Multipole decomposition of potentials in relativistic heavy ion collisions

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Abstract

In relativistic heavy ion collisions an exact multipole decomposition of the Lorentz transformed time dependent Coulomb potentials in a coordinate system with equal constant, but opposite velocities of the ions, is obtained for both zero and different from zero impact parameter. The case of large values of $\gamma$ and the gauge transformation of the interaction removing both the $\gamma$ dependence and the $\ln b$ dependence are also considered.

1 Introduction

Relativistic heavy ion collisions offer us the opportunity to investigate the properties of nuclear matter under very extreme conditions of energy and temperature [1]. Information on the collision processes is only obtained indirectly from the energy and angular distributions of the produced particles and from fragment distributions. Electromagnetic probes like the photon and dilepton can yield essential information on the evolution of relativistic heavy ion collisions, since these signals leave the reaction zone without distortion by strong interaction. Photon and dilepton production are traditionally considered to be one of the possible probes for detecting the quark-gluon plasma [2].

Relativistic heavy ion collisions provide a tool for the investigation of electrons in extremely strong electromagnetic fields [3]. Different methods were used for studying the atomic physics effects – coupled channel equations, perturbation theory [4], finite difference equations (electron-positron pair production, pair production with capture). The field of electron-positron pair creation in relativistic heavy ion collisions is reviewed in Refs. [4, 5]. Different processes were studied in Refs. [6-9]. Electron-positron pair creation in relativistic heavy ion collisions was non-perturbatively described by coupled channel equations in a coordinate system with equal constant, but opposite velocities of the ions [10]. Electron-positron pairs are produced by the electromagnetic fields of high $Z$-ions in atomic collisions at relativistic velocities. Atomic collisions mean collisions with impact parameters which are larger than the sum of the nuclear radii,
i.e., the nuclear forces have no influence on the collision. The problem of dileptons excited through the mechanism of virtual bremsstrahlung was investigated in Ref. [11].

In Sec. II we examine the basic step of the calculational technology: the multipole expansion. An expansion in $1/\gamma$ produces the multipole expansion as compact, explicit and simple functions of space and time. We will fix the coordinate system in the centrum of mass of the colliding ions, which is the more appropriate system for studying the multiple pair production process. We proceed to a multipole decomposition of the two potentials, in order to approximate the two-center Dirac equation by a simpler one-center Dirac equation. We shall consider both the cases of large values of $\gamma$ and exact multipole decomposition, for both different from zero and zero impact parameter. In Sec. III we discuss about the gauge transformation of the interaction removing both the $\gamma$ dependence and the $\ln b$ dependence.

## 2 Classical form of the interaction

In the consideration of the electromagnetic interaction of relativistic heavy ions, their motion is assumed to be well described by straight line, classical paths and unperturbed by recoil effects. Since we are interested in the multiple pair production process, it is more natural to fix the coordinate system in the centrum of mass (or center of momentum – we consider the same type of colliding ions, with the same $A$ and $Z$ and equal constant, but opposite velocities) of the colliding ions, rather than on one of the ions, which is the case, for example, for bound electron-positron creation. The interaction of the electron-positron field with the moving ions is then given by the Lorentz transformed Coulomb potentials (Liénard-Wiechert potentials)

$$V_1(\rho, z, t) = \frac{eZ(1 - v\alpha)}{\{[(b/2 - \rho)/\gamma]^2 + (z - vt)^2\}^{1/2}}, \tag{1}$$

$$V_2(\rho, z, t) = \frac{eZ(1 + v\alpha_z)}{\{[-(b/2 - \rho)/\gamma]^2 + (z + vt)^2\}^{1/2}}. \tag{2}$$

Here $b$ is the distance between the ion straight line paths, which are taken along the $z$ axis (see Fig. 1); $eZ$ are the charges and $\mathbf{v}, -\mathbf{v}$ the velocities of the ions, $\gamma = 1/(1 - v^2)^{1/2}$, $\rho, z$ and $t$ are the coordinates of the electron-positron field relative to the c.m. system and $\alpha_z$ is the Dirac matrix. The characteristic effects of the electromagnetic interactions $eV_1$ and $eV_2$ produced by the ions are contained in their time dependence and the very severe compression of the spatial dependences (equivalently – the sharp
pulse description). The time-dependent two-center Dirac equation for the electron-positron motion is given by
\[
i \frac{\partial}{\partial t} \Psi(r, t) = H_D \Psi(r, t) \tag{3}
\]
(we employ the natural unit system with \(\hbar = c = m_e = 1\)). The Dirac Hamiltonian \(H_D\) is given by
\[
H_D = H_0 - eV_1 - eV_2, \quad (4)
\]
\[
H_0 = \alpha \cdot p + \beta. \quad (5)
\]

