Asymptotic channels and gauge transformations of the time-dependent Dirac equation for extremely relativistic heavy-ion collisions

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We discuss the two-center, time-dependent Dirac equation describing the dynamics of an electron during a peripheral, relativistic heavy-ion collision at extreme energies. We derive a factored form, which is exact in the high-energy limit, for the asymptotic channel solutions of the Dirac equation, and elucidate their close connection with gauge transformations which transform the dynamics into a representation in which the interaction between the electron and a distant ion is of short range. We describe the implications of this relationship for solving the time-dependent Dirac equation for extremely relativistic collisions.

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I. INTRODUCTION

Particle production via electromagnetic processes in peripheral collisions of relativistic heavy ions has received significant study recently, both experimentally\cite{1,2} and theoretically (for reviews, see\cite{4–5}), due to anticipated experimental opportunities at colliding-beam accelerators, and the importance of this phenomena for the operation and performance of such facilities. Also of interest is the opportunity to study strong-field QED effects in particle production over a wide range of charge and collision energy\cite{Fig:4,5}. The high-energy limit of peripheral relativistic heavy-ion collisions has been recently examined, and closed-form expressions for the amplitudes describing electron-ion collisions has been recently examined, and closed-form expressions for the amplitudes describing electron-ion collisions have been obtained\cite{26–29}. These new results offer significant insight into the understanding of relativistic heavy-ion collision dynamics\cite{26,27}. In these works, the consequences of allowing the collision velocity to approach the speed of light, i.e. $\beta \equiv v/c \rightarrow 1$, and thus the collision energy to approach infinity, $\gamma \equiv (1 - \beta^2)^{-1/2} \rightarrow \infty$, have been investigated. This limit has been motivated by the progress toward new colliding-beam heavy-ion accelerator facilities currently in various stages of construction and planning. The Relativistic Heavy-ion Collider (RHIC) at Brookhaven National Laboratory will begin operation in 1999, offering collision velocities in the collider frame of $\beta_C \approx 0.999999$. Indeed, in experiments recently performed at CERN’s SPS\cite{26–29}, in which heavy-ions collide in a fixed-target mode, the equivalent collider-frame collision velocity exceeds 0.99c, suggesting that the high-energy limit is already a meaningful and relevant approximation for use in interpreting the experimental results\cite{29}. Of central importance to recent investigations of the high-energy limit is the use of a simplified form, accurate to leading order in the small parameter $\gamma^{-2}$, for the Lorentz-boosted Coulomb potential\cite{4,5,27} acting between the active electron and a bare nucleus. In this form, the dependence of the interaction on the transverse electron coordinates separates from the dependence on the longitudinal coordinate $z$ and the time $t$. Moreover, the dependence on the latter arises in combinations identified as the lightfront variables, e.g. $\tau \equiv (z \pm t)/2$, in the form of a zero-range or sharp potential. The separability of this interaction in the time-dependent, two-center Dirac equation allows for its closed-form solution\cite{26,27}. However, this useful form becomes apparent at the high energy limit only after applying phase transformations so as to remove the long-range $z$ dependence of the interaction\cite{27,23}.

In this present work, we study these phase transformations and show how they constitute well-defined gauge transformations while from a parallel perspective they formally define an interaction-representation in which the asymptotic (i.e. $|t| \to \infty$) interaction of an electron with a distant ion is absorbed into a redefinition of the electronic states. In this representation, which we call the short-range representation, the asymptotic channel states are free from effects of the distant ion, and in the high energy limit of infinite $\gamma$ the interaction has zero range. In the high-energy limit, the separation is exact. For finite $\gamma$, the short-range interaction is an approximation correct to order $\gamma^{-2}$, and so are the asymptotic channel wave functions. Neither the two-center Dirac equation, nor its boundary conditions, are rigorously separable for finite $\gamma$.

In this context, we review the pioneering work of Eichler and co-workers\cite{4,5} referred to by the name Coulomb-boundary conditions, where the long-range Coulomb or Liénard-Wiechert interaction was replaced by an effective short-range interaction. We show how
corrections of order $\gamma^{-2}$, explicit in our formal definition of the short-range representation, are implicit in the replacement procedure of the electron-projectile distance by the target-projectile distance that was used to obtain the asymptotic channels with these Coulomb-boundary conditions.

In Sec. II, we discuss the asymptotic channel solutions for the two-center Dirac equation for extremely relativistic ($\beta \rightarrow 1, \gamma \rightarrow \infty$) heavy-ion collisions. We derive factored forms for the asymptotic solutions which are accurate to order $\gamma^{-2}$, i.e. they are exact in the high-energy limit ($\gamma \rightarrow \infty$). In Sec. II A, we consider the case where the electron is asymptotically referred to the target reference frame (i.e. the electron is near to the target as $|t| \rightarrow \infty$), while in Sec. II B, we consider the case were the electron is asymptotically near to neither the target nor the projectile ion, and is most naturally referred to the collider (center-of-velocity) frame. In Sec. III, we define and present the short-range representation and derive from it the high-energy or sharp limit for the two-center Dirac equation in a simple form. In Sec. IV, we show that the phase transformation defining the short-range representation constitutes a gauge transformation. In so doing, we make explicit the connection between the Coulomb-boundary conditions and the gauge transformations first used by Baltz, Rhoades-Brown, and Weneser in numerically solving the two-center Dirac equation via coupled-channel methods. Alternative treatments of the asymptotic electron-projectile distance and alternative phase choices for the asymptotic channels are discussed in the appendices.

