Electron Collisional Excitation Between Magnetic Sublevels: A Factorization Interpolation Approach

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Abstract

It is shown that the factorization theory of distorted-wave electron collisional excitation can be generalized to treat the excitation between magnetic sublevels, which is needed to model the line polarization resulting from the collisional excitation of electron beams. In this theory, the collision strengths are factorized into two parts. A radial part involving one-electron radial wavefunctions only, and an angular part involving the angular coupling of the target states. Such factorization facilitates the rapid evaluation of collision strengths between magnetic sublevels within an entire transition array through the appropriate use of interpolation procedures.

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I. INTRODUCTION

Electron collisional excitation cross sections are required for calculation of the level population and line emission of hot plasmas, such as those encountered in astrophysical environments. In many cases, only the total excitation cross sections are of importance, at least when the electron distribution functions are isotropic. However, there exist situations where aligned excitation produces polarized line emission. Suggestions have been made to use such polarized light to study beam-plasma interactions in solar flares [**? ?**] and the properties of tokamak plasmas [**?**]. Line polarization is also an important factor to take into account in the analysis of laboratory spectroscopic data involving a directional electron beam, such as electron beam ion traps [**? ?**].

In order to determine the degree of polarization and angular distribution of emitted lines driven by electron collisional excitation, one needs detailed cross sections between the magnetic sublevels of lower and upper states. Several authors have made calculations of such cross sections involving magnetic sublevels. **?**] and **?**] used a nonrelativistic LS-coupling approach. **?**] made distorted-wave (DW) calculations using nonrelativistic radial wavefunctions, but they included intermediate-coupling effects by transforming the reactance matrices from LS-coupling to relativistic pair-coupling scheme [**? ?**]. **?**] performed the first fully relativistic DW calculations of magnetic sublevel collision strengths with a modified version of their previous program for total cross sections.

Since the pioneering work of **?**], the factorization theory of DW collisional excitation is in wide use for calculating total cross sections. This theory enables one to obtain a complete collisional excitation array without calculating a large number of radial integrals by using appropriate interpolation procedures. However, DW calculations of magnetic sublevel sollision strengths have not utilized such factorization-interpolation techniques. In this paper, we generalize the theory of **?**] to the excitation of magnetic sublevels and present its computer implimentation.

II. FACTORIZATION THEORY

The scattering amplitude $B_{m_{si}}^{m_{sf}}$ can be written as (given in Zhang, Sampson, and Clark, 1990, PRA, 41, 198)

$$\begin{aligned} B_{m_{si}}^{m_{sf}} &= \frac{2\pi}{k_i} \sum_{\substack{l_i, m_{li}, j_i, m_i \\ l_f, m_{lf}, j_f, m_f}} (i)^{l_i - l_f + 1} \exp[i(\delta_i + \delta_f)] Y_{l_i}^{m_{li}*}(\hat{\mathbf{k}}_i) Y_{l_f}^{m_{lf}}(\hat{\mathbf{k}}_f) \\ &\quad \times C(l_i \frac{1}{2} m_{li} m_{si}; j_i m_i) C(l_f \frac{1}{2} m_{lf} m_{sf}; j_f m_f) T(\alpha_i, \alpha_f) \end{aligned} \tag{1}$$

where $T(\alpha_i, \alpha_f)$ is the transition matrix elements in the representation where the free electrons are uncoupled to the targets,

$$\alpha_i = k_i \tilde{j}_i m_i J_i M_i, \;\; \alpha_f = k_f \tilde{j}_f m_f J_f M_f, \tag{2}$$

where $\tilde{j}$ denotes $\{l, j\}$. The differential cross section is

$$\frac{d\sigma}{d\hat{k_f}} = \left| B_{m_{si}}^{m_{sf}} \right|^2 . \tag{3}$$

Choosing the direction of the incident electron as the z axis, integrating over $\hat{k_f}$, summing over m_{sf}, and averaging over m_{si} gives

$$\begin{aligned} \sigma(J_f M_f, J_i M_i) &= \frac{\pi}{2k_i^2} \sum_{\substack{\tilde{j}_i, \tilde{j}_i', \tilde{j}_f \\ m_{si}, m_f}} (i)^{l_i - l_i'} \exp[i(\delta_i - \delta_{i'})]([l_i][l_i'])^{\frac{1}{2}} \\ &\quad \times (-1)^{j_i + j_i' + 2m_i} ([j_i][j_i'])^{\frac{1}{2}} \begin{pmatrix} j_i & \frac{1}{2} & l_i \\ -m_i & m_{si} & 0 \end{pmatrix} \begin{pmatrix} j_i' & \frac{1}{2} & l_i' \\ -m_i & m_{si} & 0 \end{pmatrix} \\ &\quad \times T(\alpha_i, \alpha_f) T^*(\alpha_i', \alpha_f) \end{aligned} \tag{4}$$

