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Computation of a generalized Nordsieck integral

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Abstract

In this work we introduce two analytical representations of a generalized Nordsieck integral. These integrals arise in the calculations of scattering properties of systems of Coulomb-charged particles using the natural base, which includes general solutions of the two-body Coulomb equation. We study the numerical convergence of these representations against the direct Fortran numerical integration. We test the performance of the different strategies as a function of the momentum transfer, which is typically a relevant variable in collision processes. We also discuss the advantages and disadvantages of the different approaches.

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1. Introduction

In this paper we investigate the numerical solution of a particular case of integrals that we call *generalized* Nordsieck integral [1]. This type of integrals arises in the calculation of the transition elements involving three Coulomb interacting particles. Along the years, it has been customary to write down the final state for the continuum of these systems as

$$\Psi_{C3} = N_{C3}\Phi_{PW}\prod_{l=1}^{3}{}_1F_1[ia_l;1;-ik_l\xi_l], \tag{1}$$

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where $\xi_l = r_l + \mathbf{r}_l \cdot \widehat{\mathbf{k}}_l$, $\mathbf{k}_l$ and $\mathbf{r}_l$ stand respectively for the relative momentum and distance between particles j and k, $j \neq k \neq l$. The Φ_{PW} represents the free motion of the particles

$$\Phi_{\mathrm{PW}} = e^{i\mathbf{K}\cdot\mathbf{R}+i\mathbf{k}\cdot\mathbf{r}}, \tag{2}$$

where $\{\mathbf{R}, \mathbf{r}\}$ are Jacobi coordinates and $\{\mathbf{K}, \mathbf{k}\}$ are their conjugated momenta. As usual, $a_l = Z_j Z_k \mu_{jk}/k_l$ is the Sommerfeld parameter for the interaction between particles j and k. This is the well-known C3 approximation [2]. It is based upon the approximate separability of the Schrödinger equation for three charged particles: When the coupling terms of the Hamiltonian are neglected, the solution can be written as the product of three two-body Coulomb wave functions.

However, it is possible to construct a basis of continuum Coulomb functions that can be used to expand the exact wave function. This basis was proposed to deal with any kind of three-body Coulomb system [3,4]. The so-called Δ basis can be written as:

$$\Phi_{\Delta} = \Phi_{\mathrm{PW}} \sum_{\mathbf{m},\mathbf{n}=0}^{\infty} A_{\mathbf{m},\mathbf{n}} \Phi_{\mathbf{m},\mathbf{n}}, \tag{3}$$

$$\Phi_{\mathbf{m},\mathbf{n}} = \prod_{l=1}^{3} \Delta_{m_j,n_j}(a_j, b_j, c_j; -ik_j\xi_j, -ik_j\eta_j), \tag{4}$$

where ξ_j and $\eta_j = r_j - \mathbf{r}_j \cdot \widehat{\mathbf{k}}_j$, are generalized parabolic coordinates (see [5] for details),

$$\Delta_{m,n}(a, b, c; x, y) = (ia)_m (-x)^m {}_1F_1[ia + m; b; x](-y)^n {}_1F_1[n; c; y], \tag{5}$$

$\mathbf{m} = \{m_1, m_2, m_3\}$ and $\mathbf{n} = \{n_1, n_2, n_3\}$. The coefficients $A_{\mathbf{m},\mathbf{n}}$, and b_i, c_i are determined when a particular approximate form of the non-orthogonal kinetic energy is used and the Schrödinger equation is solved. Also, it is possible to obtain these coefficients by satisfying different physical requirements like Redmond asymptotic behavior, Kato cusp conditions, etc. [3]. It has been shown in the same reference, that in some cases the coefficients b and c may, for instance, adopt the form $b = 1 + 2m$ and $c = 1 + 2n$, the one observed by the Φ_2 model [6]. For those cases, the function $\Delta_{m,n}(a, b, c; x, y)$ can be associated with the two-body Coulomb wave function where the magnetic number is different from zero.

