Exact relativistic second Born approximation for electron capture

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We derive the exact asymptotic behavior of the second Born approximation for electron capture. The transfer probability as a function of impact parameter and the cross section is shown to go like $(\ln E)^2/E$, where E is the collision energy. This result is the same as for the impulse approximation, and is independent of the initial- and final-state wave functions. In particular, it is also true for capture to the continuum.

An interesting aspect of the nonrelativistic treatments of electron capture in ion-atom collisions is that at asymptotically high collision energies E the total capture cross section (σ) calculated from the second Born approximation (BA2) behaves as $\sigma \sim E^{-5.5}$, and dominates the first-order Oppenheimer-Brinkman-Kramers (OBK) result[1] ($\sigma \sim E^{-6}$). This has been related to the fact that the BA2 contains the Thomas double-scattering amplitude, which for capture of a free electron is the lowest-order term compatible with energy-momentum conservation.[2] However, the asymptotic dominance of the nonrelativistic Thomas amplitude for total cross sections is of somewhat academic interest, as opposed to the case of differential cross sections, where it has recently been experimentally confirmed,[3] since it only occurs at energies where a relativistic description is mandatory.

Now it is known[4,5] that for a relativistic collision the Thomas cross section behaves asymptotically as E^{-3}, and is dominated by the corresponding OBK cross section[6] ($\sigma \sim E^{-1}$). One might thus believe that the OBK approximation gives the right result as $E \to \infty$ in this case. It has been shown, however, that the relativistic impulse approximation (IA), which contains terms of arbitrary high order in one of the nuclear potentials, and in particular includes BA2, leads to an asymptotic behavior[7] $\sigma \sim (\ln E)^2/E$ (the derivation in Ref. 7 goes through also without making a peaking approximation). Since it is believed that the IA is asymptotically correct for relativistic collisions, as it is in the nonrelativistic case,[8,9] it becomes an intriguing question how this asymptotic behavior arises.

In this Brief Report we show that the exact relativistic BA2 indeed has the same asymptotic behavior as the IA, even though this cannot be ascribed to the Thomas mechanism. The discrepancies between our results and those recently reported by Humphries and Moiseiwitsch[10] for a peaked BA2 can be traced back to a peaking approximation used by these authors, as discussed below. Throughout this Brief Report we use atomic units ($\hbar = e = m_e = 1$), and our conventions for the Dirac matrices α and γ_0 are those of Bjorken and Drell.[11]

We shall, for definiteness, consider capture from the target to a bound projectile state, and shall use the semiclassical (impact-parameter) picture, although this is not essential for our derivation. The exact scattering state $\Psi_f^{(-)}$ in the projectile rest frame (denoted throughout by a prime), which asymptotically develops into a projectile state ψ_f^P, is in BA2 approximated by ($\bar{\psi} = \psi^+ \gamma_0$):

$$\bar{\psi}_f'(\mathbf{r}',t') = \bar{\psi}_f^{P'}(\mathbf{r}',t') + \frac{1}{2\pi} \sum_{s=1}^{4} \int d\mathbf{q}\, d\omega_q \frac{1}{\omega_q - q^2/2 + i\epsilon} (\bar{\psi}_f^{P'} | (\gamma_0 V_T)' | q_s') \bar{q}_s' \quad , \tag{1}$$

where the free propagator G_0 has been written in its spectral representation, $|q_s\rangle$ is the sth component of a free spinor of momentum $\mathbf{q}$, and $(\gamma_0 V_T)' = T^{-1}(\gamma_0 V_T) T$ is the target Coulomb potential (charge Z_T) in the projectile frame. The transformation matrix T is given by[11]

$$T = [(1+\gamma)/2]^{1/2} [1 + \gamma\beta/(1+\gamma)\alpha_z] \quad ,$$

with $\beta = v/c$ and $\gamma = (1-\beta^2)^{-1/2}$, v being the collision velocity, and T^{-1} is found by replacing β by $-\beta$. Finally, we use the notation $(\phi^+ | A | \psi)$ to denote the matrix element $\langle \phi(t) | A(t) | \psi(t) \rangle$ integrated over time t.

Using ψ_f' from Eq. (1), the exact transfer amplitude can be approximated as

$$a_{fi} = -i(\bar{\Psi}_f^{(-)\prime} | \gamma_0 V_P' | \psi_i^{T'}) \approx -i \int dt'\, d\mathbf{r}'\, \bar{\psi}_f'(\mathbf{r}',t') (\gamma_0 V_P') [T^{-1} \psi_i^T(\mathbf{r},t)] \equiv a_{fi}^{BK} + a_{fi}^{B2} \quad ,$$

$$a_{fi}^{B2} = -i \frac{1}{2\pi} \sum_{s=1}^{4} \int d\mathbf{q}\, d\omega_q \frac{1}{\omega_q - q^2/2 + i\epsilon} \left(\psi_f^{P'+} \left| \gamma(1+\beta\alpha_z) \frac{Z_T}{r} \right| q_s' \right) \sum_{\sigma=1}^{4} \int d\mathbf{k}\, d\omega_k \left(q_s'^+ \left| \frac{Z_P}{r'} \right| T^{-1} k_\sigma(\mathbf{r},t) \right) (k_\sigma^+(\mathbf{r},t) | \psi_i^T(\mathbf{r},t)) \quad . \tag{2}$$

Here the first term, a_{fi}^{BK}, is the well-known OBK amplitude, which will not be considered further, and V_P is the projectile potential (charge Z_P). In order to facilitate the transformation of the initial target state ψ_i^T to the projectile frame, we have inserted a complete set of free states $|k_\sigma\rangle$ into the expression in Eq. (2).