II. ASYMPTOTIC SOLUTIONS TO TWO-CENTER DIRAC EQUATION

We study relativistic heavy-ion collisions with a single active electron, e.g. we neglect electron-electron interactions in comparison to the strong electron-ion interactions. An external-field approach to the influence of the ions on the electron is appropriate for peripheral impact parameters, heavy-ions, and high energies, where, to a very good approximation, the ions travel on parallel, straight-line trajectories, and ion recoil is negligible. We are using natural units ($c = 1, m_e = 1$, and $\hbar = 1$). The quantity $\alpha$ is the fine-structure constant, $\alpha$ and $\gamma^\mu$ are Dirac matrices in the Dirac representation, as in Ref. [1], and $1_4$ is the 4-dimensional unit matrix.

A. States referred to a target-fixed inertial frame

Consider first a collision of a heavy, point-like projectile ion having charge $Z_P$ with a target ion having charge $Z_T$. We consider the dynamics of a single electron interacting with the external, time-dependent electromagnetic field created by the two heavy ions (see Fig. [1]). The position of the target nucleus is the origin of the electron coordinates, and the electron has position vector $\vec{r}_T = \vec{r} = (x, y, z)$, and time coordinate $t$. The projectile moves with constant velocity, $\beta$, parallel to the $z$ axis along a trajectory displaced from the target by the impact parameter $\vec{b}$. The projectile is located at the origin of the moving inertial frame, and in the projectile frame the electron’s position vector is $\vec{r}'' = (x'', y'', z'')$, and time coordinate $t''$. Coordinates in the target and projectile inertial frames are related by an inhomogeneous Lorentz transformation (Lorentz boost) parallel to the $z$ axis such that

$$
\begin{align*}
\vec{r}''_\perp &= \vec{r}_\perp - \vec{b} \\
z'' &= \gamma(z - \beta t) \\
t'' &= \gamma(t - \beta z),
\end{align*}
$$

where $\vec{r}_\perp = (x, y)$ are the transverse spatial coordinates of the electron in the target frame. The Lorentz boost implies that the electron-projectile distance in the projectile frame, $r''_{\perp} \equiv \sqrt{(x'')^2 + (y'')^2 + (z'')^2}$, is represented in target-frame coordinates as

$$
r''_{\perp}(t) = \sqrt{(\vec{r}_\perp - \vec{b})^2 + \gamma^2(z - \beta t)^2}. 
$$

Equivalently, we may refer all coordinates to the projectile nucleus. The resulting relations are obtained by the replacements $P \leftrightarrow T$, $\beta \rightarrow -\beta$ and $\vec{b} \rightarrow -\vec{b}$.

1. Two-center Dirac equation

The single-center Dirac equation describing the bound and continuum states of the target ion has the following form in the target frame,

$$
\frac{i}{\gamma} \frac{\partial}{\partial t} |\psi_T(\vec{r}, t)\rangle = \left[\hat{H}_0 + \hat{H}_T\right] |\psi_T(\vec{r}, t)\rangle, 
$$

where $\hat{H}_0$ is the free Dirac Hamiltonian, and $\hat{H}_T$ is the interaction of the electron with the target nucleus,

$$
\hat{H}_0 \equiv -i\alpha \cdot \vec{\nabla} + \gamma^0, 
$$

$$
\hat{H}_T \equiv -Z_T \alpha \cdot \vec{b}/r_T.
$$

By $\{ |\psi_T^{(j)}(\vec{r}, t)\rangle \}$, we denote the stationary states of the target ion with quantum numbers $j$ (e.g. see for details Ref. [14]).

The two-center, time-dependent Dirac equation in the target frame for an electron interacting with both target and projectile ions is

$$
\frac{i}{\gamma} \frac{\partial}{\partial t} |\Psi(\vec{r}, t)\rangle = \left[\hat{H}_0 + \hat{H}_T + \hat{H}_P(t)\right] |\Psi(\vec{r}, t)\rangle,
$$

where $|\Psi(\vec{r}, t)\rangle$ is the Dirac spinor wave function of the electron, and
\[ \hat{H}_P(t) = \frac{-Z_P \alpha \gamma (I_4 - \beta \alpha_z)}{\sqrt{(\vec{r}'_\perp - \vec{b}_t)^2 + \gamma^2(z - \beta t)^2}} \] (7)

is the electron-projectile interaction.

2. Coulomb-boundary conditions

The interactions appearing in the two-center, time-dependent Dirac equation, Eq. (1), are of long-range form, so that the distortion of the electron’s wavefunction induced by a distant ion should not, in principle, be neglected \[13\] [8]. Asymptotic channel wavefunctions are therefore defined as the solution of the two-center Dirac equation for asymptotic times. The importance of including the electron’s interaction with asymptotically distant ions has been discussed extensively by Eichler and coworkers \[39–41\] for relativistic atomic collisions in their work on the asymptotic solutions known as the Coulomb-boundary conditions (see Ref. \[4\], Sec. 5.3.3).

