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Second Born approximation for relativistic electron capture: Exact Monte Carlo calculations for C^{6+}-Au and Ar^{18+}-Ag collisions

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The second-order Oppenheimer-Brinkman-Kramers approximation for relativistic electron capture is formulated, and rigorously calculated K-K cross sections are presented. Theoretical cross sections for electron capture in collisions of C^{6+}-Au at 400 MeV/u and Ar^{18+}-Ag at 400 and 1050 MeV/u projectile energy are compared with the experimental data and other approximate second Born results. It is shown that exact second Born cross sections grossly overestimate the experimental data.

In the past several years, there has been considerable interest in electron capture at relativistic projectile energies. Electron capture has been successfully treated employing the relativistic eikonal,[1] boundary-corrected first Born,[2] and coupled-channel theory.[3] Earlier calculations using a relativistic first-order Oppenheimer-Brinkman-Kramers (OBK1) approximation[4] resulted in cross sections that were almost an order of magnitude larger than the experimental data.[5] In order to overcome this difficulty, a relativistic second-order OBK (OBK2) approximation, or second Born approximation, has been adopted,[6] and extensive calculations have been carried out.[7-9] While several approximations of unknown validity have been employed, recently reported OBK2 cross sections[9] show good agreement with the experimental data[5] in most cases. These findings, however, are surprising in view of the analogous nonrelativistic situation, where *exact* OBK2 cross sections[10,11] are generally *larger* than the corresponding first-order cross sections for experimentally accessible projectile energies. Nonrelativistic OBK2 cross sections overestimate the experimental data even more than the OBK1 results.

The aim of the present paper is to demonstrate that the OBK2 approximation also fails to describe *relativistic* electron capture. In this work, the fully relativistic second Born transition amplitude is evaluated numerically without any approximation. Exact OBK2 cross sections for the case of non-spin-flip transitions are presented and compared with the experimental data[5] and approximate OBK2 results given by Humphries and Moiseiwitsch[7] and Moiseiwitsch.[9] Initial and final states are represented by exact hydrogenic Dirac wave functions. Intermediate states of negative energy, which have been neglected in previous studies,[6-9] are explicitly taken into account. Atomic units are used throughout unless specifically stated otherwise.

It is convenient to describe the collision in the impact parameter $\mathbf{b}$ picture with an electron bound to a target (charge Z_T) at rest and the bare projectile (charge Z_P) moving with a velocity $\mathbf{v}$ along a straight-line trajectory.

The second-order OBK transition amplitude is then given in the post form by

$$A^{+}_{\mathrm{OBK2}} = -i\int dt\int d^3r_T[\phi'_P(\mathbf{r}'_P,t')]^{\dagger}S^{-1}\left(-\frac{Z_T}{r_T}\right)\phi_T(\mathbf{r}_T,t) + (-i)\int dt\int d^3r_T\int dt_1\int d^3r_{T_1}[\phi'_P(\mathbf{r}'_P,t')]^{\dagger}S^{-1}\left(-\frac{Z_T}{r_T}\right)G_0^{+}(\mathbf{r}_T,\mathbf{r}_{T_1},t-t_1)S^2\left(-\frac{Z_P}{r'_{P_1}}\right)\phi_T(\mathbf{r}_{T_1},t_1)\,, \tag{1}$$

where

$$G_0^{+}(\mathbf{r}_T,\mathbf{r}_{T_1},t-t_1) = \frac{1}{2\pi}\int G_0^{+}(\mathbf{r}_T,\mathbf{r}_{T_1},\varepsilon)\exp[-i\varepsilon(t-t_1)]d\varepsilon \tag{2}$$

and

$$G_0^{+}(\mathbf{r}_T,\mathbf{r}_{T_1},\varepsilon) = \sum_{\mathbf{k},s}\left[\frac{\psi^{(+)}_{\mathbf{k},s}(\mathbf{r}_T)(\psi^{(+)}_{\mathbf{k},s})^{\dagger}(\mathbf{r}_{T_1})}{\varepsilon - E^{(+)}_{\mathbf{k}} + i\eta} + \frac{\psi^{(-)}_{\mathbf{k},s}(\mathbf{r}_T)(\psi^{(-)}_{\mathbf{k},s})^{\dagger}(\mathbf{r}_{T_1})}{\varepsilon + E^{(-)}_{\mathbf{k}} - i\eta}\right]. \tag{3}$$