For the further evaluation, we write $\langle r | k_\sigma(t) \rangle = u_k^\sigma \exp(i\mathbf{k}\cdot\mathbf{r} - i\omega_k t)$, where u_k^σ is a constant spinor. We choose the projectile velocity $\mathbf{v}$ as the z axis, so that the target and projectile systems are connected by the Lorentz transformations

$t=\gamma(t'+\beta z'/c)$, $z=\gamma(z'+vt')$, and $\mathbf{r}_\perp=\mathbf{r}'_\perp+\mathbf{b}$, where $\mathbf{b}$ is the impact parameter. The last two space-time integrals in Eq. (2) can then be carried out, yielding

$$(k_\sigma^+(\mathbf{r},t)|\psi_i^T(\mathbf{r},t))=\sqrt{2\pi}\,\delta(E_i-\omega_k)(u_k^{\sigma+}\phi_i(\mathbf{k}))\ ,$$

$$\left(q_s'^{+}\left|\frac{Z_P}{r'}\right|T^{-1}k_\sigma(\mathbf{r},t)\right)=\frac{Z_P}{(2\pi)^3}e^{i\mathbf{k}_\perp\cdot\mathbf{b}}\delta(\omega_q+k_z\gamma v-\gamma\omega_k)(u_q^{s+}T^{-1}u_k^\sigma)\int d\mathbf{r}'\frac{1}{r'}e^{-i\mathbf{q}\cdot\mathbf{r}'}e^{i\mathbf{k}_\perp\cdot\mathbf{r}'_\perp}e^{i\gamma z'(k_z-\beta\omega_k/c)}\ , \tag{3}$$

where E_i is the initial electron energy, and $\phi_i(\mathbf{k})$ the corresponding momentum-space wave function. We now introduce the Bethe representation for the Coulomb potential, so that

$$\left(\psi_f^{P+}\left|\gamma(1+\beta\alpha_z)\frac{Z_T}{r}\right|q_s'\right)=\frac{\gamma Z_T}{\sqrt{2}\pi^{3/2}}\int\frac{d\mathbf{s}_0}{s_0^2}e^{i\mathbf{s}_{0\perp}\cdot\mathbf{b}}\delta(s_{0z}\gamma v+E_f-\omega_q)(\phi_f^+(\mathbf{s}_{0\perp}+\mathbf{q}_\perp,\gamma s_{0z}+q_z)(1+\beta\alpha_z)u_q^s)\ , \tag{4}$$

where E_f is the energy of the final state ψ_f^P, and $\phi_f(\mathbf{k}_\perp,k_z)$ its Fourier transform for momentum $\mathbf{k}=(\mathbf{k}_\perp,k_z)$. When Eqs. (3) and (4) are inserted in Eq. (2), the integrals over ω_k and ω_q can immediately be carried out.

In order to extract the high-energy ($\gamma\to\infty$) behavior of the BA2 amplitude a_{fi}^{B2}, we change variables from $\mathbf{k}$ to $\mathbf{k}'$, with $k_z'=\gamma k_z-E_i\gamma\beta/c$ and $\mathbf{k}'_\perp=\mathbf{k}_\perp$. One finds that the following expressions occurring in Eqs. (3) and (4) remain finite as $\gamma\to\infty$:

$$-\gamma\omega_k+k_z\gamma v=-\gamma E_i+vk_z'+E_i\gamma\beta^2=-E_i/\gamma+vk_z'\ ,\quad k_z=E_i\beta/c+k_z'/\gamma\ ,\quad \gamma s_{0z}=-E_f/v+E_i/(\gamma v)-k_z'\equiv Q(k_z')\ . \tag{5}$$

Doing also the s_{0z} integration, the transition amplitude reads

$$a_{fi}^{B2}=-i\frac{Z_PZ_T}{4\pi^4\gamma v}\sum_{s,\sigma=1}^{4}\int d\mathbf{q}\,d\mathbf{k}'\frac{1}{E_i/\gamma-vk_z'-q^2/2+i\epsilon}(u_k^{\sigma+}\phi_i(\mathbf{k}))e^{i\mathbf{k}'_\perp\cdot\mathbf{b}}(u_q^{s+}T^{-1}u_k^\sigma)\frac{1}{(\mathbf{q}-\mathbf{k})^2}$$
$$\times\int\frac{d\mathbf{s}_{0\perp}}{s_{0\perp}^2+Q^2(k_z')/\gamma^2}e^{i\mathbf{s}_{0\perp}\cdot\mathbf{b}}(\phi_f^+\mathbf{s}_{0\perp}+\mathbf{q}_\perp,Q(k_z')+q_z(1+\beta\alpha_z)u_q^s)\ . \tag{6}$$

This expression is still exact.