In defining the asymptotic channel solutions for the two-center Dirac equation, Eq. (1), the asymptotic electron-projectile separation \( r_P''(\vec{r}, t \to \infty) \) is approximated in Refs. \[14, 41\] by the internuclear separation \( R'' \) (see Appendix A, Eq. (A6)), that is

\[ r_P''(\vec{r}, |t| \to \infty) \to R'' = \sqrt{b^2 + \gamma^2(3z - \beta t)^2}. \] (8)

This approximation transforms Eq. (1) to the form

\[ i\frac{\partial}{\partial t}|\Phi_T^{R\infty}(\vec{r}, t)\rangle = \left[ \hat{H}_0 + \hat{H}_T + \hat{H}_P^{R\infty}(t) \right]|\Phi_T^{R\infty}(\vec{r}, t)\rangle, \] (9)

where \( |\Phi_T^{R\infty}(\vec{r}, t)\rangle \) is the asymptotic solution, and

\[ \hat{H}_P^{R}(t) \equiv -\frac{Z_P \alpha \gamma (I_4 - \beta \alpha_z)}{\sqrt{b^2 + \gamma^2(3z - \beta t)^2}}. \] (10)

is an approximate asymptotic electron-projectile interaction.

Equation (11) can be solved exactly for any value of \( \beta \). Consider an ansatz which is a product of a space-time dependent phase factor and a single-center state (i.e. a function of the electron-target distance),

\[ |\Phi_T^{R\infty}(\vec{r}, t)\rangle = e^{-i\chi_T(\vec{z}, t)}|\psi_T^{R\infty}(\vec{r}, t)\rangle, \] (11)

where the argument of the space-time dependent phase factor is

\[ \chi_T(\vec{z}, t) \equiv \frac{Z_P \alpha}{\beta} \ln(R'' - \beta t'') \]
\[ = \frac{Z_P \alpha}{\beta} \ln \left[ \gamma(\beta^2 z - \beta t) + \sqrt{b^2 + \gamma^2(3z - \beta t)^2} \right]. \] (12)

Substituting this ansatz into Eq. (11), multiplying from the left by \( e^{i\chi_T(\vec{z}, t)} \), and collecting like terms gives

\[ i\frac{\partial}{\partial t}|\psi_T^{R\infty}(\vec{r}, t)\rangle = \left[ \hat{H}_0 + \hat{H}_T \right]|\psi_T^{R\infty}(\vec{r}, t)\rangle. \] (13)

With the ansatz (11), both the scalar and the vector components of the asymptotic interaction (10) are canceled exactly, and Eq. (13) is identical to Eq. (3). This means that \( |\Phi_T^{R\infty}(\vec{r}, t)\rangle \) of Eq. (11) factors exactly into a space-time dependent phase factor and a single-center target eigenstate \( |\psi_T^{R\infty}(\vec{r}, t)\rangle = |\psi_T(\vec{r}, t)\rangle \).

The relativistic asymptotic solutions of the form (11) are exact only in the \( \gamma \to \infty \) limit. For large, finite \( \gamma \), the factored forms are very useful, approximate asymptotic solutions.

In the derivation reviewed here, the approximation occurs in using Eq. (8) to obtain Eq. (9), and not in the solution to Eq. (1). The asymptotic distance, Eq. (8), is accurate in the nonrelativistic limit \( \beta^2 \ll 1, \gamma \approx 1 \) \[39\], but becomes approximate for larger values of \( \gamma \), when its accuracy is of the order \( \gamma^{-2} \) (see Appendix A).

3. Asymptotic two-center Dirac equation

Here we present an alternative derivation of the factored asymptotic channel states. Formally, at the asymptotic limit, Eq. (8) gives an asymptotic two-center Dirac equation, (Eq. (11) below), that is exact in the following sense: it is the rigorous mathematical limit of Eq. (8) as \( |t| \to \infty \). We obtain this exact equation and then solve it approximately, to order \( \gamma^{-2} \).

Consider again the case with the electron near to the target at asymptotic times. In this limit, the electron-projectile distance is (A10),

\[ \lim_{|t| \to \infty} r_P''(\vec{r}, t) \equiv r_P''(\vec{r}, t) = \sqrt{b^2 + \gamma^2(3z - \beta t)^2}. \] (14)

This expression differs from (2) by neglecting the transverse electron coordinate \( z \), while the longitudinal coordinate \( z \) is retained, since it enters into the Lorentz transformation (see Appendix A). Using this distance to obtain the asymptotic limit of the electron-projectile interaction, the asymptotic, two-center Dirac equation in the target frame is

\[ i\frac{\partial}{\partial t}|\Phi_T^{\infty}(\vec{r}, t)\rangle = \left[ \hat{H}_0 + \hat{H}_T + \hat{H}_T^{\infty}(t) \right]|\Phi_T^{\infty}(\vec{r}, t)\rangle, \] (15)

where \( |\Phi_T^{\infty}(\vec{r}, t)\rangle \) is the asymptotic channel solution for an electron referred to the target frame, and \( \hat{H}_T^{\infty}(t) \) is the exact asymptotic interaction of the electron with the distant projectile,

\[ \hat{H}_T^{\infty}(t) \equiv -\frac{Z_P \alpha \gamma (I_4 - \beta \alpha_z)}{\sqrt{b^2 + \gamma^2(3z - \beta t)^2}}. \] (16)

