Relativistic second-order Born theory for electron capture

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The asymptotic dependence of the second-order Born term on the collision energy E is reexamined. In contrast to previous work, a *relativistic* free-particle propagator is used, and allowance is made for the spectator electrons of the target by means of a screened potential. These modifications do not change the behavior of the capture cross section like $(\ln E)^2/E$.

In a recent study[1,2] of electron capture by swift bare ions in collisions with target atoms the second-order Born approximation has been used to extract the high-energy behavior of the capture cross section, as it is known from nonrelativistic theories that the second-order term in the Born series is asymptotically the dominating one for rearrangement collisions.[3] Two approximations were made in these calculations, first, a nonrelativistic propagator was used in the second-order Born term and second, the target atom was idealized by a one-electron ion. In addition, in the work by Humphries and Moiseiwitsch[1] a peaking approximation was introduced and only the lowest-order terms in the fine-structure constant were retained. Their result, an asymptotic E^{-1} dependence of the capture cross section, differs, however, from the logarithmic energy dependence, $(\ln E)^2/E$, which has been found without this peaking approximation.[2]

In the present communication we improve upon our previous work[2] by replacing the nonrelativistic free-particle propagator by a relativistic one and by adding to the interaction between the active target electron and the target nucleus an average field caused by the presence of the spectator electrons. Atomic units ($\hbar=e=m=1$) are used.

In the semiclassical theory, the exact transition amplitude for electron capture by a bare projectile with charge Z_P is given by

$$a_{fi}=-i\int dt'd\mathbf{r}'\bar{\psi}_f^{(-)\prime}(r')\gamma_0 V_P'(r')[T^{-1}\psi_i^T(r)] , \qquad (1)$$

with $\bar{\psi}=\psi^\dagger\gamma_0$ and γ_0 a Dirac matrix. The quantities defined in the projectile frame of reference are denoted by a prime, and $V_P'(r')=-Z_P/|\mathbf{r}'|$ is the electron-projectile interaction. $\psi_i^T(r)$ describes the bound target electron, and the operator T^{-1} transforms this function into the projectile reference frame. The coordinates $r'=(ct',\mathbf{r}')$ and $r=(ct,\mathbf{r})$ are connected by a Lorentz transformation.

The second-order Born approximation is obtained upon expanding the exact electronic scattering state $\psi_f^{(-)}$ which asymptotically develops into a projectile bound state ψ_f^P in terms of the electron-target and electron-projectile interactions, V_T and V_P, respectively, and retaining only the first two terms[4]

$$\psi_f^{(-)}(r_1)=\psi_f^P(r_1)+\frac{1}{c}\int d^4r_2 S_F^{(-)}(r_1-r_2)A_T(r_2) \times\psi_f^P(r_2) . \qquad (2)$$

The electromagnetic potential of the residual target ion is $A_T=\gamma_0 V_T$ with

$$V_T(r)=-(1/|\mathbf{r}|)[1+(Z_T-1)\exp(-\mu|\mathbf{r}|)] ,$$

where Z_T is the nuclear target charge and, for definiteness, an exponential screening function is used to represent the presence of the Z_T-1 spectator electrons; the precise form of the screening function is, however, not important in the present context. For $\mu=0$, the pure Coulomb field $V_T=-Z_T/|\mathbf{r}|$ of Ref. 2 is recovered.

The relativistic free-particle propagator S_F is most readily given by its Fourier representation. It can be expressed in terms of the normalized Dirac plane waves

$$q_s(r)=(2\pi)^{-2}u_q^s\exp(i\mathbf{q}\cdot\mathbf{r}-i\delta_s\omega t) ,$$

where u_q^s is a Dirac spinor,

$$u_q^s=[(\omega+mc^2)/2\omega]^{1/2}[1+\delta_s\boldsymbol{\alpha}\cdot\mathbf{q}c/(\omega+mc^2)]e_s ,$$

with $\alpha_{x,y,z}$ Dirac matrices and e_s a four-dimensional unit vector[5] (these spinors obey the conventional completeness relation, $\sum_{s=1}^4 u_q^s u_q^{s\dagger}=1$, in contrast to the spinors as defined in Ref. 4):

$$S_F^{(\pm)}(r_1-r_2) =\int_{-\infty}^{\infty}d\omega\int d\mathbf{q}\frac{1}{\omega-q_0c\pm i\epsilon}\sum_{s=1}^{4}\delta_s q_s(r_1)\bar{q}_s(r_2) \qquad (3)$$

with $\epsilon\to 0+$,

$$\delta_s=\begin{cases}1, & s=1,2\\ -1, & s=3,4,\end{cases}$$

$q_0c\equiv E_q=(\mathbf{q}^2c^2+m^2c^4)^{1/2}$ and $\bar{q}_s=q_s^\dagger\gamma_0$. The different sign for $s=1,2$ and $s=3,4$ is a consequence of the relativistic propagation of positive-energy states ($s=1,2$) forward in time and negative-energy states ($s=3,4$) backward in time in case of $S_F^{(+)}$ and vice versa for $S_F^{(-)}$.