We can now readily extract the asymptotic γ dependence of a_{fi}^{B2}. Apart from the factor γ^{-1} from the prefactor and a factor $\gamma^{1/2}$ from T^{-1}, there is a nontrivial γ dependence arising from the $\mathbf{s}_{0\perp}$ integration. This is because $Q(k_z')/\gamma\to 0$, while the rest of the integrand remains finite, so that the integral becomes singular at $s_{0\perp}=0$ in that limit. Since $\exp(i\mathbf{s}_{0\perp}\mathbf{b})$ and ϕ_f are generally nonzero in this region, they can be taken outside the integral without affecting the behavior at $s_{0\perp}=0$. The remaining integral is elementary, and one finds a contribution $\sim\ln(Q/\gamma)$ from the lower limit (the divergence as $s_{0\perp}\to\infty$ vanishes if the above-mentioned factors are retained inside the integral). Since the expressions in Eqs. (5) remain finite, all other factors are seen to be independent of γ as $\gamma\to\infty$, and the total cross section, obtained by integrating $|a_{fi}^{BK}+a_{fi}^{B2}|^2$ over impact parameters behaves like

$$\sigma=\text{const}\times\frac{(\ln E)^2}{E},\quad \text{as } E\to\infty\ , \tag{7}$$

since $E\sim\gamma$. This is the same functional dependence as previously found for the IA.[7] Thus the BA2 contributes at least partially to the asymptotic behavior of charge transfer.

It should be noted that in deriving Eq. (7), no explicit assumptions have been made for ϕ_i or ϕ_f, since the integrals in Eq. (6) converge for arbitrary initial and final bound states. If, on the other hand, capture to continuum (CTC) is considered, the wave functions will introduce additional singularities in the integrands. A detailed analysis shows that this will not change the asymptotic energy dependence of σ, when integrated over a finite detector resolution for the momenta of the ejected electrons, although for certain critical momentum values the differential CTC cross section may even increase with γ.

The discrepancies between the present results and those obtained by Humphries and Moiseiwitsch[10] can be traced back to a peaking approximation employed by these authors to facilitate the integration over momentum transfer. In the Bethe integral (our $\mathbf{s}_{0\perp}$ integral), they replace the denominator with the squared difference between the initial and final internuclear momenta [their Eq. (16)], which does not depend on the integration variables, but becomes a constant factor in the transition amplitude, independent of γ as $\gamma\to\infty$. Translated to our formulation, they approximate Q in such a manner that Q/γ no longer vanishes in this limit, so that the $\mathbf{s}_{0\perp}$ integral only gives a constant contribution. From their exact BA2 expression [their Eq. (15)], one can indeed derive Eq. (7), following the same steps as above.

The asymptotic dependence of Eq. (7) for the ultrarelativistic capture cross section has also been found by Moiseiwitsch and Stockman,[12] using a modified OBK formula incorporating the two-state correction of Bates.[13] However, this correction does not include all second-order terms of importance, as can be seen from the fact that the corresponding nonrelativistic theory still predicts $\sigma\sim E^{-6}$. Thus, the result of Moiseiwitsch and Stockman[12] that the constant in Eq. (7)—for which we derive no result—is of higher order in the fine-structure constant α than the constant for the $1/E$ term from Ref. 10, need not hold in the full BA2.

At first sight the result that $\sigma\sim(\ln E)^2/E$ appears to be at variance with the physical picture underlying the IA, namely, that the transfer process can be described as ionization of the target atom, followed by capture in the form of an overlap with a traveling projectile state.[8] It is known that the ionization probability for a given impact parameter asymptotically approaches a constant,[14] while the transformation of the projectile state to the target system only can introduce powers of γ (cf. above). However, for ionization this result depends critically on the relation between energy and momentum transfer, and if this relation were changed, as it effectively is for electron capture, the ionization probability would indeed grow asymptotically as[14] $(\ln\gamma)^2$. Thus, also at relativistic velocities the simple physical idea behind the IA remains valid.

The physical origin of the $\ln(E)$ dependence of a_{fi}^{B2} (and correspondingly for the IA) is the transverse electromagnetic field of a moving charge, which has no nonrelativistic counterpart. The instantaneous Coulomb potential alone (the longitudinal field) would also give a contribution like Eq. (6), but with the term Q^2/γ^2 in the denominator of the $\mathbf{s}_{0\perp}$ integral replaced by Q^2. The resulting cross section will indeed have the same asymptotic behavior as the OBK. The transverse field does not contribute to the OBK amplitude due to Lorentz invariance, as one can always transform it away by going into the projectile rest frame.

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