For solutions to the asymptotic Dirac equation, Eq. (15), consider an ansatz which is a product of a space-time dependent phase factor and a single-center state,
\[ |\Phi_F^\infty(\vec{r}, t)\rangle = e^{-i\chi_F(\vec{r}, t)}|\psi^\infty(\vec{r}, t)\rangle, \]

where the argument of the space-time dependent phase factor is
\[ \chi_F(\vec{r}, t) = \frac{Z\rho(\vec{r}, t)}{\beta} \ln \left[ \sqrt{\gamma(z - \beta t)^2 + b^2 + \gamma^2(z - \beta t)^2} \right]. \]

Substituting this ansatz into Eq. (13), multiplying from the left by \( e^{i\chi_F(\vec{r}, t)} \), and collecting like terms gives
\[ i\frac{\partial}{\partial t}|\psi^\infty(\vec{r}, t)\rangle = \left[ \hat{H}_0 + \hat{H}_T \right]|\psi^\infty(\vec{r}, t)\rangle - \left( \frac{1}{\gamma^2 - 1} \right) \frac{Z\rho(\vec{r}, t)}{\sqrt{b^2 + \gamma^2(z - \beta t)^2}} |\psi^\infty(\vec{r}, t)\rangle. \]

The scalar component of the asymptotic electron-projectile interaction is canceled exactly. The remaining vector component is of order 1, and
\[ \langle \gamma \to \infty \lim \frac{|\psi^\infty(\vec{r}, t)\rangle}{\psi_T(\vec{r}, t)} \] a space-time dependent phase factor,
\[ \lim_{\beta \to 1} |\Psi_F^\infty(\vec{r}, t)\rangle = e^{-i\chi_F(\vec{r}, t)}|\psi_T(\vec{r}, t)\rangle. \]

We have discussed two alternative derivations of the factored forms for the asymptotic solutions for the two-center Dirac equation and have shown that they provide identical results in the high-energy limit: Equations (1) and (13), as well as their respective solutions, Eqs. (11) and (20), are identical as \( \beta \to 1 \). The physical reason for this is simple. As \( \beta \to 1 \), the target atom, as seen from the projectile, shrinks to a disk, so that the distinction between the \( z \)-coordinate of the nucleus and that of the electron disappears.

For large, finite \( \gamma \), both derivations provide slightly different, but equally useful, approximate solutions accurate to order \( \gamma^{-2} \). Other equally valid choices of the argument of the phase factor in Eq. (18) can be made which differ only in factors of \( \beta^2 \) (see Appendix B).

**B. Collider frame**

For electrons distant from both the target and projectile ion at asymptotic times, the collider (i.e., center-of-mass) inertial frame is a natural choice. The origin of the collider frame is reached from the origin of the target frame, for example, by an inhomogeneous Lorentz transformation in the \( z \) direction to a frame of velocity \( \beta_C = \sqrt{1 - \gamma^2} \) and Lorentz factor \( \gamma_C = (\gamma + 1)/2 \). In the transverse direction, the origin of the collider frame is located equidistant from the target and projectile trajectories (see Fig. 3). The position vector of the electron in the collider frame is \( \vec{r}_C' = \vec{r}' = (x', y', z') \), and the associated time is \( t' \). Coordinates in the projectile and target frames are each related to the coordinates in the collider frame by equal, but oppositely directed, Lorentz transformations in the \( z \) direction,
\[ \vec{r}_C' = \vec{r}_C' - \vec{b}/2 \]
\[ z = \gamma C(z' + \beta_C t') \]
\[ t = \gamma C(t' + \beta_C z') \]
and,
\[ \vec{r}_C' = \vec{r}_C' + \vec{b}/2 \]
\[ z = \gamma C(z' + \beta_C t') \]
\[ t = \gamma C(t' + \beta_C z') \]

As a consequence of the Lorentz boosts, the electron-projectile distance in collider-frame coordinates is
\[ r_C'(\vec{r}', t') = \sqrt{(\vec{r}_C' - \vec{b}/2)^2 + \gamma C^2 z' - \beta_C t')^2}, \]
and the electron-target distance in collider-frame coordinates is
\[ r_T(\vec{r}', t') = \sqrt{(\vec{r}_C' + \vec{b}/2)^2 + \gamma C^2 z' + \beta_C t')^2}. \]

1. Two-center Dirac equation

The free-particle Dirac equation in the collider frame has the form
\[ i\frac{\partial}{\partial t}|\phi_C(\vec{r}, t')\rangle = \hat{H}_0^C|\phi_C(\vec{r}, t')\rangle, \]
where \( \hat{H}_0^C \) is the free Dirac Hamiltonian in the collider frame,
\[ \hat{H}_0^C = -i\vec{\alpha} \cdot \vec{\nabla} + \gamma C. \]

The set \( \{\phi_C^{(j)}(\vec{r}, t')\} \) represents the Dirac plane-wave eigenstates with quantum numbers \( j' \), namely, the three components of the momentum, \( \vec{\gamma} \), the sign of the energy, and the spin.

