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THE INCLUSION OF THE ELECTRON SCREENING POTENTIAL IN IMPACT-PARAMETER CALCULATION

A.Orbán, B.Sulik

Institute of Nuclear Research, Hungarian Academy of Sciences,
P.O. Box 51, H-4001 Debrecen, Hungary

We investigate the electron screening effect of the projectile on the amplitude of a target atomic transition within the framework of the semiclassical approximation (SCA). The aim is to provide a general tool for accounting projectile electron screening effect in impact parameter calculations, even when the target or projectile wave functions are numerical.
In the implementation of this problem we need the modified spherical Bessel functions of the first and third kind and their derivatives. We have elaborated closed expressions for the *n*th order derivation of the modified spherical Bessel function of first and third kind. The numerical stability against the arguments, the order of functions and the order of derivation has also been analyzed.

Theory

In atomic collisions, where the projectile is a neutral atom or an ion carrying electrons the target excitation processes are strongly influenced by the projectile electrons, which screen the Coulomb field of the projectile nucleus. In this work, we focus on the electron screening effect of the projectile on the amplitude of a target transition, within the framework of the semiclassical approximation. Our calculation is based on Ref.[1].

If the target transition is described within the framework of the time dependent perturbation theory, the transition amplitude has the following form:

$$a=-i\int_{-\infty}^{\infty}dt'\,e^{i(E_b-E_a)t'}\langle b|V(t')|a\rangle+(-i)^2\sum_k\int_{-\infty}^{\infty}dt'\int_{-\infty}^{t'}dt''\,e^{-i(E_b-E_k)t'}\langle b|V(t')|k\rangle e^{-i(E_k-E_a)t''}\langle k|V(t'')|i\rangle+\dots$$

We denote the initial and final target states with $|a\rangle$ and $|b\rangle$, and their energies with E_a, and E_b, respectively.

Considering one target electron, the interaction potencial *V(t)* may be approximated as a sum of target electron – projectile nucleus and target electron – projectile electron Coulomb potential terms.

$$V(\mathbf{R}-\mathbf{r})=\frac{-Z_{proj}}{|\mathbf{R}-\mathbf{r}|}+\sum_{j=1}^{N}\frac{1}{|\mathbf{R}+\mathbf{r}_j-\mathbf{r}|}\quad .$$

Supposing no electronic transitions on the projectile, the electron screening effect can be taken into account by introducing the electron screening potential $V_s(\mathbf{R}-\mathbf{r})$. This function is defined by the diagonal matrix element of the projectile ground state.

$$V_s(\mathbf{R}-\mathbf{r})=\sum_{k=1}^{N}\int dr_k\,\chi_k^*(\mathbf{r}_k)\frac{1}{|\mathbf{R}+\mathbf{r}_k-\mathbf{r}|}\chi_k(\mathbf{r}_k),$$

where N is the number of projectile electrons, $\mathbf{R}$ is the internuclear position vector, $\mathbf{r}$, $\mathbf{r}_k$ are the position vectors of the target and projectile electron and $\chi_k(\mathbf{r}_k)$ is the projectile one-electron ground state wave function.

When the projectile electron wave functions are approximated by hydrogenic or Slater-type orbitals [2], a spherically symmetric screening potential has the following form:

$$V_s(|\boldsymbol{R}-\boldsymbol{r}|)=\frac{N}{|\boldsymbol{R}-\boldsymbol{r}|}-\sum_{k=0}^{F}c_k|\boldsymbol{R}-\boldsymbol{r}|^{n_k-1}e^{-a_k|\boldsymbol{R}-\boldsymbol{r}|},$$

where F and n_k are positive integers, c_k is real and a_k is a positive number.

For numerical projectile wave functions we use a nonlinear least-squares fitting technique to estimate the screening potential parameters [3].

For evaluation of $V_s(|\boldsymbol{R}-\boldsymbol{r}|)$, following Ref.[1], we utilized the multipole expansion

$$\frac{e^{-a|\boldsymbol{R}-\boldsymbol{r}|}}{|\boldsymbol{R}-\boldsymbol{r}|}=\sum_{L=0}^{\infty}\frac{2L+1}{\sqrt{Rr}}I_{L+1/2}(ar_>)K_{L+1/2}(ar_>)P_L(\hat{R},\hat{r}) ,$$

and the identity

$$x^n e^{-ax}=\frac{d^{n+1}}{d(-a)^{n+1}}\frac{e^{-ax}}{x} ,$$

where $I_{L+1/2}$, $K_{L+1/2}$ are the Lth order spherical Bessel function of the first and third kind, $r_<=\min(R,r)$, $r_>=\max(R,r)$.