It is clear then, that to compute the transition matrix element with a final state expanded in the Δ Coulomb basis, one has to deal with the integral:

$$J'_{mn} = Q_{mn} \int \frac{\mathrm{d}\mathbf{r}}{r} e^{-\lambda r + i\mathbf{q}\cdot\mathbf{r}} (-ik\xi)^m {}_1F_1[-ia + m; 1 + 2m; ik\xi](-ik\eta)^n {}_1F_1[n; 1 + 2n; ik\eta] \tag{6}$$

with $Q_{mn} = C^*_{mn}(-ia)_m N_0 N_\lambda$. The factors $N_0 = (2\pi)^{-3/2}$ and $N_\lambda = (\lambda^3/\pi)^{1/2}$ are the normalization constants of the final plane wave state and the initial ground state of the hydrogenic system, respectively. In Eq. (6), λ is associated to the charge of the bound state, $1/r$ to the Coulomb potential, $\mathbf{q}$ to the momentum transfer, a represents a Sommerfeld parameter and $\mathbf{k}$ stands for the final momentum of the system. The factor C_{mn} is the normalization factor to satisfy the asymptotic Coulomb wave condition,

$$C_{mn} = \frac{(-1)^{m+n}}{(ia)_m} \frac{\Gamma[1 + m - ia]}{\Gamma[1 + 2m]} \frac{\Gamma[1 + n]}{\Gamma[1 + 2n]} e^{-\pi\frac{a}{2} + i\pi(m+n)}. \tag{7}$$

We call Eq. (6) the *extended* Nordsieck integral to distinguish it from the *generalized* one given by

$$J'_1 = J'_1 \begin{pmatrix} z & a_1 & b_1 & \mathbf{p}_1 \\ \mathbf{q} & a_2 & b_2 & \mathbf{p}_2 \end{pmatrix} = \int \frac{\mathrm{d}\mathbf{r}}{r} e^{-zr + i\mathbf{q}\cdot\mathbf{r}} {}_1F_1[ia_1; b_1; ip_1\xi_1] {}_1F_1[ia_2; b_2; ip_2\xi_2] \tag{8}$$

and the *elementary* version in which in particular $b_1 = b_2 = 1$. Note that J'_{00} is a special case of the already computed elementary Nordsieck integral [1,7]. The integral in Eq. (6) can be reduced to a finite sum of generalized Nordsieck integrals which were studied by Colavecchia [8].

In this work, we introduce two groups of representations for the extended form of the generalized Nordsieck integral and test them against the numerical quadrature. In Section 2 we present the main formulas related to these representations, while in Section 3 the numerical results are shown. We summarize the results and discuss future developments in Section 4. Atomic units are used throughout this paper.

2. Mathematics

2.1. A single series expansion

Provided that in the generalized parabolic coordinates system the radius vector is given by

$$\mathbf{r} = \left(\sqrt{\xi\eta}\cos\phi, \sqrt{\xi\eta}\sin\phi, (\xi-\eta)/2\right) \tag{9}$$

and the element of volume is $\mathrm{d}\mathbf{r} = (\xi+\eta)/4\,\mathrm{d}\xi\,\mathrm{d}\eta\,\mathrm{d}\phi$ we find, after performing the integration in the ϕ-coordinate, that the integral in Eq. (6) can be written as

$$J'_{mn} = R_{mn}\int_0^{+\infty}\int_0^{+\infty} \mathrm{d}\xi'\,\mathrm{d}\eta'\,J_0\left[\sqrt{\xi'\eta'}\right]\xi'^m e^{\alpha'\xi'} \times {}_1F_1\left[-ia+m;1+2m;\frac{ik}{q_t}\xi'\right]\eta'^n e^{\beta'\eta'}\,{}_1F_1\left[n;1+2n;\frac{ik}{q_t}\eta'\right], \tag{10}$$

where $q_t = (q_x^2+q_y^2)^{1/2}$ stands for the transversal momentum transfer, $\xi' = \xi q_t$ and $\eta' = \eta q_t$. The remaining parameters are,

$$R_{mn} = 2\pi\,Q_{mn}\frac{1}{2q_t^2}\left(-\frac{ik}{q_t}\right)^{m+n}, \tag{11}$$

$$\alpha' = \frac{\alpha}{q_t} = \frac{-\lambda+iq_z}{2q_t} \quad \text{and} \quad \beta' = \frac{\beta}{q_t} = \alpha'^*. \tag{12}$$