The two-center, time-dependent Dirac equation in the collider frame for an electron interacting with both target and projectile ions is
\[ i\frac{\partial}{\partial t}|\Psi'(\vec{r}', t')\rangle = \left[ \hat{H}_0^C + \hat{H}_T(\vec{r}') + \hat{H}_P(\vec{r}') \right]|\Psi'(\vec{r}', t')\rangle, \]
where \( |\Psi'(\vec{r}', t')\rangle \) is the Dirac spinor wave function of the electron, \( \hat{H}_T(\vec{r}') \) is the electron-target interaction, and \( \hat{H}_P(\vec{r}') \) is the electron-projectile interaction,
\[
\hat{H}_T(t') = -\frac{Z_T \alpha \gamma_C (I_4 + \beta_C \partial_z)}{\sqrt{(r_\perp + b/2)^2 + \gamma_C^2 (z' - \beta_C t')^2}} \tag{32}
\]

\[
\hat{H}_P(t') = -\frac{Z_P \alpha \gamma_C (I_4 - \beta_C \partial_z)}{\sqrt{(r_\perp - b/2)^2 + \gamma_C^2 (z' - \beta_C t')^2}} \tag{33}
\]

2. Asymptotic two-center Dirac equation

Consider, in the collider frame, at asymptotic times, an electron distant from both the target and projectile ions. The electron-projectile and electron-target distances then have the following asymptotic limits,

\[
\lim_{|\nu'| \to \infty} r_P'(\hat{r}', t') \equiv r_P^\infty(\hat{r}', t') = \sqrt{(b/2)^2 + \gamma_C^2 (z' - \beta_C t')^2},
\]

\[
\lim_{|\nu'| \to \infty} r_T(\hat{r}', t') \equiv r_T^\infty(\hat{r}', t') = \sqrt{(b/2)^2 + \gamma_C^2 (z' + \beta_C t')^2}. \tag{34}
\]

Using these distances, the asymptotic, two-center Dirac equation is

\[
\frac{i}{\partial t'} |\Phi_C^\infty(\hat{r}', t')\rangle = \left[ \hat{H}_0' + \hat{H}_T^\infty(\hat{t}') + \hat{H}_P^\infty(\hat{t}') \right] |\Phi_C^\infty(\hat{r}', t')\rangle, \tag{35}
\]

where \(|\Phi_C^\infty(\hat{r}', t')\rangle\) is the Dirac spinor wave function of the electron asymptotic channel solution, \(\hat{H}_T^\infty(\hat{t}')\) is the asymptotic electron-target interaction, and \(\hat{H}_P^\infty(\hat{t}')\) is the asymptotic electron-projectile interaction,

\[
\hat{H}_T^\infty(\hat{t}') \equiv -\frac{Z_T \alpha \gamma_C (I_4 + \beta_C \partial_z)}{\sqrt{(b/2)^2 + \gamma_C^2 (z' + \beta_C t')^2}} \tag{36}
\]

\[
\hat{H}_P^\infty(\hat{t}') \equiv -\frac{Z_P \alpha \gamma_C (I_4 - \beta_C \partial_z)}{\sqrt{(b/2)^2 + \gamma_C^2 (z' - \beta_C t')^2}} \tag{37}
\]

For the solutions of Eq. (34), consider an ansatz of a space-time dependent phase factor times a Dirac plane-wave state,

\[
|\Phi_C^\infty(\hat{r}', t')\rangle = e^{-i\chi_C'(z', t')} |\phi^\infty(\hat{r}', t')\rangle, \tag{38}
\]

where

\[
\chi_C'(z', t') = \frac{Z_P \alpha}{\beta} \ln \left[ \frac{\gamma_C (z - \beta_C t') + \sqrt{(b/2)^2 + \gamma_C^2 (z' - \beta_C t')^2}}{\gamma_C (z + \beta_C t') + \sqrt{(b/2)^2 + \gamma_C^2 (z' + \beta_C t')^2}} \right]. \tag{39}
\]

Substituting Eq. (39) into Eq. (33), multiplying from the left by \(e^{+i\chi_C'(z', t')}\), and collecting like terms gives

\[
\frac{i}{\partial t'} |\phi^\infty(\hat{r}', t')\rangle = \left[ \hat{H}_0' + \frac{1}{\gamma_C^2 - 1} \frac{Z_T \alpha \beta C \partial_z}{\sqrt{(b/2)^2 + \gamma_C^2 (z' + \beta_C t')^2}} \right] |\phi^\infty(\hat{r}', t')\rangle \tag{40}
\]

As in the target-centered case, the scalar component of the asymptotic-electron-projectile and electron-target interactions cancel exactly, and the vector component vanishes in the \(\beta_C \to 1\) limit. In this limit, the remaining equation is identical to the free Dirac equation, Eq. (23), and \(|\phi^\infty(\hat{r}', t')\rangle \to |\phi_C'(\hat{r}', t')\rangle\), is a Dirac plane-wave eigenstate. We conclude that in the extreme, high-energy limit, the ansatz in Eq. (33) with the Dirac plane wave, is the exact solution to the asymptotic, two-center Dirac equation, Eq. (35),

\[
\lim_{\beta_C \to 1} |\Phi_C^\infty(\hat{r}', t')\rangle = e^{-i\chi_C'(z', t')} |\phi_C'(\hat{r}', t')\rangle. \tag{41}
\]

III. SHORT-RANGE REPRESENTATION

The factored forms of the asymptotic solutions to the two-center Dirac equation, Eqs. (11, 20, 41), obtained in the previous section, invite the definition of a new representation for the time-dependent Dirac equation. In this section, we introduce this representation, which we call the short-range representation, within the context of computing amplitudes for direct reactions first in the target frame, and then the collider frame.