Since a method for constructing continuum wave functions for the two-center Dirac equation is known only for the static case (only for scalar potentials) [12, 13], we proceed to a multipole decomposition of \(V_1\) and \(V_2\), in order to approximate the two-center Dirac equation (3) by a simpler one-center Dirac equation. We will consider the following cases:

A. - large values of \(\gamma\) and \(b \neq 0\) (but not too large);
B. - exact multipole decomposition and \(b \neq 0\);
C. - exact multipole decomposition and \(b = 0\);
D. - large values of \(\gamma\) and \(b = 0\).

2.1 A. The case of large values of \(\gamma\) and \(b \neq 0\) (but not too large)

In [14] there were derived simple closed forms for the multipole \(M^m_l\) that are accurate for large values of \(\gamma\) (asymptotic-large \(\gamma\) limit) for the transformed Coulomb potential \(V_p\) in the case of a moving projectile and the coordinate system fixed on the target nucleus:
\[
V_p(\rho, z, t) = eZ_p(1 - v_p\alpha_z) \frac{1}{\{(b - \rho)/\gamma\}^2 + (z - v_gt)^2}^{1/2}, \tag{6}
\]
where \(Z_p, v_p\) and \(b\) are respectively the charge, the velocity and the impact parameter of the projectile. This multipole decomposition of the potential \(V_p\) reads
\[
M^m_l(r, t) = \int d\Omega Y^m_l(\theta, \phi) \quad \frac{1}{\{(b - \rho)/\gamma\}^2 + (z - v_gt)^2}^{1/2}, \tag{7}
\]
\[
V_p(\rho, z, t) = eZ_p(1 - v_p\alpha_z) \sum_{l,m} M^m_l(r, t)Y^m_l(\theta, \phi) = eZ_p(1 - v_p\alpha_z) \sum_{l,m} V^m_l(r, t). \tag{8}
\]
The derivation consists of an almost straightforward expansion about the near singular point \( z = v_p t \), after some careful rearrangements of the integrand. It is important to note that the expansion requires that \( b/(r - v_p t) \ll \gamma \); assuming that the nature of the physical problem confines \( r \) and \( v_p t \) to moderate multiples of \( \hbar/m_c \), the requirement of \( b \) becomes \( b \ll \gamma \hbar/m_c \) [14]. Defining \( \theta_t \) by

\[
\begin{align*}
(1) & \quad |v_p t| < r, \quad \cos \theta_t = \frac{v_p t}{r}, \quad \sin \theta_t = \sqrt{1 - \left(\frac{v_p t}{r}\right)^2}, \\
(2) & \quad |v_p t| > r, \quad \cos \theta_t = 1, \quad \sin \theta_t = 0,
\end{align*}
\]

replacing \( v_p \) by 1 (they differ only by \( O(1/\gamma^2) \)) and noting that to order \( \ln \gamma/\gamma^2 \) the \( (b - \rho)^2/\gamma^2 \) term in the denominator can be replaced by its value at \( \theta = \theta_t \), the asymptotic form of the multipole decomposition of \( V_p(\rho, z, t) \) (where \( z = r \cos \theta \)) is given for \( m > 0 \) by [14, 15]

\[
M^m_l(r, t) = \frac{Y^m_l(t, 0)}{r} \times \begin{cases} 
2\pi \left(\frac{r^2 - t^2}{b^2}\right)^{l/2}, & r < t < \sqrt{b^2 + t^2} \\
0, & r < t \\
\frac{2\pi}{m} \left(\frac{b^2}{r^2 - t^2}\right)^{l/2}, & r > \sqrt{b^2 + t^2}.
\end{cases}
\]