The series expansion that we work out in this section is obtained directly from Eq. (10), once the Bessel J_0 function that couples the integration variables is expressed in terms of its power series expansion, e.g., $J_0[\sqrt{\xi'\eta'}] = \sum_{l=0}^{\infty}(-1/4)^l\xi'^l\eta'^l/l!^2$ [9]. The two integrals in variables ξ' and η' resulting from the substitution, are the integral representations of the Gauss hypergeometric functions in the parameters X and Y [5], respectively, involved in the next

$$J'_{mn} = S_{mn}\sum_{t=0}^{\infty}\frac{(m+1)_t(n+1)_t}{1_t}\frac{Z^t}{t!} \times {}_2F_1[-ia+m, m+1+t; 1+2m; X]\,{}_2F_1[n, n+1+t; 1+2n; Y], \tag{13}$$

$$X = -\frac{ik}{\alpha} = \frac{-2kq_z}{\lambda^2+q_z^2} + i\frac{2k\lambda}{\lambda^2+q_z^2}, \tag{14}$$

$$Z = -\frac{q_t^2}{4\alpha\beta} = -\frac{q_t^2}{4|\alpha|^2} = -\frac{q_x^2+q_y^2}{\lambda^2+q_z^2}, \tag{15}$$

$Y = -ik/\beta = -X^*$ and

$$S_{mn} = 2\pi\,Q_{mn}\frac{2}{\lambda^2+q_z^2}(-X)^m(-Y)^n 1_m 1_n. \tag{16}$$

The above series expansion converges absolutely if $|X| < X_0$, $|Y| < Y_0$ and $|Z| < Z_0$, whenever X_0, Y_0 and Z_0 satisfy that $(1 - X_0)(1 - Y_0) = Z_0$ or $(1 - X_0)^2 = Z_0$, the convergence radius X_0 determined by the parameters of the main integral. This condition holds because the last series expansion has the same absolute convergence properties than the triple hypergeometric function in the variables X, Y and Z, obtained when both Gauss ${}_2F_1$ hypergeometric functions in Eq. (13) are written in terms of their corresponding power series expansions [10]. The resulting triple power series expansion converges absolutely for suitable constrained values of X, Y and Z and the corresponding convergence intervals are related as stated before. This triple power series expansion is named by Srivastava and Manocha [11] as the Lauricella's F_3 or Saran's F_K hypergeometric function of three variables. The series expansion in Eq. (13) and the triple series expansion must converge absolutely within the same domain, since the only difference between both of them stems from the way the infinite terms of the two series are added. Even though in this case there is no doubt about the *analytic* convergence, the *numerical* convergence may be a source of problems.

As shown below, the expansion in Eq. (13) is suitable for numerical purposes in the region of low transversal momentum transfer q_t. This representation is divergent within the range of high values of q_t were the corresponding analytic continuation in the Z direction must be used to compute the main integral. This issue will be considered in the next section.

2.2. The multiple series expansion

A second series expansion is obtained from Eq. (13), first performing the summation with respect to the variable Z and then in the remaining variables, X and Y. After some algebra involving the Pochhammer coefficients, we obtain the double series expansion

$$J'_{mn} = S_{mn} \sum_{r=0}^{\infty} \sum_{s=0}^{\infty} \frac{(-ia+m)_r (m+1)_r}{(1+2m)_r} \frac{X^r}{r!} \frac{(n)_s (n+1)_s}{(1+2n)_s} \frac{Y^s}{s!} {}_2F_1[m+1+r, n+1+s; 1; Z]. \tag{17}$$

The series expansion in Eq. (17) keeps the same absolute convergence properties as the series in Eq. (13), since again, the only difference between the two of them stems from the way in which the terms of the series are added. It is worth noting that, from the numerical standpoint, this last expansion is a suitable representation of the main integral in Eq. (6) only at small values of the parameters k and $m+n$ for which the series remains convergent within all the range of momentum transfer q_t. This happens to be so because even though formally the series expansion is a representation of the main triple Nordsieck integral (it is an expansion in the variable Z), absolutely convergent only for suitable constrained values of Z, the analytical continuation of the involved Gauss hypergeometric function (which is an expansion in the variable Z^{-1}) is already well known and included in the computer software. As a result, the series expansion behaves in practice as if it were absolutely convergent within all the range of Z. However, as the parameters k and $m+n$ increase, the series expansion in Eq. (17) becomes numerically divergent at low values of q_t and remains a suitable representation only at high values of the parameter q_t. It behaves like an actual analytic continuation of the main triple series expansion. Since the expansion of Eq. (13) converges, numerically speaking, within the range of low momentum transfer, the triple series must be absolutely convergent at least for those low q_t values. For that reason the expansion in Eq. (17) is divergent at low q_t, but only due to numerical computer limitations.