In nonrelativistic \([39]\) as well as in relativistic collisions \([40, 41]\), it has been previously shown to be useful to introduce a formulation that substitutes the long-range Coulomb or Liénard-Wiechert interaction by an effective short-range interaction, jointly with an appropriate phase transformation, thus rendering formal scattering theory applicable. The essence of these approaches has been to replace the electron-projectile separation for an electron close to the target and asymptotically far from the projectile, by the internuclear separation \(R_0'\) given by the expression \([8]\). Then, with an ansatz like Eq. (11), the approximate asymptotic electron-projectile interaction \([11]\) can be removed completely from the Hamiltonian, so that for finite electron-projectile separations, one has to deal with a short-range interaction obtained from the original long-range one by the replacement

\[
\frac{1}{r_p'} \to \frac{1}{r_p'} - \frac{1}{R_0'}. \tag{42}
\]

The effects of subtracting the asymptotic long-range part have been demonstrated numerically for direct and rearrangement collisions using perturbation theory and coupled-channel methods \([41]\).
We have shown in the previous section and in appendix A that in the relativistic regime $R'\gamma$ differs from a more rigorous asymptotic limit for the electron-projectile separation $|\mathbf{r}|$ or $|\mathbf{A}|$, by terms of the order of $1/\gamma^2$. This approach revealed that a complete and exact removal of the asymptotic electron-projectile interaction is possible only in the $\beta \to 1$ limit (see Eqs. (19) and (23)).

For finite relativistic energies, terms of the order $1/\gamma^2$ remain in either the scalar or vector components of the electron-projectile asymptotic interaction, but are small for large $\gamma$. In the following, we are concentrating on the high-energy limit, in which the description becomes simple and unique.

### A. Exact Transition Amplitudes

Following the notation of Ref. [13], let $|\Psi_j^+(t_f)\rangle$ be the exact outgoing-wave solution evolving from an initial channel solution $|\Phi_j^+(t_i)\rangle$, i.e.

$$\lim_{t_i \to -\infty} |\Psi_j^+(t)\rangle = |\Phi_j^+(t)\rangle,$$  \hspace{1cm} (43)

and $|\Phi_k^\infty(t_f)\rangle$ be the final asymptotic channel. Then, by definition, the exact transition amplitude is given in the post form as

$$A_{kj}^{(+)} = \lim_{t_i \to -\infty} \langle \Phi_k^\infty(t_f) | \Phi_j^+(t) \rangle.$$  \hspace{1cm} (44)

The prior form of the amplitude is defined at $t \to -\infty$ as the projection of the exact incoming wave solution $|\Psi_j^-(t_i)\rangle$ evolving backward in time from the final channel $|\Phi_k^\infty(t_f)\rangle$, i.e.

$$\lim_{t_i \to -\infty} |\Psi_k^-(t)\rangle = |\Phi_k^\infty(t)\rangle,$$  \hspace{1cm} (45)

onto the initial channel solution $|\Phi_j^+(t)\rangle$,

$$A_{kj}^{(-)} = \lim_{t_i \to -\infty} \langle \Phi_j^+(t_i) | \Phi_k^\infty(t) \rangle.$$  \hspace{1cm} (46)

The post and prior forms of the amplitude may be unified using the time-evolution operator $\hat{U}(t_f, t_i)$ to relate the full outgoing-wave (incoming-wave) solution to its initial (final) state as

$$|\Psi_j^+(t_f)\rangle = \hat{U}(t_f, t_i)|\Phi_j^+(t_i)\rangle$$

$$|\Psi_k^-(t_i)\rangle = \hat{U}^\dagger(t_f, t_i)|\Phi_k^\infty(t_f)\rangle.$$  \hspace{1cm} (47)

Inserting Eqs. (47) into Eq. (44) or Eq. (46), one obtains,

$$A_{kj} = \lim_{t_i \to -\infty} \langle \Phi_k^\infty(t_f) | \hat{U}(t_f, t_i)| \Phi_j^+(t) \rangle.$$  \hspace{1cm} (48)

Reference [13] considered these states in the target inertial frame. Yet, the definitions presented here apply to the projectile or collider as well. In direct reactions, the initial and final channels in Eq. (48) are both solutions of the same asymptotic Hamiltonian associated with a single collision partner (e.g. atomic excitation or ionization). In rearrangement collisions, the initial and final channels may be solutions of different asymptotic Hamiltonians associated with different collision partners (e.g. charge exchange).

### B. Short-range Dirac equation

In this section, we discuss the short-range representation for the Dirac equation within the context of computing transition amplitudes for direct reactions in the high-energy limit.