This expression is valid for positive \( m \) and \( t \). Negative \( m \) and \( t \) expressions are given by symmetry. For \( m = 0 \), the asymptotic form is [14, 15]

\[
M^0_l(r, t) = \frac{\sqrt{\pi}(2l + 1)}{r} \times \begin{cases} 
P_l(t/r)(2 \ln 2 \gamma + \ln \frac{r^2 - t^2}{b^2} - 2 \sum_{n=1}^{l-1} \frac{1}{n}), & t < r < \sqrt{b^2 + t^2} \\
2Q_l(t/r), & r < t \\
P_l(t/r)(2 \ln 2 \gamma - 2 \sum_{n=1}^{l} \frac{1}{n}), & r > \sqrt{b^2 + t^2}.
\end{cases}
\]

valid for positive \( t \), with the negative \( t \) form again to be obtained by symmetry. Here \( Q_l \) is the Legendre function of the second kind. Unless the \( m = 0 \) multipole terms are to be integrated together with functions that vary sharply in the \( r \sim v_p t \) region, the need for the bridge function at \( r \sim t \) disappears [14]. The evaluation of time-dependent matrix elements for use in coupled-channels calculations will be facilitated by the form of the above interaction (which will have an analogous structure for our two-center case). In Eqs. (10),(11) all terms can be expressed in terms of polynomials and/or convergent series in \( t/r \) for \( t < r \) and in \( r/t \) for \( r < t \). Thus the matrix element to be integrated over \( r \) can have its interaction expressed as a series of negative and positive powers of \( r \). In each of the terms of the series in \( r, t \) is effectively a coefficient: \( r \) and \( t \).
have become separable term by term. These asymptotic forms provide a simple means of calculating matrix elements. In addition they allow to straightforwardly look at the \( \gamma \) dependence of any set of matrix elements or amplitudes. As one can see directly, the \( \gamma \) dependence of the multipole operators appears only in the \( m = 0 \) terms and only in the one form [14]

\[
2(\ln 2\gamma) e Z_p (1 - \alpha_z) \sum_l Y^0_l(\theta) \sqrt{\pi(2l+1)} P_l(\frac{t}{r}) = 2(\ln 2\gamma) e Z_p (1 - \alpha_z) \delta(z - t), \quad r > t; (12)
\]

the condition \( r \geq t \) is automatically contained in the \( \delta(z - t) \). But as we shall see in Sec. III, this set of terms is entirely removable by a gauge transformation. Once having removed this explicit dependence on \( \gamma \), we are left only with the implicit dependence inherent in the limitation already noted that the above forms are valid only for the region \( b \ll \gamma h/m_\text{e}c \). However, when \( b \) is not small, perturbation theory is valid.

The multipole expansion for the potential \( V_1 \) is given also by the formulas (10),(11), but with \( b \) replaced by \( b/2 \), \( Z_p \) by \( Z \) and \( v_p \) by \( v \) with \( v = 1 \). We have proven that the multipole expansion for \( V_2 \) can be obtained from that for \( V_1 \), by replacing \( 1 - \alpha_z \) by \( 1 + \alpha_z \) and by multiplying the whole expression by \( (-1)^l \).

1. Monopole approximation

In the case \( l = 0, m = 0 \), we have

\[
V^{(0)}_1 = e Z (1 - \alpha_z) \frac{1}{2r} \times \begin{cases} 
2Q_0(\frac{t}{r}), & r < t \\
2 \ln 2\gamma + \ln \frac{r^2 - t^2}{b^2/4}, & t < r < \sqrt{b^2/4 + t^2} \\
2 \ln 2\gamma, & r > \sqrt{b^2/4 + t^2}
\end{cases} (13)
\]

and \( V^{(0)}_2 = V^{(0)}_1 (\alpha_z \to -\alpha_z) \). Then

\[
V^{(0)} = V^{(0)}_1 + V^{(0)}_2 = \frac{2eZ}{r} \times \begin{cases} 
2Q_0(\frac{t}{r}), & r < t \\
2 \ln 2\gamma + \frac{1}{2} \ln \frac{r^2 - t^2}{b^2/4}, & t < r < \sqrt{b^2/4 + t^2} \\
2 \ln 2\gamma, & r > \sqrt{b^2/4 + t^2}
\end{cases} \quad (14)
\]

Here

\[
Q_0(\frac{t}{r}) = \frac{1}{2} \ln \frac{t + r}{t - r}. \quad (15)
\]

2. Dipole approximation \((l = 1)\)
The dipole term is given by

\[ V^{(1)} = V^{(1)}_1 + V^{(1)}_2 = -\frac{3eZ\alpha z}{r} \sin \theta \cos \phi \sin \theta_t \times \begin{cases} 0, & r < t \\ \left( \frac{t^2 - t^2}{b^2/4} \right)^{3/2}, & t < r < \sqrt{b^2/4 + t^2} \\ \left( \frac{b^2/4}{r^2 - t^2} \right)^{1/2}, & r > \sqrt{b^2/4 + t^2} \end{cases} \]

\[ + \cos \theta \times \begin{cases} \frac{2Q_1 \left( \frac{t}{r} \right)}{2} \frac{2}{r} \left( 2 \ln 2 + \ln \frac{r^2 - t^2}{b^2/4} - 2 \right), & t < r < \sqrt{b^2/4 + t^2} \\ \left( \frac{-2}{r} \ln 2\gamma - 1 \right), & r > \sqrt{b^2/4 + t^2}. \end{cases} \] (16)

