}$$

δh_T will be treated as a small perturbation. Only the electric-dipole contribution to the target-field interaction, Eq. (2.17), will be retained here. [The first two terms in Eq. (2.17) represent magnetic-dipole and electric-quadrupole corrections, as well as corrections of still higher order.] For the case of linear polarization the interaction, call it h', then takes the form

$$h' = i\left(\frac{2\pi e^2\hbar\omega}{L^3}\right)^{1/2}\left(\sum_j^{(T)} \vec{r}_j\cdot\vec{\lambda}\right)(a-a^\dagger). \tag{4.2}$$

In the absence of the perturbation δh_T the eigenvalue equation to be solved is

$$(h_T+H_F+h')|d_{in}\rangle = e_{in}|d_{in}\rangle, \quad i=1,2. \tag{4.3}$$

We look for a solution in the form

$$|d_{in}\rangle = \sum_{m=-\infty}^{\infty}\sum_{k=1}^{2} a_m^{(k)}(i,n)|\chi_k\rangle|m+n\rangle \tag{4.4}$$

subject to the condition

$$|d_{in}\rangle \to |\chi_i\rangle|n\rangle, \quad h'\to 0. \tag{4.5}$$

Substituting the expansion (4.4) into the Schrödinger equation (4.3) and projecting onto an arbitrary basis vector, we obtain a set of coupled recursion relations for the expansion coefficients. These become decoupled when they are reexpressed in terms of the combinations $a_m^{(1)}\pm a_m^{(2)}$. By comparison with the recursion relations for the Bessel functions, and after imposing the constraint (4.5), we readily find

$$\begin{aligned} a_m^{(k)}(i,n) &= e^{-m\pi/2}\,\tfrac{1}{2}[J_{-m}(\sigma)+J_m(\sigma)], \quad k=i\\ a_m^{(k)}(i,n) &= e^{-im\pi/2}\,\tfrac{1}{2}[J_{-m}(\sigma)-J_m(\sigma)], \quad k\neq i. \end{aligned} \tag{4.6}$$

Here we define

$$\tfrac{1}{2}\hbar\omega\sigma = \left(\frac{2\pi e^2\hbar n\omega}{L^3}\right)^{1/2}\left\langle\chi_2\left|\sum_j^{(T)}\vec{r}_j\cdot\vec{\lambda}\right|\chi_1\right\rangle. \tag{4.7}$$

(The matrix element on the right is taken to be real for simplicity.) The energy eigenvalue is determined by the requirement that the state vector be normalizable[11]; this leads to the result

$$e_{in} = \tfrac{1}{2}(\epsilon_1+\epsilon_2)+n\hbar\omega. \tag{4.8}$$

The orthonormality relations

$$\langle d_{i'n'}|d_{in}\rangle = \delta_{i'i}\delta_{n'n} \tag{4.9}$$

are readily verified using the integral representation

$$J_m(\sigma) = \int_0^{2\pi}\frac{d\phi}{2\pi}e^{im\phi-i\sigma\sin\phi} \tag{4.10}$$

along with the closure relation (3.15).

To improve on this lowest-order solution we follow a standard procedure and introduce the projection operators

$$p(n) = \sum_{i=1}^{2}|d_{in}\rangle\langle d_{in}|, \quad q(n)=1-p(n), \tag{4.11}$$

and let $|d_n\rangle$ represent an as yet undetermined linear combination of $|d_{1n}\rangle$ and $|d_{2n}\rangle$. A formal solution of the eigenvalue equation

$$(h_T+\delta h_T+H_F+h')|D_{in}\rangle = E_{in}|D_{in}\rangle \tag{4.12}$$

is given by

$$|D_{in}\rangle = N_{in}(1+g_q(E_{in})\delta h_T)|d_n\rangle, \tag{4.13}$$

where N_{in} is a normalization constant and g_q satisfies the resolvent equation

$$q(n)(E-h_T-\delta h_T-H_F-h')q(n)g_q(E) = q(n). \tag{4.14}$$

Equation (4.13) will in fact represent a solution provided E_{in} and $|d_n\rangle$ are chosen such that the condition

$$\{E_{in}-e_{in}-p(n)[\delta h_T+\delta h_T g_q(E_{in})\delta h_T]p(n)\}|d_n\rangle = 0 \tag{4.15}$$

is satisfied.

