Relativistic calculations of charge transfer probabilities in $^{92+}U$–$^{91+}(1s)$ collisions using the basis set of cubic Hermite splines

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Abstract
A new approach for solving the time-dependent two-center Dirac equation is presented. The method is based on using the finite basis set of cubic Hermite splines on a two-dimensional lattice. The Dirac equation is treated in the rotating reference frame. The collision of $^{92+}$ (as a projectile) and $^{91+}$ (as a target) is considered at energy $E_{\text{lab}} = 6 \text{ MeV u}^{-1}$. The charge transfer probabilities are calculated for different values of the impact parameter. The results obtained are compared with previous calculations (Tupitsyn et al 2010 Phys. Rev. A 82 042701), where a method based on atomic-like Dirac–Sturm orbitals was employed. This work can provide a new tool for the investigation of quantum electrodynamics effects in heavy-ion collisions near the supercritical regime.

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1. Introduction

Heavy-ion collisions can be used as a powerful tool for the test of quantum electrodynamics at supercritical Coulomb fields [1]. To date, many approaches have been employed to treat such collisions [2–14]. In our previous work [14, 15], a method for solving the time-dependent Dirac equation in the basis of atomic-like Dirac–Fock–Sturm orbitals was developed.

In this paper, we develop an alternative approach to the treatment of low-energy heavy-ion collisions. The method is based on using the cubic Hermite spline basis set on a two-dimensional uniform grid. The Dirac equation is considered in a rotating reference frame. Previously, the time-dependent Schrödinger equation was treated in a rotating coordinate frame in [16]. The basis of cubic Hermite splines was used for non-relativistic time-dependent calculations [17, 18] and for relativistic time-dependent calculations in the monopole approximation [19]. To the best of our knowledge, however, the Hermite splines have not been employed before for solving the time-dependent Dirac equation for the real two-center problem.

The theoretical methods are described in section 2. The results of our calculations of the charge-transfer probabilities for the $^{92+}$–$^{91+}(1s)$ collisions are presented in section 3. Atomic units ($\hbar = e = m = 1$) are used throughout the paper.
Figure 1. The charge transfer probability as a function of the impact parameter. Signs ‘+’ and ‘×’ indicate the results of one channel and six channel calculations, respectively. The solid line corresponds to the results of [14].

2. Theory

2.1. Basis of the Hermite splines

In this paper, a basis of cubic Hermite splines is used. This basis can be defined in the following way. The interval \([a, b]\) is partitioned into \(N\) equal subintervals \(a = x_0 < x_1 < \cdots < x_N = b\), with the length \(h = x_{i+1} - x_i\) \((i = 1, \ldots, N - 1)\). For each node \(x_i\) two functions are introduced:

\[
s_i^0(x) = f^0 \left( \frac{x - x_i}{h} \right), \quad s_i^1(x) = hf^1 \left( \frac{x - x_i}{h} \right),
\]

where

\[
f^0(x) = \begin{cases} 0, & |x| \geq 1, \\ (1-x)^2(1+2x), & 0 < x < 1, \\ (1+x)^2(1-2x), & -1 < x < 0. \end{cases}
\]

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\]

Since only adjacent splines overlap, the Hamiltonian and overlapping matrices are sparse. It is a significant advantage of this basis. The two-dimensional basis Hermite splines are defined as

\[
\phi_j(x, y) = s_i^0(x) \cdot s_j^0(y).
\]

Here \(j = j(\mu, \nu, l, m)\) enumerates the splines \(\phi_j(x, y)\) in a certain way.

2.2. Solution of the time-dependent two-center Dirac equation

We consider a collision of \(\text{U}^{92+}\) (target) and \(\text{U}^{91+}(1s)\) (projectile). The position of the target is fixed; the projectile moves along a straight line with a constant velocity.