Here

\[ Q_1 \left( \frac{t}{r} \right) = \frac{t}{r} Q_0 \left( \frac{t}{r} \right) - 1 = \frac{t}{2r} \ln \frac{t + r}{t - r} - 1. \] (17)

We remind that \( v = 1 \) in the case A. In the dipole approximation we have to add the terms \( V^{(0)} \) and \( V^{(1)} \) given by Eqs. (14) and (16):

\[ V = V^{(0)} + V^{(1)}. \] (18)

### 2.2 B. Exact multipole decomposition \((b \neq 0)\)

The exact multipole decomposition is given as the series [14]:

\[ V_1 = eZ(1 - v\alpha z) \sum_{l,m} Y_l^m(\theta, \phi) \sum_{l'} Y_{l'}^m(\theta_u, 0) R(l, l'; r, u) A(m; l, l'; \frac{1}{v}), \] (19)

where

\[ u = \left( \frac{b^2}{4} + (vt)^2 \right)^{1/2}, \quad \cos \theta_u = \frac{vt}{u}, \quad \sin \theta_u = \frac{b}{2u} \] (20)

and

\[ R(l, l'; r, u) = \frac{\pi}{4} \frac{u'}{r^{l+1}} \frac{\Gamma \left( \frac{l + l' + 1}{2} \right)}{\Gamma \left( \frac{l - l' + 1}{2} \right)} F \left( \frac{l + l' + 1}{2}, \frac{l - l' + 3}{2}, \frac{u^2}{r^2} \right) \] for \( r > u \). (21)

\[ A(m; l, l'; \frac{1}{v}) = \frac{1}{4\pi} (-1)^m \sqrt{(2l + 1)(2l' + 1)} \sum_L C_{l''m\nu} C_{000}^{l''L} \frac{2}{v} Q_L \left( \frac{1}{v} \right). \] (22)

For \( r < u \), we have to do the interchange \( r \leftrightarrow u, l \leftrightarrow l' \) in \( R \). For the special case \( r = u \),

\[ R(l, l'; r, r) = \frac{\pi}{4} \frac{1}{r^{l+1}} \frac{\Gamma \left( \frac{l + l' + 1}{2} \right)}{\Gamma \left( \frac{l - l' + 1}{2} \right) \Gamma \left( \frac{l' + 1}{2} \right) \Gamma \left( \frac{l - l' + 1}{2} \right)}. \] (23)
This form for the multipole expansion is equivalent with that appearing in the literature. There is a set of special cases that is particularly simple [14]. For \( r > u \) the sum over \( l' \) in Eq. (19) is cut off by the spherical Bessel function integral (for \( \mathcal{R} \)) (the occurrence of a negative-integer value of the argument of the gamma function ensures that \( l' \leq l \)); furthermore, for \( l' \leq l \) the hypergeometric function is just a polynomial. Thus the exact result for \( Y_1^1 \) component of \( V_1 \) is for \( r > u \):

\[
Y_1^1(\theta, \phi) \sqrt{\frac{3\pi}{2}} \frac{b}{2r^2} \left[ \frac{1}{v^2} - 1 \right] Q_0\left(\frac{1}{v}\right) - \frac{1}{v^2} \right].
\]

(24)

As \( \gamma \to \infty, v \to 1 \), then the term in square brackets approaches \(-1\), in agreement with the corresponding expression in the case A. Similarly, the \( Y_1^0 \) component of \( V_1 \) is for \( r > u \):

\[
Y_1^0(\theta, \phi) \sqrt{3\pi} \frac{t}{r} \left[ \frac{2}{v^2} Q_0\left(\frac{1}{v}\right) - 2 \right].
\]

(25)

As \( \gamma \to \infty \), the term in square brackets approaches \( 2(\ln 2 - 1) \), in agreement with the case A. The difference between exact and asymptotic values is \( O(\ln \gamma / \gamma^2) \).