The preceding formulation may be used to construct a solution in the form of an expansion in powers of δh_T. Working only to first order we see from Eq. (4.15) that the level shift is determined by diagonalizing the matrix $\langle d_{in}|\delta h_T|d_{jn}\rangle$. But the matrix is diagonal as it stands. Evaluating the diagonal elements we find

$$\begin{aligned} E_{1n} &\cong \tfrac{1}{2}(\epsilon_1+\epsilon_2)+n\hbar\omega+\tfrac{1}{2}(\epsilon_1-\epsilon_2)J_0(2\sigma),\\ E_{2n} &\cong \tfrac{1}{2}(\epsilon_1+\epsilon_2)+n\hbar\omega-\tfrac{1}{2}(\epsilon_1-\epsilon_2)J_0(2\sigma). \end{aligned} \tag{4.16}$$

The normalized state vectors are then determined, to first order, as

$$|D_{in}\rangle \cong [1+g_q(E_{in})\delta h_T)|d_{in}\rangle. \tag{4.17}$$

For the resolvent g_q we may use the lowest-order approximation

$$g_q \cong \sum_{n'\neq n}\sum_{i=1}^{2}\frac{|d_{in'}\rangle\langle d_{in'}|}{(n-n')\hbar\omega}. \tag{4.18}$$

A straightforward calculation leads to the result

$$|D_{in}\rangle \cong |d_{in}\rangle + \sum_{m=-\infty}^{\infty}\sum_{k=1}^{2} b_m^{(k)}(i,n)|\chi_k\rangle|m+n\rangle, \tag{4.19}$$

with

$$\begin{aligned} b_m^{(k)}(i,n) &= \Delta_i e^{-im\pi/2}\sum_{s\neq 0}\frac{1}{s}J_{-s}(2\sigma)J_{-s-m}(\sigma)\tfrac{1}{2}[1+(-1)^m], \quad k=i\\ &= \Delta_i e^{-im\pi/2}\sum_{s\neq 0}\frac{1}{s}J_{-s}(2\sigma)J_{-s-m}(\sigma)\tfrac{1}{2}[1-(-1)^m], \quad k\neq i. \end{aligned} \tag{4.20}$$

Here s runs over all nonzero integral values and

$$\Delta_i = \begin{cases} (\epsilon_1 - \epsilon_2)/2\hbar\omega, & i=1 \\ (\epsilon_2 - \epsilon_1)/2\hbar\omega, & i=2 \end{cases}. \tag{4.21}$$

B. Transition amplitude

In lowest order the approximation (3.22) reduces to

$$T_{B'B} \cong \sum_m \sum_{m'} \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i(m'-m)\phi} f^*_{\vec{p}'}(\phi) f_{\vec{p}}(\phi) t_{m'm}, \tag{4.22}$$

with $t_{m'm}$ given by Eq. (3.6), the scalar variables being fixed by the conditions (3.9). Since the initial target state $|\chi_i\rangle$ has been taken to be nondegenerate we may make the replacement $|D_m(i,n)\rangle \to |\chi_i\rangle \delta_{mn}$ in Eq. (3.6), the corrections being of second order. The final target state $|\chi_{i'}\rangle$ is one of a pair of almost degenerate states. According to Eqs. (4.4) and (4.19) we have the approximation

$$|D_{m'}(i',n')\rangle = \sum_{k=1}^{2} [a^{(k)}_{m'-n'}(i',n') + b^{(k)}_{m'-n'}(i',n')] \, |\chi_k\rangle. \tag{4.23}$$

Since at this point we are working only to lowest order we may drop the b coefficient in Eq. (4.23). This leads to the approximation

$$t_{m'm} \cong \sum_{k=1}^{2} a^{(k)}_{m'-n'}(i',n') t^{ki} \delta_{mn}, \tag{4.24}$$

where

$$t^{ki} = \langle \vec{p}' | \langle \chi_k \| [V_B + V_{B'} G(E) V_B] |\chi_i\rangle \, |\vec{p}\rangle \tag{4.25}$$

is the on-shell amplitude for the transition taking the target from state $|\chi_i\rangle$ to state $|\chi_k\rangle$ in the absence of the field. Given this explicit dependence on the indices m and m' in Eq. (4.22) the sums can be performed. We are left to evaluate

$$T_{B'B} \cong \sum_{m'} \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i(m'-n)\phi} \exp i[S_{\vec{p}}(\phi) - S_{\vec{p}'}(\phi)] \times \sum_{k=1}^{2} a^{(k)*}_{m'-n'} t^{ki}. \tag{4.26}$$

With the field taken to be linearly polarized, and with corrections of order $p/\mu c$ ignored we have

$$S_{\vec{p}}(\phi) - S_{\vec{p}'}(\phi) = \rho_{\vec{p}\vec{p}'} \sin\phi, \tag{4.27}$$

with

$$\rho_{\vec{p}\vec{p}'} = \frac{2}{\hbar\omega} \left(\frac{2\pi\hbar e^2 n}{\mu^2 \omega L^3}\right)^{1/2} (\vec{p} - \vec{p}') \cdot \vec{\lambda}. \tag{4.28}$$