The transition amplitude in the second-order Born approximation is obtained by inserting (2) into (1). In the following, only the second-order Born term to a_{fi}, denoted by a_{fi}^{B2} [which follows from inserting the second term on the right-hand side of (2) into (1)] will be considered. As we have chosen to evaluate the transition matrix element in the projectile reference frame, the target field A_T has to be transformed according to[2]

$$A_T'(r')=T^{-1}A_T(r)T=\gamma\left[1+\frac{v}{c}\alpha_z\right]V_T(r)$$

$$=-\frac{1}{2\pi^2}\gamma\left[1+\frac{v}{c}\alpha_z\right]\int d\mathbf{s}_0 e^{i\mathbf{s}_{0\perp}\cdot(\mathbf{r}_\perp'+\mathbf{b})}e^{is_{0z}\gamma(z'+vt')}\left[\frac{1}{s_0^2}+\frac{Z_T-1}{s_0^2+\mu^2}\right], \tag{4}$$

where the z direction is defined by the collision velocity $\mathbf{v}$ and $\gamma=(1-v^2/c^2)^{-1/2}$. In the last step, the Fourier representation of V_T has been used together with the transformation from r to r' at impact parameter $\mathbf{b}$.

By introducing a complete set of Dirac plane waves $k_\sigma(r)$ into (1) after T^{-1}, the evaluation of the transition amplitude proceeds in the same way as done in Ref. 2 and will not be repeated here. We only give the final result for the second-order Born term

$$a_{fi}^{B2}=-i\frac{Z_P}{4\pi^4\gamma v}\sum_{s,\sigma=1}^{4}\delta_s\int d\mathbf{q}\,d\mathbf{k}'\frac{1}{\delta_s(E_i/\gamma-vk_z')-q_0c+i\epsilon}[u_k^{\sigma\dagger}\phi_i(\mathbf{k})]e^{i\mathbf{k}_\perp'\cdot\mathbf{b}}(u_q^{s\dagger}T^{-1}u_k^{\sigma})\frac{1}{(\mathbf{q}-\mathbf{k}')^2}$$

$$\times\int d\mathbf{s}_{0\perp}\left[\frac{1}{s_{0\perp}^2+s_{0z}^2}+\frac{Z_T-1}{s_{0\perp}^2+s_{0z}^2+\mu^2}\right]e^{i\mathbf{s}_{0\perp}\cdot\mathbf{b}}\left[\phi_f^\dagger(\mathbf{s}_{0\perp}+\mathbf{q}_\perp,\gamma s_{0z}+q_z)\left[1+\frac{v}{c}\alpha_z\right]u_q^s\right], \tag{5}$$

where $s_{0z}=\gamma^{-1}[-E_f/v+E_i/(\gamma v)-k_z']$ is fixed by energy conservation, E_f and E_i are the energies and $\phi_i(\mathbf{p})$ and $\phi_f(\mathbf{p}_\perp,p_z)$ the Fourier transforms of the final and initial bound states, respectively. The vectors $\mathbf{k}$ and $\mathbf{k}'$ are related by $\mathbf{k}_\perp=\mathbf{k}_\perp'$ and $k_z=k_z'/\gamma+E_iv/c^2$ [note that in Eq. (6) of Ref. 2, $(\mathbf{q}-\mathbf{k})^2$ should read $(\mathbf{q}-\mathbf{k}')^2$].

Equation (5) differs from the corresponding equation of our previous work in the energy denominator $\delta_s(E_i/\gamma-vk_z')-q_0c$ and in the multiplicative sign factor δ_s which results from the proper propagation of the electron and positron states; in the case of a nonrelativistic propagator, $\delta_s\Longrightarrow1$ and $q_0c\Longrightarrow\mathbf{q}^2/2$. Moreover, consideration of the presence of the spectator electrons introduces an additional term in the $\mathbf{s}_{0\perp}$ integrand which is *finite* as $s_0\rightarrow0$.

Let us now consider the energy dependence of the transition amplitude as $E=\gamma M_Pc^2\rightarrow\infty$ (M_P being the projectile mass). A $\gamma^{-1/2}$ dependence arises from the combination of the prefactor γ^{-1} in (5) and from the asymptotic dependence of T^{-1} like $\gamma^{1/2}$. Moreover, s_{0z} behaves like γ^{-1} which implies that the integral over $ds_{0\perp}$ of the term proportional to $(s_{0\perp}^2+s_{0z}^2)^{-1}$ diverges asymptotically like $\ln\gamma$, while the integral over the second term containing the screening constant μ is independent of γ as $\gamma\rightarrow\infty$. All other quantities in (5) remain finite in this limit. Hence $a_{fi}^{B2}\sim\gamma^{-1/2}\ln\gamma$, and the energy dependence of the capture cross section σ as obtained by adding the first-order Born term (which behaves asymptotically[6] like $\gamma^{-1/2}$) to a_{fi}^{B2} and squaring the amplitude is $\sigma\sim(\ln E)^2/E$ for $E\rightarrow\infty$. This energy dependence is the same as found in our previous work.[2]

The omission of the two above-mentioned approximations affects, however, the magnitude of the $\gamma^{-1/2}\ln\gamma$ term in the transition amplitude and hence its importance for finite γ. In particular, the consideration of screening—with a contribution to a_{fi}^{B2} proportional to $\gamma^{-1/2}$—will strongly reduce the prefactor of the $\gamma^{-1/2}\ln\gamma$ term (with $1/Z_T$) as compared to a pure Coulomb target field.

If, on the other hand, allowance is made for an ultimate *complete* screening of the target potential, the Coulombic term in (5) proportional to s_0^{-2} is no longer present. In this case, the first and second-order Born term will show the same asymptotic energy dependence, leading to $\sigma\sim E^{-1}$ for $E\rightarrow\infty$.

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