Another form of the exact multipole decomposition can be obtained if we write the denominator of \( V_1 \) as

\[
1 - \frac{1}{\sqrt{(x - b/2)^2 + y^2 + \gamma^2(z - vt)^2}} = \frac{1}{|\mathbf{r}' - \mathbf{R}'(t)|},
\]

with the vectors \( \mathbf{r}' = (x, y, \gamma z) \) and \( \mathbf{R}' = (b/2, 0, \gamma vt) \). The expansion in multipoles is then given by [3, 16]:

\[
1 - \frac{1}{|\mathbf{r}' - \mathbf{R}'|} = \begin{cases} 
\sum_{l=0}^{\infty} \frac{4\pi}{2l + 1} \frac{R_l^{q+1}}{R_l^q} \sum_{m=-l}^{l} Y_l^m(\hat{\mathbf{R}}') Y_l^m(\hat{\mathbf{r}}'), & r' \leq R' \\
\sum_{l=0}^{\infty} \frac{4\pi}{2l + 1} \frac{R_l^{q+1}}{R_l^q} \sum_{m=-l}^{l} Y_l^m(\hat{\mathbf{R}}') Y_l^m(\hat{\mathbf{r}}'), & r' \geq R'.
\end{cases}
\]

(27)

\( \hat{\mathbf{R}}' \) and \( \hat{\mathbf{r}}' \) represent the angular arguments of the spherical harmonics \( Y_l^m \) which give the direction of \( \mathbf{R}' \) and \( \mathbf{r}' \). As usual the scattering plane is taken to be \( \phi = 0 \). In consequence the spherical harmonics \( Y_l^m(\hat{\mathbf{R}}') \) is real-valued.

1. Monopole approximation \((l = 0)\)

We have (with \( \gamma^2 v^2 = \gamma^2 - 1 \) and \( R' = \sqrt{b^2/4 + \gamma^2 v^2 t^2 / \gamma} \)):

\[
V_1^{(0)}(\theta, \phi) = eZ(1 - v\alpha_z) \times \begin{cases} 
\frac{1}{R'} & r' \leq R' \\
\frac{1}{r'} & r' \geq R'
\end{cases}
\]

(28)
and \( V_2^{(0)} = V_1^{(0)}(\alpha_z \rightarrow -\alpha_z) \). Then

\[
V^{(0)} = 2eZ \times \left\{ \begin{array}{ll}
\frac{1}{R'} & r' \leq R' \\
\frac{1}{r'} & r' \geq R'.
\end{array} \right.
\]  

(29)

2. Dipole approximation

For \((l = 1)\) we have:

\[
V_1^{(1)} = eZ(1 - v\alpha_z) \times \left\{ \begin{array}{ll}
\frac{r'}{R} \cos \delta, & r' \leq R' \\
\frac{r'}{r'^2} \cos \delta, & r' \geq R'.
\end{array} \right.
\]  

(30)

where \(\delta\) is the angle between the vectors \(r'\) and \(R'\) and \(V_2^{(1)} = -V_1^{(1)}(\alpha_z \rightarrow -\alpha_z)\). Then the dipole term is given by

\[
V^{(1)} = -2eZv\alpha_z \cos \delta \times \left\{ \begin{array}{ll}
\frac{r'}{R^2}, & r' \leq R' \\
\frac{R'}{r'^2}, & r' \geq R'.
\end{array} \right.
\]  

(31)

and in the dipole approximation

\[
V = V^{(0)} + V^{(1)} = 2eZ \times \left\{ \begin{array}{ll}
\frac{1}{R} - v\alpha_z \cos \delta \times \left\{ \begin{array}{ll}
\frac{r'}{R^2}, & r' \leq R' \\
\frac{R'}{r'^2}, & r' \geq R'.
\end{array} \right.
\end{array} \right.
\]  

(32)

2.3 C. Exact multipole decomposition. The case \(b = 0\)

For the calculation of electron-positron pair production in heavy ion reactions the situation as \(b \rightarrow 0\) is of particular interest because it is in this lowest impact regime that the failure of perturbation theory is greatest. Since the scale at which nuclear effects contribute for two interacting large nuclei \((b \leq 15\) fm) is much smaller than the atomic scale for electrons and positrons \((\hbar/m_e c = 386\) fm), the \(b = 0\) solution should be of interest as closely approximating the situation at the smallest impact parameter for which nuclear effects are not applicable (or for which we omit all nuclear reactions). Sample calculations show \(b = 0\) and \(b = 15\) fm results to be \(\leq 1\%\) apart [15, 17].