Using Eq. (4.6), along with the representation (4.10) for the Bessel function and the relation (3.15), the sum over m' can be carried out with the result

$$T_{B'B} \cong \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i(n'-n)\phi} \exp i(\rho_{\vec{p}\vec{p}'} \sin\phi) \times [\cos(\sigma\cos\phi) t^{i'i} - i \sin(\sigma\cos\phi) t^{\hat{i}'i}], \tag{4.29}$$

where $\hat{i}'=1$ for $i'=2$ and $\hat{i}'=2$ for $i'=1$. To perform the ϕ integration we write

$$\rho_{\vec{p}\vec{p}'} \sin\phi + \sigma\cos\phi = (\rho^2_{\vec{p}\vec{p}'} + \sigma^2)^{1/2} \times (\sin\phi\cos\psi + \cos\phi\sin\psi) \tag{4.30}$$

with $\tan\psi = \sigma/\rho_{\vec{p}\vec{p}'}$, and make use of Eq. (4.10) once again. The result is of the form

$$T_{B'B} = \sum_{k=1}^{2} \Gamma^{i'k}_{n-n'} t^{ki}, \tag{4.31}$$

where we have defined

$$\begin{aligned} \Gamma^{11}_m &= \Gamma^{22}_m = J_m([\rho^2_{\vec{p}\vec{p}'} + \sigma^2]^{1/2}) \cos m\psi, \\ \Gamma^{12}_m &= \Gamma^{21}_m = -iJ_m((\rho^2_{\vec{p}\vec{p}'} + \sigma^2)^{1/2}) \sin m\psi. \end{aligned} \tag{4.32}$$

The above results, along with the relations $\sum_m J^2_m(x) = 1$ and $\sum_m J^2_m(x) \sin 2m\psi = 0$, imply the sum rule

$$\sum_{n'=-\infty}^{\infty} \sum_{i'=1}^{2} \left| \sum_{k=1}^{2} \Gamma^{i'k}_{n-n'} t^{ki} \right|^2 = \sum_{k=1}^{2} |t^{ki}|^2. \tag{4.33}$$

It follows that in this lowest-order approximation the differential cross section for scattering into one or the other of the two nearly degenerate states of the target reduces, when summed over final states of the field, to the corresponding differential cross section for scattering in the absence of the field.[12]

In arriving at Eq. (4.31) we used only the lowest-order contribution to the dressed-atom state in Eq. (4.23). The first-order correction to the expansion coefficient is given by Eq. (4.20). When this correction is included we again find the transition amplitude in the form (4.31) but with Eqs. (4.32) replaced by

$$\begin{aligned} \Gamma^{11}_m = \Gamma^{22}_m &= J_m((\rho^2_{\vec{p}\vec{p}'} + \sigma^2)^{1/2}) \cos m\psi + \Delta_{i'} \sum_{s\neq 0} \frac{1}{s} J_{-s}(2\sigma) J_{m+s}((\rho^2_{\vec{p}\vec{p}'} + \sigma^2)^{1/2}) \cos[m\psi + s(\psi + \pi/2)], \\ \Gamma^{12}_m = \Gamma^{21}_m &= -iJ_m((\rho^2_{\vec{p}\vec{p}'} + \sigma^2)^{1/2}) \sin m\psi - i\Delta_{i'} \sum_{s\neq 0} \frac{1}{s} J_{-s}(2\sigma) J_{m+s}((\rho^2_{\vec{p}\vec{p}'} + \sigma^2)^{1/2}) \sin[m\psi + s(\psi + \pi/2)]. \end{aligned} \tag{4.34}$$

[The derivation of this result is straightforward, based once again on Eqs. (3.15) and (4.10), and the details are omitted here.]

The remaining first-order correction terms in Eq. (3.22) are those proportional to the derivatives of the t matrix with respect to the scalar variables. The lowest-order approximation (4.24) suffices here since the term being calculated is itself of first order. After performing the sums over m and m' we arrive at the complete first-order approximation for this model[13]:

$$T_{\beta'\beta} \cong \sum_{k=1}^{2} \Bigg[\Gamma^{i'k}_{n-n'} t^{ki} + (\Gamma^{i'k}_{n-n'+1} + \Gamma^{i'k}_{n-n'-1}) \times \left(\tfrac{1}{2}\hbar\omega(\rho_{\vec{p}} + \rho_{\vec{p}'}) \frac{1}{2} \frac{\partial t^{ki}}{\partial \nu} - \rho_{\vec{p}\vec{p}'} (\vec{p}' - \vec{p}) \cdot \hbar\vec{k} \frac{\partial t^{ki}}{\partial \tau} \right) + (\Gamma^{\hat{i}'k}_{n-n'+1} - \Gamma^{\hat{i}'k}_{n-n'-1})(i\tfrac{1}{2}\hbar\omega\sigma) \frac{\partial t^{ki}}{\partial \xi'} \Bigg] . \tag{4.35}$$

In determining the coefficient of $\partial t^{ki}/\partial\xi'$ we have used the identity

$$2(n'-n)\Gamma^{ik}_{n-n'} + \rho_{\vec{p}\vec{p}'}(\Gamma^{ik}_{n-n'+1} + \Gamma^{ik}_{n-n'-1}) = i\sigma(\Gamma^{\hat{i}k}_{n-n'+1} - \Gamma^{\hat{i}k}_{n-n'-1}) , \tag{4.36}$$

which is easily derived from the integral representation of the Γ coefficients [see Eq. (4.29)] by integration by parts. It is then evident that in the limit $\sigma \to 0$ the off-shell derivative makes no contribution, the result (4.35) reducing to the low-frequency approximation derived previously for the case of nondegenerate target states.[2,8]

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