Ionization of heavy atoms by polarized relativistic protons

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Ionization of heavy atoms by polarized relativistic protons

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The effect due to the polarization of the incident high-energy ($\sim$GeV) proton beam on the ionization cross section of heavy atoms is investigated. In particular, with the use of Darwin wave functions for the atomic electron, the effect for hydrogenlike atoms is worked out. A numerical illustration shows that the polarization effect is completely insignificant. We also conclude that the K-shell ionization process is completely insensitive to the polarization of the incident beam.

In recent years considerable theoretical and experimental effort has been made to study the relativistic effects in the ionization process of medium-heavy and heavy atoms by high-energy projectiles. In particular, the recent experiment by Anholt *et al.*[1] on the K-vacancy production by protons of 4.88 GeV in energy obtained from the Lawrence Berkeley Laboratory Bevatron (Bevalac) showed that, in addition to Coulomb interaction between the projectile proton and the target K electron, the transverse and the spin-flip effects contribute significantly in such a process. The transverse effect which accounts for the retardation in the interaction between the proton and the atomic electron increases as the proton becomes more relativistic and the spin-flip effect, caused by the change of spin of the atomic electron while being ionized, contributes significantly for targets of heavy atoms.[1-3] Thus it would be of interest to see if this spin-flip effect can be isolated from other effects so that one can better understand the relativistic nature of the target atom. One way of achieving this will be to study the ionization of a polarized target by a polarized beam of high-energy protons and investigate the analyzing power for such a process. In the following we shall make a study of such polarization effects and shall restrict ourselves to hydrogenlike atoms.

The interaction of an atom with a beam of high-energy protons in the first Born approximation is described, in the notation of Ref. 4, by the following cross-section formula[4]:

$$\frac{d\sigma}{d\Omega_{p'}}=\frac{4M^2e^4}{q^4}\frac{|\vec{\mathrm{P}}'|}{|\vec{\mathrm{P}}|}\sum_{\underline{S},\underline{S}'}|\bar{u}(\underline{P}',\underline{S}')\gamma_\mu u(\underline{P},\underline{S})J^\mu|^2 \ , \quad (1)$$

where $\underline{P},\underline{P}'$, $\underline{S},\underline{S}'$ are, respectively, the initial and final four-momentum and spin of the proton, the three vectors are denoted by arrows, M is the mass of proton, $\underline{q}=\underline{P}'-\underline{P}$ is the four-momentum transfer, and

$$J^\mu\equiv\langle n|e^{i\vec{q}\cdot\vec{r}}\gamma^0\gamma^\mu|0\rangle \quad (2)$$

is the transition matrix element for the atomic electron. For unpolarized incident protons, the $\sum_{\underline{S},\underline{S}'}$ can be carried out by the usual trace method:

$$\sum_{\underline{S},\underline{S}'}|\bar{u}(\underline{P}',\underline{S}')\gamma_\mu u(\underline{P},\underline{S})|^2=\tfrac{1}{2}\mathrm{Tr}\left[\gamma_\mu\left(\frac{\not P+M}{2M}\right)\gamma_\nu\left(\frac{\not P'+M}{2M}\right)\right]$$
$$=\frac{1}{2M^2}\left(P'_\mu P_\nu+P_\mu P'_\nu+g_{\mu\nu}\frac{q^2}{2}\right) \ , \quad (3)$$

where $\not P=\gamma^\alpha P_\alpha$, and the summation over the repeated index α is implied. Substitution of (3) into (1) gives the usual formula for unpolarized incident protons[5]:

$$\frac{d\sigma}{d\Omega_{p'}}=\frac{2e^4}{\underline{q}^4}\frac{|\vec{\mathrm{P}}'|}{|\vec{\mathrm{P}}|}\left(P_\mu P'_\mu+P'_\mu P_\nu+\frac{g_{\mu\nu}q^2}{2}\right)J^\mu J^{\nu *} \ . \quad (4)$$

This formula is covariant and exact and can be reduced to the Fano-Anholt three-dimensional form in the forward scattering approximation applied to the incident proton.