Let us consider the \(b = 0\) case without any approximation in \(1/\gamma\). Here we assume \(t > 0\). To obtain appropriate expressions for \(t < 0\) one can make use of the symmetry relation \(M_0^0(r, -t) = (-1)^l M_0^0(r, t)\). By definition we have [15, 17] in the case of \(V_1\):

\[
M_l^{m(1)}(r, t) = \int d\Omega Y_l^m \frac{1}{\{\rho^2/\gamma^2 + (z - vt)^2\}^{1/2}}.
\]  

(33)
By symmetry only \( m = 0 \) is non-vanishing and we immediately integrate over \( \phi(\rho = r \sin \theta, z = r \cos \theta) \):

\[
M_{m}^{1}(r, t) = 2\pi \delta_{m, 0} \int_{-1}^{1} \frac{Y_{0}^{0}(\cos \theta) d(\cos \theta)}{\{r^2 \sin^2 \theta / \gamma^2 + (r \cos \theta - vt)^2\}^{1/2}}. \quad (34)
\]

Let us define \( x = \cos \theta \) and note that \( 1 / \gamma^2 = 1 - v^2 \) to rewrite

\[
M_{m}^{1}(r, t) = \sqrt{2\pi(2l + 1)} \frac{2}{rv} \int_{-1}^{1} \frac{P_{l}(x) dx}{(\frac{1}{v^2} + \frac{t^2}{r^2} - 1 - \frac{2xt}{vr} + x^2)^{1/2}}. \quad (35)
\]

This expression is symmetric in \( 1 / v \) and \( t/r \) and the integral over \( x \) can be carried out in closed form for each value of \( l \). The authors of Refs. [15, 17] recently found the following simple exact result for the multipole moments of the \( b = 0 \) case:

\[
M_{l}^{1}(r, t) = \delta_{m, 0} \frac{2\sqrt{\pi(2l + 1)}}{rv} \times \begin{cases} 
P_{l}(\frac{1}{v})Q_{l}(\frac{t}{r}), & r < vt \\
Q_{l}(\frac{1}{v})P_{l}(\frac{t}{r}), & r > vt.
\end{cases} \quad (36)
\]

Then

\[
V_{1} = eZ(1 - v\alpha_{z}) \sum_{l} Y_{0}^{0}(\theta) \frac{2\sqrt{\pi(2l + 1)}}{rv} \times \begin{cases} 
P_{l}(\frac{1}{v})Q_{l}(\frac{t}{r}), & r < vt \\
Q_{l}(\frac{1}{v})P_{l}(\frac{t}{r}), & r > vt.
\end{cases} \quad (37)
\]

We obtain for \( V_{2} \) the expression

\[
V_{2} = eZ(1 + v\alpha_{z}) \sum_{l} (-1)^{l} Y_{l}^{0}(\theta) \frac{2\sqrt{\pi(2l + 1)}}{rv} \times \begin{cases} 
P_{l}(\frac{1}{v})Q_{l}(\frac{t}{r}), & r < vt \\
Q_{l}(\frac{1}{v})P_{l}(\frac{t}{r}), & r > vt.
\end{cases} \quad (38)
\]

1. **Monopole approximation** (\( l = 0 \))

We obtain:

\[
V^{(0)} = V_{1}^{(0)} + V_{2}^{(0)} = \frac{2eZ}{r} \frac{1}{v} \times \begin{cases} 
Q_{0}(\frac{t}{r}), & r < vt \\
Q_{0}(\frac{1}{v}), & r > vt.
\end{cases} \quad (39)
\]

By taking the limit \( v \to 0, \lim_{v \to 0} \frac{1}{v}Q_{0}(\frac{1}{v}) = 1 \), so that in the non-relativistic limit we have \( V_{\text{non-rel}} = 2eZ/r \), as it should be.

2. **Dipole approximation** (\( l = 1 \))

In this case we have:

\[
V_{1}^{(1)} = eZ(1 - v\alpha_{z}) Y_{1}^{0}(\theta) \frac{2\sqrt{3\pi}}{rv} \times \begin{cases} 
\frac{1}{v}Q_{1}(\frac{t}{r}), & r < vt \\
\frac{1}{r}Q_{1}(\frac{1}{v}), & r > vt
\end{cases}. \quad (40)
\]
and $V_2^{(1)} = -V_1^{(1)}(\alpha_z \to -\alpha_z)$. Then

$$V^{(1)} = V_1^{(1)} + V_2^{(1)} = -\frac{6eZ\alpha_z}{r} \cos \theta \times \left\{ \begin{array}{ll}
\frac{1}{\sqrt{t}} Q_1\left(\frac{t}{r}\right), & r < vt \\
\frac{1}{\sqrt{r}} Q_1\left(\frac{r}{v}\right), & r > vt. 
\end{array} \right.$$