The formal expression for the last partial analytical continuation in the Z direction of the Lauricella's triple hypergeometric function may be obtained from Eq. (17), performing the substitution of the compact form of the ${}_2F_1$ Gauss hypergeometric function in variable Z by its analytical continuation to obtain, after some algebra and for the case with $m \geqslant n$, the following

$$\begin{aligned} J'_{mn} = {} & S_{mn} (-1)^{m+n+1} \binom{m}{n} Z^{-(m+1)} \sum_{t=0}^{\infty} \frac{(m+1)_t (m+1)_t}{(m+1-n)_t} \frac{Z^{-t}}{t!} \\ & \times {}_2F_1[-ia+m, -t; 1+2m; X] {}_2F_1[n, n-m-t; 1+2n; Y]. \end{aligned} \tag{18}$$

The corresponding expansion for case with $m < n$ keeps a similar structure to the last one with the indexes m and n exchanged.

2.3. Connection with the generalized Nordsieck integrals

We have also computed a finite expansion of the extended Nordsieck integral in terms of generalized Nordsieck integrals, given by

$$J'_{mn} = Q_{mn}(1+m)_m(1+n)_n \sum_{r=0}^{m}\sum_{s=0}^{n}(-1)^{r+s}\binom{m}{r}\binom{n}{s} J'_1\begin{bmatrix} z & -a-ir & 1+m & \mathbf{k} \\ \mathbf{q} & -is & 1+n & -\mathbf{k} \end{bmatrix}. \tag{19}$$

On the other hand, Colavecchia et al. [12] computed from the integral representation of the Kummer functions included in the generalized Nordsieck integral in Eq. (8), a power series representation of the generalized integral J'_1 in terms of a particular case of the Lauricella generalized hypergeometric $F^{(3)}$ function of three variables [11]. Since the convergence properties of the expansion $F^{(3)}$ are not well known, two more expansions were computed and presented in the same cited reference. These expansions are given by (for short we write J'_1 in terms of the parameters given in [7])

$$J'_1 = 4\pi \frac{A_1^{-ia_1}A_2^{-ia_2}}{D}\sum_{k=0}^{\infty}\frac{(ia_1)_k(ia_2)_k 1_k}{(b_1)_k(b_2)_k}\frac{x_0^k}{k!} \times {}_2F_1[b_1-1, ia_1+k; b_1+k; z_1]\,{}_2F_1[b_2-1, ia_2+k; b_1+k; z_2] \tag{20}$$

and

$$J'_1 = 4\pi \frac{A_1^{-ia_1}A_2^{-ia_2}}{D}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\frac{(b_1-1)_l(ia_1)_l}{(b_1)_l}\frac{[z_1]^l}{l!}\frac{(b_2-1)_m(ia_2)_m}{(b_2)_m}\frac{[z_2]^m}{m!} \times {}_3F_2[1, ia_1+l, ia_2+m; b_1+l, b_2+m; x_0], \tag{21}$$

where

$$D = z^2 + \mathbf{q}^2, \tag{22}$$

$$S_i = \mathbf{q}\cdot p_i - izp_i, \quad i = 1,2, \tag{23}$$

$$S_3 = p_1q_2 - \mathbf{p}_1\cdot\mathbf{p}_2, \tag{24}$$

$$U_i = 2S_i/D, \qquad A_i = 1+U_i, \quad i = 1,2,3, \tag{25}$$

$$x_0 = 1 - \frac{A_1+A_2-A_3}{A_1A_2}, \tag{26}$$

$$z_1 = U_i/A_i, \quad i = 1,2. \tag{27}$$

Combining Eq. (19) with Eqs. (20) and (21), two additional representations of the extended generalized Nordsieck integral are obtained. We found, as it will be shown later, that the numerical convergence properties of each of these two representations are similar to those of representations in Eqs. (13) and (17), at least for the smaller values of the parameters m and n.