Now let us consider a polarized proton beam with its polarization completely described by the four-covariant spin vector S^μ which is defined to be $(0,\hat{S})$ in the rest frame.[4] With such a polarized proton beam, Eq. (1) becomes

$$\frac{d\sigma}{d\Omega_{p'}}=\frac{4M^2e^4}{q^4}\frac{|\vec{\mathrm{P}}'|}{|\vec{\mathrm{P}}|}\times\mathrm{Tr}\left[\gamma^\mu\left(\frac{1+\gamma_5 S}{S}\right)\left(\frac{\not P+M}{2M}\right)\gamma^\nu\left(\frac{\not P'+M}{2M}\right)\right]J_\mu J_\nu^* \ , \quad (5)$$

where we have introduced the spin projection operator $(1+\gamma_5\not S/2)$ for the proton. Keeping in mind that

$$\mathrm{Tr}\gamma_5\ (\text{odd number of } \gamma^\mu\text{'s})=0$$

and

$$\mathrm{Tr}(\gamma_5\gamma_\alpha\gamma_\beta\gamma_\delta\gamma_\rho)=4i\epsilon_{\alpha\beta\delta\rho} \ ,$$

with $\epsilon_{\alpha\beta\delta\rho}$ as the complete (fourth-ranked) antisymmetric tensor,[4] we work out the extra contribution due to the term $\gamma_5\not S$ in Eq. (5) and obtain

$$\mathrm{Tr}(\gamma^\mu\gamma_5\not S\not P\gamma^\nu M+\gamma^\mu\gamma_5 SM\gamma^\nu\not P')J_\mu J_\nu^*$$
$$=-4Mi(\epsilon_{\mu\alpha\beta\nu}S_\alpha P_\beta+\epsilon_{\mu\delta\nu\rho}S_\delta P'_\rho)J_\mu J_\nu^* \ . \quad (6)$$

Note that this extra contribution does not vanish, in general, even though the tensors ϵ imply that the terms inside the bracket must be antisymmetric in μ and ν since $J_\mu J_\nu^*\neq J_\nu J_\mu^*$, in general. However, in the case of an unpolarized free-electron target, one can show that $J_\mu J_\nu^*$ is indeed symmetric in μ,ν and hence Eq. (6) vanishes, giving back the well-known result that polarizing the incident beam does not give any different scattering cross sections in this case in the first Born approximation.

In order to investigate the contribution of (6) to scattering processes with bound atomic electrons, let us denote the contribution in Eq. (6) by symbol C:

$$C=-4Mi(\epsilon_{\mu\alpha\beta\nu}S_\alpha P_\beta+\epsilon_{\mu\delta\nu\rho}S_\delta P'_\rho)J_\mu J_\nu^* \quad . \tag{7}$$

Also, J_μ can be identified with the electronic form factors F_n and $\vec{G}_n$ of Fano[6] and Anholt[1] as

$$\begin{aligned} J_0&=F_n(q)=\langle n|e^{i\vec{q}\cdot\vec{r}}|0\rangle \ , \\ \vec{J}&=\vec{G}_n(q)=\langle n|\vec{\alpha}e^{i\vec{q}\cdot\vec{r}}|0\rangle \ . \end{aligned} \tag{8}$$

Since ϵ in (7) implies $\mu\neq\nu$ and since there are no cross terms $F_n\vec{G}_n$ for atomic transitions due to different selection rules, therefore $\mu\neq\nu\neq0$, and Eq. (7) can finally be written in three-dimensional form as

$$C=4M[(E-E')\vec{S}-S_0(\vec{P}-\vec{P}')]\cdot i(\vec{G}_n\times\vec{G}_n^*) \quad . \tag{9}$$

We have denoted $\vec{P}=(E,\vec{P})$ and $\underline{P}'=(E',\vec{P}')$ for the incident proton. To evaluate the term $\vec{G}_n\times\vec{G}_n^*$, let us follow Anholt's approach[2] for hydrogenlike atoms.

Anholt treats the atomic electron by using semirelativistic Darwin wave functions[7]:

$$\psi_{ns}=Na_s\phi_n \ , \tag{10}$$

where

$$a_+=\begin{pmatrix}\frac{i}{2c}\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)\\ -\frac{i}{2c}\frac{\partial}{\partial z}\\ 0\\ 1\end{pmatrix};\quad a_-=\begin{pmatrix}\frac{i}{2c}\frac{\partial}{\partial z}\\ \frac{i}{2c}\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\\ 1\\ 0\end{pmatrix} \tag{11}$$

are the four operator spinors for spin-up and spin-down states, respectively; ϕ_n being a normalized nonrelativistic eigenfunction and N is the normalization factor. We generalize the state of the electron by letting it have the possibility of being polarized. Thus we write our electron ground-state wave function as

$$\psi_{0s}=N(Aa_++Ba_-)\phi_0 \ , \tag{12}$$

with

$$A^2+B^2=1 \ . \tag{13}$$

For ionization processes,

$$\vec{G}_n(q)\equiv\vec{G}(q)=\langle\epsilon|\vec{\alpha}e^{i\vec{q}\cdot\vec{r}}|0\rangle \ , \tag{14}$$

where $|0\rangle$ and $|\epsilon\rangle$ are the ground and continuum states, respectively. We can compute respectively, the elements G_x, G_y, and G_z by choosing $\hat{z}\parallel\vec{q}^2$, where