In the first order purterbation theory

$$T(\alpha_i, \alpha_f) = -2i < J_i M_i \tilde{j}_i m_i | V | J_f M_f \tilde{j}_f m_f > \tag{5}$$

where V is the coulomb interaction. In your derivation, you started off with the square of this matrix element, however, it is the two matrix elements involve different initial states that enter the expression for the cross sections. When both initial and final states involve one free electron, it can be expanded as

$$V = 2 \sum_t \sum_{\substack{\tilde{j}_i j_0 \\ \tilde{j}_f j_1}} \sum_{i \neq j} \left(Z^t(j_0, j_1) \cdot Z^t(\tilde{j}_i, \tilde{j}_f) \right) \Phi^t(j_0 \tilde{j}_i, j_1 \tilde{j}_f) \tag{6}$$

substitute into Eq. **??**

$$
\begin{aligned}
\sigma(J_f M_f, J_i M_i) \;=\; & \frac{8\pi}{k_i^2} \sum_{\substack{\tilde{j}_i,\tilde{j}_i',\tilde{j}_f \\ m_{si},m_f}} \sum_{\substack{j_0,j_1 \\ j_0',j_1'}} \sum_{t,t'} (i)^{l_i-l_i'} \exp[i(\delta_i-\delta_{i'})]([l_i][l_i'])^{\frac{1}{2}} \\
& \times(-1)^{j_i+j_i'+2m_i}([j_i][j_i'])^{\frac{1}{2}} \begin{pmatrix} j_i & \frac{1}{2} & l_i \\ -m_i & m_{si} & 0 \end{pmatrix} \begin{pmatrix} j_i' & \frac{1}{2} & l_i' \\ -m_i & m_{si} & 0 \end{pmatrix} \\
& \times \left\langle J_i M_i \tilde{j}_i m_i \left| Z^t(j_0 j_1)\cdot Z^t(\tilde{j}_i \tilde{j}_f) \right| J_f M_f \tilde{j}_f m_f \right\rangle \\
& \times \left\langle J_i M_i \tilde{j}_i' m_i \left| Z^{t'}(j_0' j_1')\cdot Z^{t'}(\tilde{j}_i' \tilde{j}_f) \right| J_f M_f \tilde{j}_f m_f \right\rangle \\
& \times \Phi^t(j_0\tilde{j}_i, j_1\tilde{j}_f)\Phi^{t'}(j_0'\tilde{j}_i', j_1'\tilde{j}_f) \qquad (7)
\end{aligned}
$$

Expanding the scalar product in the spherical tensors

$$
\begin{aligned}
\left\langle J_i M_i \tilde{j}_i m_i \left| Z^t(j_0 j_1)\cdot Z^t(\tilde{j}_i \tilde{j}_f) \right| J_f M_f \tilde{j}_f m_f \right\rangle \;=\; & \sum_q (-1)^q < \tilde{j}_i m_i | z^t_{-q}(\tilde{j}_f \tilde{j}_f) | \tilde{j}_i m_i > \\
& \times < J_i M_i | Z^t_q(j_0 j_1) | J_f M_f > \\
=\; & (-1)^q (-1)^{j_i-m_i} \begin{pmatrix} j_i & t & j_f \\ -m_i & -q & m_f \end{pmatrix} \\
& \times(-1)^{J_i-M_i} \begin{pmatrix} J_i & t & J_f \\ -M_i & q & M_f \end{pmatrix} \\
& \times \left\langle J_i M_i \left\| Z^t(j_0 j_1) \right\| J_f M_f \right\rangle \qquad (8)
\end{aligned}
$$