2.4. The numerical approach

To test the approximations obtained before, we developed a Fortran code for numerical integration in double precision that allowed us a straightforward determination of the actual value of the extended generalized integral in Eq. (6). The code was designed to integrate functions that are complicated only in a region of space by increasing the number of points taken in that interval. The code is based on the Simpson's method with 3 points, but including *exactly* the oscillations contained in the factors $\exp[\alpha'\xi']$ or $\exp[\beta'\eta']$.

The method so developed is much faster than the traditional Simpson scheme. Using a relative error $\varepsilon_r = 10^{-4}$, we reproduce at least 3 or 4 figures of the exact values as obtained before, only in the range of low k, say $k \lesssim 3$ a.u. for the case studied. For $k \gtrsim 3$ a.u. (incidentally the same value of the parameter k for which the divergence interval mentioned in the next section begins to unfold), the Fortran subroutine fails to compute the integral within all the ranges of the parameter q_t, for the value of ε_r considered. Smaller relative errors and extended precision (and consequently much more time consuming) are necessary in order to achieve convergency.

3. Numerical results

In this section we display some basic results obtained from the test on the numerical performance of the representations computed before against the numerical integration Fortran subroutine. All the matrix elements were computed by means of the Mathematica 4.0 program and plotted for the case with $\lambda = 2$ and $q_z = 1$ measured in atomic units, which simulate a typical double photoionization of Helium.

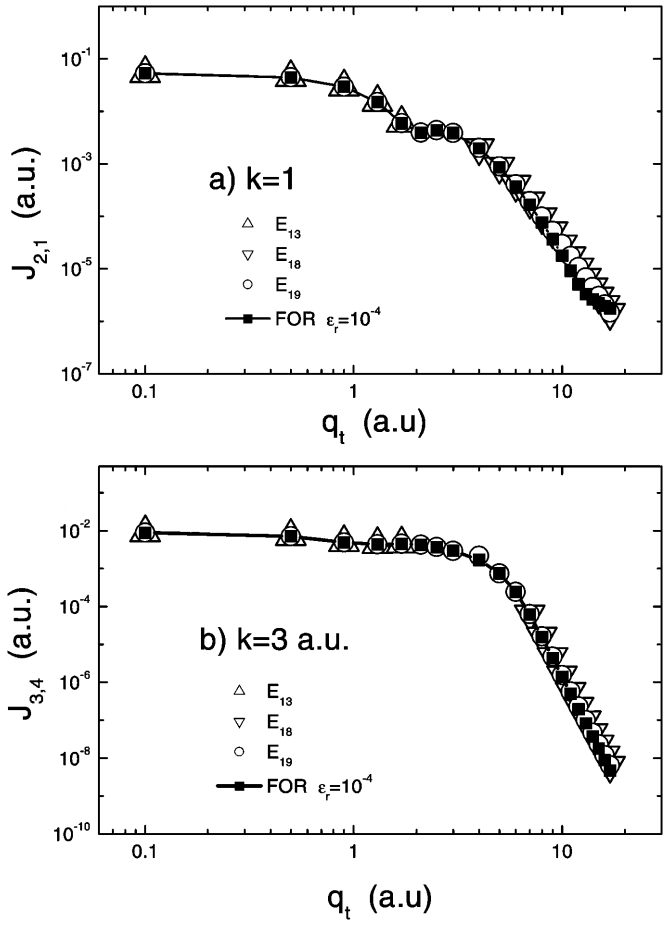

Fig. 1. Theoretical and numerical matrix element approximation for the two-body Coulomb system as a function of the transversal momentum transfer q_t at low $m+n$ and k. (a) $m = 2$, $n = 1$ and $k = 1$. (b) $m = 3$, $n = 4$ and $k = 3$.

For the sake of simplicity, we will denote each expansion by E_l where l indicates the number of equation while the numerical integral obtained by means of the Fortran subroutine will be denoted in the figures by FOR.