For the screening potential, we get the following closed formula:

$$V_s(|\boldsymbol{R}-\boldsymbol{r}|)=\frac{N}{|\boldsymbol{R}-\boldsymbol{r}|}-\sum_{k=0}^{F}c_k\sum_{L=0}^{\infty}\frac{2L+1}{\sqrt{Rr}}P_L(\hat{R},\hat{r})\frac{d^{n_k}}{d(-a_k)^{n_k}}I_{L+1/2}(a_kr_<)K_{L+1/2}(a_kr_>).$$

In the expression of the screening potential, there appears the derivate of the product of spherical Bessel functions. This factor may be written as:

$$\frac{d^{n_k}}{d(-a_k)^{n_k}}(I_{L+1/2}(a_kr_<)K_{L+1/2}(a_kr_>))=\frac{2}{\pi\sqrt{r_<r_>}}(-1)^{n_k}\left(a_k\sum_{t=0}^{n_k}C_{n_k}^{t}\frac{d^t}{da_k^{\,t}}i_L(a_kr_<)\frac{d^{n_k-t}}{da_k^{\,n_k-t}}k_L(a_kr_>)+\right.$$
$$\left.n_k\sum_{u=0}^{n_k-1}C_{n_k-1}^{u}\frac{d^u}{da_k^{\,u}}i_L(a_kr_<)\frac{d^{n_k-1-u}}{da_k^{\,n_k-1-u}}k_L(a_kr_>)\right)$$

$i_L(z)=\sqrt{\frac{\pi}{2z}}I_{L+1/2}(z)$ and $k_L(z)=\sqrt{\frac{\pi}{2z}}K_{L+1/2}(z)$ being the L-th orther modified spherical Bessel functions of the first and the third kind respectively

We developed a closed formula for calculating the kth order derivative of modified spherical Bessel function of different orders. The main advantage of this formula is that the k-th order derivative $f_n^k(z)$ of a Bessel function $f_n(z)=i_n(z),(-1)^{n+1}k_n(z)$ can be built exclusively from Bessel functions:

$$f_n^k(z)=\sum_{i=0}^{2k}A_{n-k+i}^{k}f_{n-k+i}(z),\quad i-\text{even}.$$

The expansion coefficients can be calculated by recursion:

$$A_i^p=C(i-1)A_{i-1}^{p-1}+B(i+1)A_{i+1}^{p-1} ,$$

where $A_0^0 = 1$ and B, C are simple functions of i.

Results

We have elaborated closed expressions and recursion relations for the *n*th order derivation of the modified spherical Bessel function of first and third kind and respectively for their products.

We analyzed the numerical stability against the arguments, the order of functions and the order of derivation. We tested our routines for n=0,...,10, k=1,...,6 and z=0,...,1000. Our numerical results have been compared with the Mathematica [4] software results.

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ВКЛЮЧЕННЯ ПОТЕНЦІАЛУ ЕЛЕКТРОННОГО ЕКРАНУВАННЯ В РОЗРАХУНОК ПАРАМЕТРІВ УДАРУ

А.Орбан, Б.Шулік

Інститут ядерних досліджень Угорської Академії наук, Дебрецен, Угорщина

Нами досліджено вплив ефекту електронного екранування налітаючої частинки на амплітуду атомного переходу мішені в рамках напівкласичного наближення. Метою цього є отримання загального засобу для врахування ефекту електронного екранування налітаючої частинки при розрахунках параметрів удару, навіть коли хвильові функції мішені або налітаючої частинки є чисельними.

Для розв'язання цього завдання потрібні модифіковані сферичні функції Бесселя першого і третього виду та їх похідні. Ми отримали замкнені вирази для похідної *n*-го порядку від модифікованої сферичної функції Бесселя першого і третього виду. Також проаналізовано чисельну стабільність залежно від аргументів, порядку функцій і порядку похідних.