The summation over q may be dropped since it is fixed by the $3j$ symbols and is $M_i - M_f$, therefore

$$
\begin{aligned}
\sigma(J_f M_f, J_i M_i) \;=\; & \frac{8\pi}{k_i^2} \sum_{tt'} \begin{pmatrix} J_i & t & J_f \\ -M_i & q & M_f \end{pmatrix} \begin{pmatrix} J_i & t' & J_f \\ -M_i & q' & M_f \end{pmatrix} \\
& \times \sum_{\substack{j_0 j_1 \\ j_0' j_1'}} \left\langle J_i M_i \left\| Z^t(j_0 j_1) \right\| J_f M_f \right\rangle \left\langle J_i M_i \left\| Z^{t'}(j_0' j_1') \right\| J_f M_f \right\rangle \\
& \times \sum_{\substack{\tilde{j}_i,\tilde{j}_i',\tilde{j}_f \\ m_{si},m_f}} (i)^{l_i-l_i'} \exp[i(\delta_i-\delta_{i'})]([l_i][l_i'])^{\frac{1}{2}} \\
& \times([j_i][j_i'])^{\frac{1}{2}} \begin{pmatrix} j_i & \frac{1}{2} & l_i \\ -m_i & m_{si} & 0 \end{pmatrix} \begin{pmatrix} j_i' & \frac{1}{2} & l_i' \\ -m_i & m_{si} & 0 \end{pmatrix} \\
& \times \begin{pmatrix} j_i & t & j_f \\ -m_i & -q & m_f \end{pmatrix} \begin{pmatrix} j_i' & t' & j_f \\ -m_i & -q' & m_f \end{pmatrix} \\
& \times \Phi^t(j_0\tilde{j}_i, j_1\tilde{j}_f)\Phi^{t'}(j_0'\tilde{j}_i', j_1'\tilde{j}_f) \qquad (9)
\end{aligned}
$$

or it may be written as

$$
\begin{aligned}
\sigma(J_fM_f, J_iM_i) &= \frac{8\pi}{k_i^2}\sum_{tt'}\begin{pmatrix} J_i & t & J_f \\ -M_i & q & M_f \end{pmatrix}\begin{pmatrix} J_i & t' & J_f \\ -M_i & q' & M_f \end{pmatrix} \\
&\quad \times \sum_{\substack{j_0j_1 \\ j_0'j_1'}} A^t(j_0j_1)A^{t'}(j_0'j_1')Q^{tt'}(j_0j_1, j_0'j_1') \qquad (10)
\end{aligned}
$$

with

$$
A^t(j_0j_1) = \left\langle J_iM_i \left|\left| Z^t(j_0j_1) \right|\right| J_fM_f \right\rangle \qquad (11)
$$

and

$$
\begin{aligned}
Q^{tt'}(j_0j_1, j_0'j_1') &= \sum_{\substack{\tilde{j}_i, \tilde{j}_i', \tilde{j}_f \\ m_{si}, m_f}} (i)^{l_i - l_i'} \exp[i(\delta_i - \delta_{i'})]([l_i][l_i'])^{\frac{1}{2}} \\
&\quad \times([j_i][j_i'])^{\frac{1}{2}} \begin{pmatrix} j_i & \frac{1}{2} & l_i \\ -m_i & m_{si} & 0 \end{pmatrix}\begin{pmatrix} j_i' & \frac{1}{2} & l_i' \\ -m_i & m_{si} & 0 \end{pmatrix} \\
&\quad \times \begin{pmatrix} j_i & t & j_f \\ -m_i & -q & m_f \end{pmatrix}\begin{pmatrix} j_i' & t' & j_f \\ -m_i & -q' & m_f \end{pmatrix} \\
&\quad \times\Phi^t(j_0\tilde{j}_i, j_1\tilde{j}_f)\Phi^{t'}(j_0'\tilde{j}_i', j_1'\tilde{j}_f) \qquad (12)
\end{aligned}
$$

In Eq. **??**, ony after summation over M_f and averaging over M_i, the first two $3j$ symbols produces $\delta_{tt'}\delta_{qq'}$, then the summation over m_f and q in the last two $3j$ symbols gives $\delta_{j_ij_i'}$, and finally, the summation over m_{si} and m_i gives $\delta_{l_il_i'}$, therefore cancels the phase factors, we recover the HULLAC factorization for the total cross sections.

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