Each matrix element was obtained by evaluating the series expansions E_{13}, E_{18} and E_{19} together with the numerical quadrature FOR, at different points of the space of parameters and as a function of the momentum transfer q_t. The series obtained from Eqs. (17) and (21) were excluded from the numerical analysis, since their convergence properties do not improve those of series E_{18} and E_{19}, respectively.

In all the cases we believe that the correct value for the matrix element is the one obtained when the two independent series expansions (the couple E_{13} and E_{18}, and E_{19}) coincide within the error considered.

Whenever the parameters $m+n$ and k are kept small, e.g., $m+n \lesssim 10$ and $k \lesssim 3$ a.u., the series representations E_{13} (suitable for small q_t) and E_{18} (suitable for large q_t), considered as one, the Colavecchia's E_{19} and the numerical quadrature FOR are found to be equivalent in the sense that they produce the same numerical values (see Fig. 1) and demand similar CPU times in the performance of the sum. As the parameter $k > 3$ a.u., a finite interval $[q_m, q_M]$ in which all the approximations diverge begins to unfold. This is shown in Fig. 2. Note that the

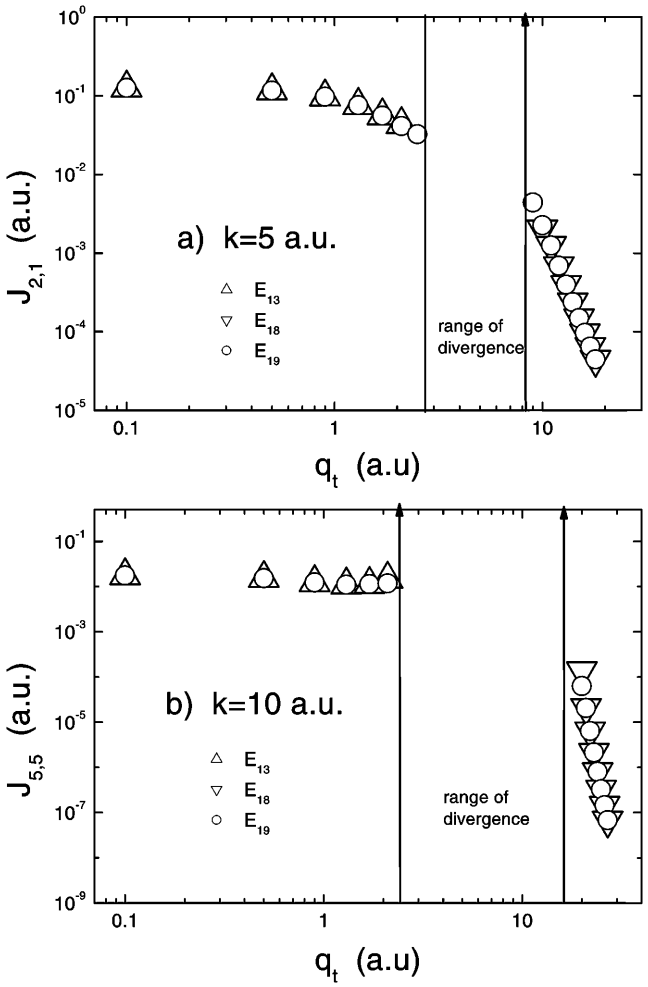

Fig. 2. Similar to Fig. 1 at low $m+n$ and high k. (a) $m=2$, $n=1$ and $k=5$. (b) $m=5$, $n=5$ and $k=10$. Between the vertical lines both theoretical representations diverge.

numerical quadrature FOR is not plotted, since the Fortran program fails to perform the integration within all the range of q_t, considering $\varepsilon_r = 10^{-4}$. In this situation, only the series representations are useful to evaluate the matrix element. The range of values of the parameter q_t for which the integral representations diverge is associated with the transition between the two characteristic regimes of the matrix element integral considered. That is, for $q_t < q_m$ the curve remains relatively constant and for $q_t > q_M$, the plot falls off as $q_t^{-2(m+1)}$ if $m \geqslant n$, which follows from Eq. (18). In this case $q_m \simeq 2$ a.u. while q_M is determined by the convergence of the series E_{19}. This latter limit depends upon the values of k, m and n. For $q_t \cong q_M$ the series E_{19} converges slowly while E_{18} does not converge. As q_t increases, both E_{18} and E_{19} converge, the former being much faster.