#### 1. Equation of motion: target frame

In the following, we consider the limit $\beta \to 1$, so that the asymptotic channels for a target-frame electron interacting with a nearby target ion and a distant projectile ion has the exact, factored solution of Eq. (20). We substitute this asymptotic solution into the expression for the exact transition amplitudes for direct reactions in the target frame, Eq. (48), for the initial state $j$ and final state $k$,

$$A_{kj} = \lim_{t_i \to -\infty} \langle \psi^j_k(t_f)| e^{-i\mathbf{P}_r \mathbf{r} (t_f)} | \psi^j_k(t_i) \rangle.$$  \hspace{1cm} (49)

Rearranging the exponential factors in the expression so that they are applied directly to the evolution operator, one obtains

$$A_{kj} = \lim_{t_i \to -\infty} \langle \psi^j_k (t_f) | e^{-i\mathbf{P}_r \mathbf{r} (t_f)} \hat{U}(t_f, t_i)| e^{-i\mathbf{P}_r \mathbf{r} (t_i)} \psi^j_k (t_i) \rangle.$$  \hspace{1cm} (50)

The transition amplitude, Eq. (50), is suggestive of a new representation for the dynamics through the operation of the space-time-dependent phase,

$$|\Psi^S(r', t)\rangle = e^{i\mathbf{P}_r \mathbf{r} (t)} |\Psi^S(r', t)\rangle,$$  \hspace{1cm} (51)

$$\hat{U}^S(t_f, t_i) = e^{i\mathbf{P}_r \mathbf{r} (t_f)} \hat{U}(t_f, t_i) e^{-i\mathbf{P}_r \mathbf{r} (t_i)},$$  \hspace{1cm} (52)

where $|\Psi^S(r', t)\rangle$ is the wavefunction, and $\hat{U}^S(t_f, t_i)$ is the time-evolution operator in the new representation. Substituting Eq. (52) into Eq. (50) gives the exact amplitude for direct reactions in the new representation,

$$A_{kj} = \lim_{t_i \to -\infty} \langle \psi^j_k (t_f) | \hat{U}^S(t_f, t_i)| \psi^j_k (t_i) \rangle.$$  \hspace{1cm} (53)

Note that Eq. (53) has the form of a transition amplitude computed between initial and final channels which are
undistorted single-center eigenstates of the target ion, as would be the case if the interaction between the electron and the distant projectile was of short range.

To understand better its utility, we transform the two-center Dirac equation into the short-range representation. Beginning with Eq. (35), and making the substitution

$$|\Psi(\vec{r}, t)\rangle = e^{-i\chi_P(z, t)}|\Psi(S)(\vec{r}, t)\rangle, \quad (54)$$
gives, after multiplying from the left by $e^{i\chi_P(z, t)}$, the equation of motion,

$$i\frac{\partial}{\partial t}|\Psi(S)(\vec{r}, t)\rangle = \left[\hat{H}_0 + \hat{H}_T + \hat{W}_P(t)\right]|\Psi(S)(\vec{r}, t)\rangle, \quad (55)$$

where $\hat{W}_P(t)$ is the time-dependent electron-projectile interaction in the new representation [35],

$$\hat{W}_P(t) \equiv \hat{H}_P(t) - \frac{Z_P e\alpha\gamma(I_4 - (1/\beta)\hat{a}_z)}{\sqrt{b^2 + \gamma^2(z - \beta t)^2}}. \quad (56)$$

In the high-energy limit, $\beta \to 1$, and

$$\lim_{\beta \to 1} \hat{W}_P(t) = \hat{H}_P(t) - \hat{H}_T^\perp(t). \quad (57)$$

$\hat{W}_P(t)$ is the original electron-projectile interaction with its long-range, asymptotic space-time dependence subtracted. The cancellation is exact only in the $\beta \to 1$ limit. Otherwise, there remains a residual long-range interaction of the order $1/\gamma^2$. As a result of this very useful characteristic, we name this new representation the short-range representation. The phase transformation used to define the short-range representation, Eq. (51), exactly cancels the phase distortion factor contained in the asymptotic solution to the two-center Dirac equation in the extreme, high-energy limit, Eq. (21). The result is a representation of the two-center Dirac equation appropriate for direct reactions in extremely relativistic heavy-ion collisions in which the electron-projectile interaction has short range and the initial and final states are effectively single-center eigenstates of the target ion. (Note that the transverse-coordinate dependence of $\hat{W}_P(t)$ remains of long-range (i.e. $1/r_{\perp}$) form. However, the transverse coordinates do not contribute to the interaction of the electron with a distant ion at asymptotic times.)

The electron-ion interaction in the short-range representation simplifies further if, in addition to the $\beta \to 1$ limit, one requires that the transverse electron coordinates $\vec{r}_\perp$ and the impact parameter $b$ are small compared to $\gamma$, i.e.

$$|\vec{r}_\perp|, b \ll \gamma. \quad (58)$$

In this limit, $\hat{W}_P(t)$ factors into a product of a Dirac-delta function of argument $(t - z)$ and a logarithmic function of the transverse coordinates (similar to the potential induced by a line of charge), (see Refs. [1], [3], [5], i.e.

$$\lim_{\frac{r_{\perp}}{\beta} \to \gamma} \hat{W}_P(t) = (I_4 - \hat{a}_z)Z_P\alpha\delta(t - z)\ln \left[\frac{(\vec{r}_\perp - \vec{b})^2}{b^2}\right]. \quad (59)$$

We refer to this as the sharp limit of the electron-projectile interaction in the short-range representation, as the interaction has zero range in the light-front coordinate $r_\perp \equiv (t - z)/2$. This behavior reflects the fact that the peak transverse electric field produced by a moving charge increases proportional to $\gamma$ while the duration $\Delta t \approx b/(\gamma\beta)$ of the collision decreases as $1/\gamma$. The interaction in this sharp limit has the character of an electromagnetic shockfront which develops as the speed of the source of the electromagnetic field, $\beta$, approaches the propagation speed, $c$, of the field [12].