The spinors $\psi^{(+)}_{\mathbf{k},s}(\mathbf{r}_T)$ and $\psi^{(-)}_{\mathbf{k},s}(\mathbf{r}_T)$ satisfy the free-field Dirac equation

$$H_0\psi^{(\pm)}_{\mathbf{k},s}(\mathbf{r}_T) = \pm E^{(\pm)}_{\mathbf{k}}\psi^{(\pm)}_{\mathbf{k},s}(\mathbf{r}_T),\ E^{(\pm)}_{\mathbf{k}} > 0\,, \tag{4}$$

where

$$H_0 = -ic\boldsymbol{\alpha}\cdot\nabla_{r_T} + c^2\gamma_4\,. \tag{5}$$

We have denoted by $\psi^{(+)}_{\mathbf{k},s}(\mathbf{r}_T)$ the positive-energy solutions, which represent electrons, and by $\psi^{(-)}_{\mathbf{k},s}(\mathbf{r}_T)$ the negative-energy solutions, which represent positrons. Here, $\mathbf{r}_T$ and $\mathbf{r}'_P$ are the electron coordinates with respect to the target nucleus in the target frame and with respect to the projectile nucleus in the projectile frame, respectively. The spinor transformation $S = [(\gamma+1)/2]^{1/2}(1$

$-\delta\alpha_z$) with $\gamma=(1-\beta^2)^{-1/2}$, $\beta=v/c$, and $\delta=[(\gamma-1)/(\gamma+1)]^{1/2}$ transforms an eigenfunction from the target to the projectile system; $c=137.04$ a.u. is the velocity of light, and $\boldsymbol{\alpha}$ and γ_4 are Dirac matrices.[12] The summation occurring in (3) is over all possible free-particle spinors with intermediate momentum $\mathbf{k}$. Clearly, if we multiply $G_0^+(\mathbf{r}_T,\mathbf{r}_{T_1},t-t_1)$ by $i\gamma_4$ the Feynman electron propagator[12] is retrieved. The initial and final wave functions ϕ_T and ϕ_P are taken as exact hydrogenic $1s_{1/2}(m_j=\pm\frac{1}{2})$ Dirac wave functions. Only non-spin-flip ($\pm\frac{1}{2}\rightarrow\pm\frac{1}{2}$) transitions are calculated since their contributions are most important for the projectile energies and collision systems under consideration. Following standard techniques,[1] we obtain the final cross section in a form that requires the numerical evaluation of seven-dimensional integrals, as compared with the three-dimensional integrals occurring in the nonrelativistic OBK2 approximation.[11] The integrations were evaluated by the Monte Carlo technique.[13] By comparing various steps in the iteration procedure we estimate the accuracy to be better than 10%. Within this accuracy the following tests of the numerical procedure have been carried out: (a) The results of exact nonrelativistic OBK2 calculations[10,11] for $p+\mathrm{H}$ collisions at 125 keV, 1 MeV, and 50 MeV have been reproduced. (b) Cross sections independently calculated in the target and in the projectile frame agree. (c) Detailed balance holds in both target and projectile frame.