In Fig. 3, where the higher index matrix elements are considered, two points deserve to be mentioned. First, the CPU time spent to compute the matrix element from representation E_{19} increases notably compared with the corresponding time of the couple E_{13} and E_{18}, because the finite expansion given in Eq. (19) involves the computation of $(m+1)(n+1)$ different terms and because the Mathematica program needs to work with extended precision in order to reproduce the same result as the series E_{13} and E_{18}. The time required to compute each matrix element from the series E_{19} increases with the number of figures required to produce the correct result and this

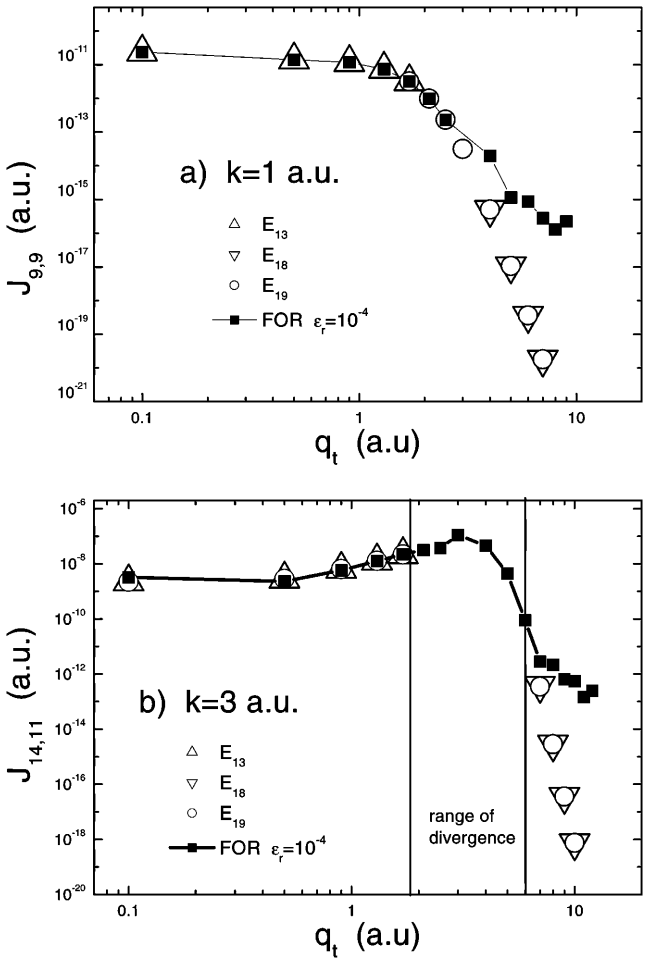

Fig. 3. Similar to Fig.1 at high $m+n$ and low k. (a) $m=9$, $n=9$ and $k=1$. (b) $m=14$, $n=11$ and $k=3$. Between the vertical lines both theoretical representations diverge.

number increase as $m + n$ increase. The second point to be noticed is that, as expected, the numerical quadrature loses its accuracy when the parameter $m + n$ increases considering $\varepsilon_r = 10^{-4}$, because for those integral indexes the correct matrix element value falls down to levels below the significance level of double precision description.

4. Conclusions

In this work we have obtained an analytical result for the extended Nordsieck integral. We have shown that this expression can be cast into a single index series expansion and a multiple series expansion, both involving Gauss hypergeometric functions. We have performed a comparative study on the performance of two analytical representations and a numerical integration subroutine, as a function of the transversal momentum transfer q_t.

We have found that the analytical models provide an accurate approximation to the actual value of the matrix element, within the range of values of the transversal momentum transfer q_t where they converge. For the higher values of the parameters $m + n$ and k, for which the Fortran subroutine fails to perform the main integral, both analytical representations converge to the same approximate value for the matrix element. In that situation it is observed that the CPU time spent by the representation E_{19} increases considerably, as compared with the time spent by the series E_{13} and E_{18}, however, near the extremes of the divergence interval, only the representation E_{19} converges.

The expansions here introduced may represent a very useful alternative to be considered and they provide a complementary strategy in the calculation of the transition matrices for the three charged particle problem. Further work has been undertaken to compute extended Nordsieck integrals in higher dimensions.

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