$$G_x=\int\psi^*_{\epsilon s'}\alpha_x\psi_{0s}e^{iqz}d^3r \ , \tag{15}$$

etc. Furthermore, in this choice of coordinate, one can show that[2]

$$G_z=\frac{\Delta E}{|\vec{q}|c}F \ , \tag{16}$$

where $\Delta E=\epsilon-\epsilon_0$. Since we have remarked that there cannot exist a cross term like $F\vec{G}$, therefore both G_xG_z and G_yG_z terms vanish. Hence only the z component may survive in the term $(\vec{G}_n\times\vec{G}_n^*)$ in (9). Following Anholt[2] and using (10) and (11), we find that

$$\begin{aligned} G_{x++}&=G_{x--}=\frac{id}{c}I_x \ , \\ G_{y++}&=G_{y--}=\frac{id}{c}I_y \ , \\ G_{x+-}&=\frac{d|\vec{q}|}{2c}I_0 \ , \\ G_{x-+}&=-\frac{d|\vec{q}|}{2c}I_0 \ , \\ G_{y+-}&=G_{y-+}=\frac{id|\vec{q}|}{2c}I_0 \ , \end{aligned} \tag{17}$$

where the symbol $G_{s's}$ denotes the electron transition with its spin changed from s to s',

$$d=N^0N'=\left[1+\left(\frac{Z\alpha}{2}\right)^2\right]^{-1/2}\left[1+\left(\frac{k\alpha^2}{2}\right)\right]^{-1/2}$$

originated from the normalization factors with $\alpha=\frac{1}{137}$, and the integrals I_0, I_x, and I_y are given by

$$\begin{aligned} I_0&=\int\phi_\epsilon^*\phi_0e^{iqz}d^3r \ , \\ I_x&=\int\phi_\epsilon^*\frac{\partial}{\partial x}\phi_0e^{iqz}d^3r \ , \\ I_y&=\int\phi_\epsilon^*\frac{\partial}{\partial y}\phi_0e^{iqz}d^3r \ . \end{aligned} \tag{18}$$

The expressions for these integrals are all given in Anholt's article.[2] Using (17), we find that only the $\hat{z}$ component of $\vec{G}_n\times\vec{G}_n^*$ survives when the electron flips its spin. The result is

$$\begin{aligned} (\vec{G}_n\times\vec{G}_n^*)_z&=G_xG_y^*-G_y-G_x^* \\ &=i\left(\frac{d^2|\vec{q}|^2}{2c^2}\right)(A^2-B^2)|I_0|^2 \ . \end{aligned} \tag{19}$$

Substituting into (9), we find the contribution to $(d\sigma/d\Omega)$ due to polarization of the incident protons given by

$$C=\frac{2d^2|\vec{q}|^2M}{c^2}(S_0|\vec{q}|-\bar{Q}S_z)(A^2-B^2)|I_0|^2 \ , \tag{20}$$

where $\bar{Q}=E-E'$ and $\vec{q}=\vec{P}-\vec{P}'$ are, respectively, the energy and momentum transfers. From (20), we see immediately that for an unpolarized atomic electron $(A=B=1/\sqrt{2})$, $C=0$. When the result in (6) is expressed in the form of Eq. (20) substituted back in (5) and the expression for $d\sigma/d\Omega_p$ is converted into three-dimensional form in the forward scattering approximation, we finally obtain a generalization of Anholt's result [Ref. 2, Eq. (16)] which may be written as $(q\equiv|\vec{q}|$ here)

$$\frac{d^2\sigma}{d\epsilon\,dq}=\frac{8\pi qd^2}{v^2}\left[\frac{|I_0|^2}{q^4}+\left|\frac{\beta(\sin\lambda)I_x}{c(q^2-q_m^2\beta^2)}\right|^2+\left(\frac{2M}{E^2}(S_0q-\bar{Q}S_z)(A^2-B^2)+\beta^2\sin^2\lambda\right)\left|\frac{I_0q}{2c(q^2-q_m^2\beta^2)}\right|^2\right] \ . \tag{21}$$

We have followed Anholt and assumed that the collision occurs in the xz plane and that λ is the angle between $\vec{\beta}$ and $\vec{q}$ where $\cos\lambda = q_m/q$ and $q_m = \Delta E/v$ is the minimum momentum transferred to the atom. Equation (21) applies for the ionization of a hydrogenlike atom from the ground state to the continuum state with energy ϵ. We see that the polarization effects of both the incident proton and the atomic electron enter only into the third term which is the spin-flip term of Anholt's original result for K-shell ionization. To apply Eq. (21) to K-shell ionization, we have to take care of the double occupancy of the K shell. Thus the first two terms in (21) (i.e., the longitudinal and transverse terms) just double, giving back the results of Anholt's equation (16).[2] We note also that the use of the generalized description of the atomic electron [Eq. (12)] does not affect Anholt's original result. For K-shell electrons, the polarization effects vanish identically since we must have A equal to B on account of Pauli's exclusion principle, and the remaining spin-flip term doubles again, reducing back once more to Anholt's result. Thus we arrive at the conclusion that, as far as the K-shell ionization is concerned, there is no difference whether a polarized or unpolarized incident proton beam is used.