In Table I we present the results of our exact OBK2 calculations for K-K capture in collisions between C^{6+}-Au at 400 MeV/u and Ar^{18+}-Ag at 400 and 1050 MeV/u projectile energy together with the experimental data.[5] The experimental data contain contributions from all initial and final states as well as spin-flip contributions. Both effects, if included, would increase our theoretical K-K cross section by about 20%–40%. We also include the results of approximate evaluations of Eq. (1) (Refs. 7 and 9) in which (a) intermediate states of negative energy have been omitted, (b) a peaking approximation has been used in order to simplify the evaluation, and (c) various terms of the order of $(\alpha Z)^2$ have been neglected. While the omission of negative-energy intermediate states turns out to be justified (see below) it is already known from nonrelativistic calculations[10] that peaking approximations may lead to entirely incorrect results. It can be seen from Table I that the exact OBK2 cross sections are about 1 order of magnitude larger than the corresponding results obtained from a first-order OBK calculation. Moreover, the exact OBK2 values are between 1 and 2 orders of magnitude larger than the experimental data. The relativistic second Born approximation hence fails to describe relativistic electron capture. We note that for C^{6+}-Au collisions the cross section ratio OBK2/OBK1 is about 17 indicating a poor convergence behavior for high-Z target atoms. Contributions from intermediate states of negative energy are found to be negligible, i.e., effects from virtual pair creation and annihilation do not contribute in accordance with calculations for electron-positron pair production.[14] The OBK2 cross sections obtained by Humphries and Moiseiwitsch[7] employing a "peaking" approximation and by Moiseiwitsch[9] using an "averaging" approximation are in flagrant disagreement with the exact results.

Finally, we wish to add some remarks on the asymptotic behavior of the relativistic second Born cross section. Two conflicting results have been reported, namely, the asymptotic E^{-1} dependence (with projectile energy E) obtained by Humphries and Moiseiwitsch,[6] and the $(\ln E)^2/E$ dependence given by Jakubassa-Amundsen and Amundsen.[15] This discrepancy can be attributed to a peaking approximation employed by the authors of Ref. 6.[15] However, the derivation given by the authors of Ref. 15 is not free from shortcomings: the relativistic second Born amplitude is defined by employing a *nonrelativistic* version of the free propagator. We have reanalyzed the problem and found that the asymptotic energy dependence derived from Eq. (1) is correctly given by $(\ln E)^2/E$. The details of the theoretical development are given in a separate publication. The second Born term is therefore asymptotically dominant over the first Born term in conformity with nonrelativistic electron capture, where the double-scattering mechanism is of particular importance.

In summary, we have presented exactly evaluated relativistic OBK2 cross sections for the first time. It has been demonstrated that the OBK2 approximation fails to describe relativistic electron capture, in agreement with observations in the nonrelativistic case. This is in sharp contrast to the results reported by Moiseiwitsch.[9] Since these results are derived from peaking type approximations, our findings cast serious doubts on such approximations which

TABLE I. Cross sections (in units of cm^2) for electron capture from K shell to K shell. Theoretical $1s$-$1s$ cross sections have been multiplied with a factor of 2 to account for the presence of two K electrons. The number in square brackets are powers of ten by which the preceding numbers have to be multiplied.

Z_P	Z_T	Energy (MeV/u)	OBK1	OBK2 (exact) (this work)	OBK2 (Ref. 7)	OBK2 (Ref. 9)[a]	Experiment (Ref. 5)[b]
6	79	400	7.16 [−25]	1.2 [−23]		6.3 [−25]	7.8 [−25]
18	47	400	1.34 [−22]	5.7 [−22]	1.08 [−22]	4.1 [−23]	1.9 [−23]
18	47	1050	3.18 [−24]	1.2 [−23]	1.21 [−24]	6.7 [−25]	2.7 [−25]

[a]Spin-flip contributions and capture from initial into final s states with principal quantum numbers 1, 2, and 3 included.

[b]Capture from all initial into all final states as well as spin-flip contributions included.

are widely used to evaluate transition amplitudes for relativistic collisions. Exact OBK2 cross sections have been shown to be between 1 and 2 orders of magnitude larger than the experimental data. Effects of virtual electron-positron pair creation and annihilation appeared to be negligible for the collision systems and projectile energies under consideration. The enormous differences between first- and second-order cross sections for high-Z target atoms point to the necessity of nonperturbative methods for the treatment of relativistic charge exchange.

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