The electron movement is considered in the cylindrical coordinate system \((\rho, z, \varphi)\) which is rotating around the target with the internuclear axis as the z-axis. In this coordinate system, the Dirac equation is written as [20]

\[
\frac{i}{\hbar} \frac{\partial \psi}{\partial t} = \hat{H} \psi,
\]

\[
\hat{H} = \hat{H}_0 - \hat{j}\omega,
\]

where \(\psi\) is the Dirac wave function, \(\hat{j}\) is the angular momentum operator, \(\omega\) is the angular velocity of the reference frame and

\[
\hat{H}_0 = c\alpha \hat{p} + \beta c^2 + V(r, t).
\]

Here \(\alpha, \beta\) are the Dirac matrices and \(V(r, t)\) is the two-center potential. In equation (5), we disregard some negligible terms [20].

The wave function is represented as

\[
\psi^k(\rho, z, \varphi, t) = \sum_{m=-M}^{M} \psi_m^k(\rho, z, t) \Phi_m^k(\varphi),
\]

where \(m\) is a half-integer quantum number, index \(k\) enumerates the components of \(\psi(\rho, z, \varphi, t)\), \(2M + 1\) is the number of \(m\)-states under consideration and

\[
\Phi_m^k(\varphi) = \frac{1}{\sqrt{2\pi}} \left\{ \exp[i(m-1/2)\varphi], k = 1, 3, \right. \\
\left. \exp[i(m+1/2)\varphi], k = 2, 4. \right\}
\]

Each component \(\psi_m^k(\rho, z, t)\) is expanded in the basis of cubic Hermite splines \(\{\phi_i(\rho, z)\}\):

\[
\psi^k(\rho, z, \varphi, t) = \sum_{m=-M}^{M} \sum_{l=1}^{N} C_{l,m}^k(t) \phi_l(\rho, z) \Phi_m^k(\varphi).
\]

Let us introduce the new notation \(C_j = C_{l,m}^k, f_j = \phi_l \Phi_m^k\). The coefficients \(C_j\) can be obtained by solving the equation

\[
i\hbar \frac{dC(t)}{dt} = \hat{H}(t) C(t).
\]

Here \(C\) is the vector of the coefficients \(C_j, H_j = (f_i | \hat{H} | f_j)\) and \(S_{ij} = (f_i | f_j)\). The matrix elements \(S_{ij}\) and \(H_{ij}\) are
calculated by numerical integration with respect to \( \rho \) and \( z \), and analytical integration with respect to the \( \varphi \) coordinate. For a sufficiently small time interval \( \Delta t \) the formal solution of equation (11) is

\[
C(t + \Delta t) = \exp \left( -i S^{-1} H \Delta t \right) C(t). \tag{12}
\]

The exponential operator is expanded as

\[
C(t + \Delta t) = \left[ 1 - i S^{-1} H \Delta t - \frac{1}{2} (S^{-1} H \Delta t)^2 + \cdots \right] C(t). \tag{13}
\]

The vector \( C(t) \) is calculated on each time step using equation (13) with the first four terms.

3. Results

The charge transfer probabilities in the \( \text{U}^{92+} - \text{U}^{91+}(1s) \) collisions were obtained for one \( (m = 1/2) \) and six channels with different \( m \) (see equation (8)) at the projectile energy \( E_{\text{lab}} = 6 \text{ MeV u}^{-1} \). The number of basis functions was 15 360 and 92 160 for one and six channels, respectively. The results are shown in figure 1.

4. Conclusion

In this work, the charge transfer probabilities in the \( \text{U}^{92+} - \text{U}^{91+}(1s) \) collisions were calculated for a wide range of impact parameters. As can be seen from figure 1, the results of the calculations with six channels are in good agreement with the corresponding values obtained in [14]. Since \( \langle \Phi_m | \mathbf{J} | \Phi_m \rangle = 0 \), the rotation of the internuclear axis is not taken into account in the case of the one channel calculations. As one can see from figure 1, the influence of this rotation is essential for the impact parameter \( b < 600 \text{ fm} \).

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