Let us now investigate the magnitude of the polarization effects for hydrogelike atoms here. Since it has been shown that for high-energy one-photon exchange scattering processes, the transverse polarization effect enters by an order of (M/E) smaller than the longitudinal effect; therefore we shall assume the intitial proton spin $\vec{S}$ to be along $\vec{\beta}$.

TABLE I. Polarization contributions as a function of incident proton energy for ^{92}U.

Proton energy (GeV)	Spin-flip term (b)	Polarization contribution (b) with $A=1$, $B=0$
1.5	2.41×10^{-1}	-1.15×10^{-5}
2.0	3.69×10^{-1}	-1.35×10^{-5}
2.5	4.55×10^{-1}	-1.33×10^{-5}
3.0	0.52	-1.25×10^{-5}
3.5	0.58	-1.19×10^{-5}
4.0	0.62	-1.08×10^{-5}
4.5	0.66	-1.0×10^{-5}
5.0	0.69	-9.29×10^{-6}

Furthermore, it can be shown that[4]

$$S_0 = \pm\beta|\vec{S}|, \quad |\vec{S}| = E/M \ , \tag{22}$$

with $\pm$ corresponding to right- and left-hand polarizations. We finally obtain the polarization contribution in (21) to be

$$\frac{2M}{E^2}(S_0 q - \bar{Q}S_z)(A^2-B^2) = \frac{2}{E}(\pm\beta q - \bar{Q}\cos\lambda)(A^2-B^2) \ . \tag{23}$$

To see the significance of (23), we compute the total cross section with this polarization effect. Since this effect enters only in the spin-flip term, we therefore compute only σ_{SF}. Following the integration variables (in atomic units) used by Anholt,[2] we finally obtain

$$\sigma_{SF} = \frac{4\pi d^2}{\eta_K Z^4}\int_{W_{min}}^{\infty} dW \int_{Q_{min}}^{\infty} \frac{dQ}{Q}\frac{(Z\alpha)^2}{[1-\beta^2(Q_{min}/Q)]^2}\left[\frac{1}{4}\right]\left[\beta^2\left[1-\frac{Q_{min}}{Q}\right]\frac{2}{E}\left(\pm\beta Z\sqrt{Q} - \frac{Z^2(W-1)}{2}\sqrt{Q_{min}/Q}\,(A^2-B^2)\right)\right]F_K \ , \tag{24}$$

where

$$W = k^2+1 = \epsilon/I_K + 1 \approx \bar{Q}/I_K + 1, \ I_K = \tfrac{1}{2}Z^2, \ Q = q^2/Z^2 \ ,$$

$Q_{min} = W^2/4\eta_K$, $W_{min} = \theta_K$, and $\eta_K = v^2/Z^2$. The function F_K is defined as

$$F_K = Z^2 I_0^2 = (3Q+W)Q\frac{2^7\exp\{-(2/k)\tan^{-1}[2k/(Q+1-k^2)]\}}{3[1-\exp(-2\pi/k)][(Q+1-k^2)^2+4k^2]^3} \ . \tag{25}$$

The first term in (24) is the usual spin-flip term, and the second one is the polarization contribution. We have computed Eq. (24) as a function of incident energy for a large Z $(=92)$ for the extreme case with $A=1$, $B=0$, and for left-hand polarized protons. The result is shown in Table I. The case when $A=0$, $B=1$ can be obtained by just changing the signs of the results.

From Table I, we see that the polarization effect is completely negligible for all energies compared to the original spin-flip contributions. However, it was shown before[2,8] that this spin-flip effect, though important, is smaller than the transverse effect in Eq. (21) at the energies considered (see Table I); therefore we see that the polarization effect is completely negligible in the atomic ionization process as treated here. Even if one extends this work to higher energies where the spin-flip effect becomes important, the polarization effect is still found to be negligible. Furthermore, the change of spin of the outgoing proton is also negligible[2] due to the conservation of helicity, and the forward scattering approximation applied here for the proton is much heavier than the atomic electron. Thus we conclude that one does not learn anything significant by ionizing a relativistic atom with polarized incident proton beam and, as far as K-shell ionization is concerned, the process does not distinguish between a polarized or an unpolarized incident beam.

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