(41)

Therefore in the dipole approximation

$$V = V^{(0)} + V^{(1)} = \frac{2eZ}{r} \left[ \frac{1}{v} \times \left\{ \begin{array}{ll}
Q_0\left(\frac{t}{r}\right), & r < t \\
Q_0\left(\frac{r}{v}\right), & r > t. 
\end{array} \right. \right] - 3\alpha_z \cos \theta \times \left\{ \begin{array}{ll}
\frac{1}{\sqrt{t}} Q_1\left(\frac{t}{r}\right), & r < vt \\
\frac{1}{\sqrt{r}} Q_1\left(\frac{r}{v}\right), & r > vt. 
\end{array} \right.$$

(42)

2.4 D. The case of large values of $\gamma$ and $b = 0$

For $b = 0$ the expression of multipole moments takes on the simple form good up to order $\ln \gamma/\gamma^2$ [15, 17]. For $V_1$

$$M_l^{m(1)}(r,t) = \delta_{m,0} \frac{2\sqrt{\pi(2l+1)}}{r} \times \left\{ \begin{array}{ll}
\frac{Q_l\left(\frac{t}{r}\right)}{r}, & r < t \\
P_l\left(\frac{t}{r}\right)(\ln 2\gamma - \sum_{n=1}^{l} \frac{1}{n}), & r > t. 
\end{array} \right.$$

(43)

Here $t > 0$. To obtain appropriate expressions for $t < 0$ one can make use again of the symmetry relation. Analogously, we have for $V_2$:

$$M_l^{m(2)}(r,t) = (-1)^l M_l^{m(1)}(r,t).$$

In this asymptotic form, the split between the two regions $r > vt, r < vt$ has been written as $r > t, r < t$, dropping the $1/\gamma^2$ differences (we remind that $v \to 1$).

1. Monopole approximation ($l = 0$)

We have:

$$V_1^{(0)} = \frac{eZ(1 - \alpha_z)}{r} \times \left\{ \begin{array}{ll}
Q_0\left(\frac{t}{r}\right), & r < t \\
\ln 2\gamma, & r > t. 
\end{array} \right.$$

(44)

and $V_2^{(0)} = V_1^{(0)}(\alpha_z \to -\alpha_z)$. Then

$$V^{(0)} = V_1^{(0)} + V_2^{(0)} = \frac{2eZ}{r} \times \left\{ \begin{array}{ll}
Q_0\left(\frac{t}{r}\right), & r < t \\
\ln 2\gamma, & r > t. 
\end{array} \right.$$

(45)

2. Dipole approximation ($l = 1$)

We have:

$$V_1^{(1)} = eZ(1 - \alpha_z)Y_1^0(\theta) \frac{2\sqrt{3\pi}}{r} \times \left\{ \begin{array}{ll}
Q_1\left(\frac{t}{r}\right), & r < t \\
\frac{t}{r}\left(\ln 2\gamma - 1\right), & r > t. 
\end{array} \right.$$

(46)
and $V_{2}^{(1)} = -V_{1}^{(1)}(\alpha_{z} \rightarrow -\alpha_{z})$. Then

$$V^{(1)} = -\frac{6eZ\alpha_{z}}{r}\cos \theta \times \begin{cases} \frac{t}{r}(\ln 2\gamma - 1), & r > t. \\ Q_{1}(\frac{t}{r}), & r < t. \end{cases}$$

Therefore in the dipole approximation

$$V = V^{(0)} + V^{(1)} = \frac{2eZ}{r} \times \begin{cases} Q_{0}(\frac{t}{r}) - 3\alpha_{z}\cos \theta \times \begin{cases} \frac{t}{r}(\ln 2\gamma - 1), & r > t. \\ Q_{1}(\frac{t}{r}), & r < t. \end{cases} \end{cases}$$

(48)

In the monopole approximation, where only the term with $l = 0$ in the multipole expansion of the two-center potential is taken into account, a charged spherical shell of radius $vt$ (case C) or $t$ (case D) simulates the Coulomb potential of the two nuclei.

3 Gauge transformation of the interaction

It has previously been shown that in the large $\gamma$ limit a gauge transformation on the considered potential can remove both the large positive and negative time contributions of the potential as well as the $\gamma$ dependence [15, 17]. If one makes the gauge transformation on the wave function [15, 17]

$$\psi = e^{-i\chi(r,t)}\psi',$$

(49)

where

$$\chi(r,t) = \frac{eZ}{v}\ln[\gamma(z - vt) + \sqrt{b^{2} + \gamma^{2}(z - vt)^{2}}],$$

(50)

the interaction $V(\rho, z, t)$ is gauge transformed to

$$V(\rho, z, t) = \frac{eZ(1 - v\alpha_{z})}{\sqrt{[(b - \rho)/\gamma]^{2} + (z - vt)^{2}}} - \frac{eZ(1 - (1/v)\alpha_{z})}{\sqrt{b^{2}/\gamma^{2} + (z - vt)^{2}}}.$$ 

(51)

This transformation removes both the $\gamma$ dependence and the $\ln b$ dependence of the interaction for the region $r < \sqrt{b^{2} + t^{2}}$. The large $\gamma$ expression for the $m = 0$ gauge transformed interaction then becomes [15, 17]

$$M_{l}^{0}(r, t) = \frac{\sqrt{\pi}(2l + 1)}{r}P_{l}(\frac{t}{r}) \times \begin{cases} 0, & r < \sqrt{b^{2} + t^{2}} \\ -\ln \frac{r^{2} - t^{2}}{b^{2}}, & r > \sqrt{b^{2} + t^{2}}. \end{cases}$$ 

(52)

Note that this transformation affects the $m = 0$ part of the interaction only. An additional computational advantage of the previous form Eq. (52) is that the large
positive and negative time contributions inherent in the term $Q_l(t/r)$ of Eq. (11) have been removed, as was shown by Baltz, Rhoades-Brown and Weneser [15]. It is very important that there is no $\gamma$ dependence in either $m = 0$ or $m \neq 0$ parts of the interaction.

In the untransformed interaction, Eq. (11), the large negative and positive time interaction is dominated by the $m = 0$ interaction for $t > r$,

$$V_0^0(r, t) = \frac{1}{2r} \ln \frac{1 + r/t}{1 - r/t} = \frac{1}{t} + \frac{r^2}{3t^3} + \frac{r^4}{5t^5} + \ldots$$

(recall that there is no $t > r$ interaction for $m \neq 0$). There is a similar $Q_l(t/r)$ dependence in the exact $b = 0$ expression [15]. For the monopole interaction

$$V_0^0(r, t) = \frac{1}{2r} \ln \frac{1 + r/t}{1 - r/t} = \frac{1}{t} + \frac{r^2}{3t^3} + \frac{r^4}{5t^5} + \ldots$$

By analyzing $Q_l(t/r)$ for $l \neq 0$, one finds that other $m = 0$ interactions, $V_1^0(r, t)$ have terms of longest range going as $1/t^{l+1}$. For $r < t$ we must consider $Q_l(t/r)$ which has a piece equal to $-\ln(t - r)$. Likewise, for $t < r < \sqrt{b^2 + t^2}$, we must consider [15]

$$\ln \frac{r^2 - t^2}{b^2} = \ln \frac{r + t}{b^2} + \ln(r - t).$$

1. Monopole approximation

In the case $l = 0, m = 0$, we have

$$V_1^{(0)} = eZ(1 - \alpha_z) \frac{1}{2r} \times \begin{cases} 0, & r < \sqrt{b^2/4 + t^2} \\ -\ln \frac{r^2 - t^2}{b^2/4}, & r > \sqrt{b^2/4 + t^2} \end{cases}$$

and $V_2^{(0)} = V_1^{(0)}(\alpha_z \rightarrow -\alpha_z)$. Then

$$V_g^{(0)} = V_1^{(0)} + V_2^{(0)} = \frac{2eZ}{r} \times \begin{cases} 0, & r < \sqrt{b^2/4 + t^2} \\ -\ln \frac{r^2 - t^2}{b^2/4}, & r > \sqrt{b^2/4 + t^2} \end{cases}$$

2. Dipole approximation ($l = 1$)

The dipole term is given by

$$V_g^{(1)} = V_1^{(1)} + V_2^{(1)} = -\frac{3eZ\alpha_z}{r} [\sin \theta \cos \phi \sin \theta_t \times \begin{cases} 0, & r < t \\ \left(\frac{r^2 - t^2}{b^2/4}\right)^{1/2}, & t < r < \sqrt{b^2/4 + t^2} \\ \left(\frac{r^2 - t^2}{b^2/4}\right)^{1/2}, & r > \sqrt{b^2/4 + t^2} \end{cases}$$
In the dipole approximation we have to add the terms $V^{(0)}_g$ and $V^{(1)}_g$ given by Eqs. (57) and (58):

$$V_g = V^{(0)}_g + V^{(1)}_g.$$  

(59)

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