The short-range, two-center Dirac equation, Eq. (55), in the sharp limit, (i.e. using the interaction in Eq. (59)), has been recently used by Baltz to compute the high-energy limit of the impact-parameter dependent probabilities for bound-free electron-positron pair production in peripheral, relativistic heavy-ion collisions [26]. In reflecting on this achievement, it is important to recall that the derivation of Eq. (55) given here assumes asymptotic channels which correspond to direct reactions only. Asymptotic channels which correspond to the electron being distant from the target as either $t_i \to -\infty$ or $t_f \to +\infty$ are not considered in this description. As a result, the charge-transfer mechanism for bound-free pair production [4, 5] is not included in the solutions given in Ref. [26]. The extreme high-energy behavior of the charge-transfer mechanism for pair production has not received detailed study.

An analogous short-range representation may be defined for direct reactions in the projectile frame, with similar interpretation. The construction of the short-range representation in the collider frame is also similar, but differs in that the asymptotic interaction of the electron with both projectile and target ions must be considered. We discuss the collider-frame case in the next section.

2. Equation of motion: collider frame

Consider the extreme, high-energy limit $\beta_C \to 1$ of the two-center Dirac equation in the collider frame, Eq. (22), so that the asymptotic channels for an electron interacting with distant target and projectile ions has the factored form of Eq. (11). We substitute this exact solution into the expression for the exact transition amplitudes for the collider frame for the initial state $j$ and final state $k$,

$$A_{kj} = \lim_{\substack{t_i' \to -\infty \\to t_i' \to \infty}} \langle e^{-i\chi_C(\vec{r}', t_f')}\phi_{C}^{(k)}(t_f')|\hat{U}(t_f, t_i')e^{-i\chi_C(\vec{r}', t_i')}\phi_{C}^{(j)}(t_i')\rangle. \quad (60)$$
Rearranging the exponential factors in the expression so that they are applied directly to the evolution operator, one obtains,

\[ A_{kj} = \lim_{t_j' \to -\infty} \langle \phi_C^{(j)}(t'_j) | \langle \phi_C^{(k)}(t'_j') | \chi_{C}(z',t') \rangle e^{i\tau \chi_C(z',t') | \chi_{C}(z',t') \rangle} . \]  

(61)

Defining the short-range representation in the collider frame,

\[ |\Psi(S)(r',t')\rangle = e^{i\tau \chi_C(z',t')} |\Psi(S)(r',t')\rangle \]  

(62)

\[ \tilde{U}(S)(t'_j, t'_j) = e^{i\tau \chi_C(z',t')} \tilde{U}(t'_j, t'_j) e^{-i\tau \chi_C(z',t')} . \]  

(63)

gives the formal expression for the exact transition amplitude between plane-wave states in the collider frame using the short-range representation,

\[ A_{kj} = \lim_{t_j' \to -\infty} \langle \phi_C^{(k)}(t'_j) | \tilde{U}(S)(t'_j, t'_j) | \phi_C^{(j)}(t'_j) \rangle . \]  

(64)

To obtain the two-center Dirac equation in the collider frame in the short-range representation, we begin with Eq. (81), and make the substitution

\[ |\Psi'(r',t')\rangle = e^{-i\tau \chi_C(z',t')} |\Psi(S)(r',t')\rangle . \]  

(65)

After multiplying from the left by \( e^{+i\tau \chi_C(z',t')} \), the equation of motion has the form

\[ \frac{\partial}{\partial t} |\Psi(S)(r',t')\rangle = \left[ \tilde{H}_0 + \tilde{W}_T(t') + \tilde{W}_P(t') \right] |\Psi(S)(r',t')\rangle , \]  

(66)

where \( \tilde{W}_T(t') \) and \( \tilde{W}_P(t') \) are the time-dependent electron-target and electron-projectile interactions in the short-range representation,

\[ \tilde{W}_T(t') = \tilde{H}_T(t') - \frac{Z_T \alpha \gamma C (I_4 + (1/\beta_C) \alpha_z)}{\sqrt{(b/2)^2 + \gamma^2 (z' + \beta_C t')^2}} , \]  

\[ \tilde{W}_P(t') = \tilde{H}_P(t') - \frac{Z_P \alpha \gamma C (I_4 - (1/\beta_C) \alpha_z)}{\sqrt{(b/2)^2 + \gamma^2 (z' - \beta_C t')^2}} . \]  

(67)

In the high-energy limit, \( \beta_C \to 1 \), and

\[ \lim_{\beta_C \to 1} \tilde{W}_T(t') = \tilde{H}_T(t') - \tilde{H}_T^\infty(t') , \]  

\[ \lim_{\beta_C \to 1} \tilde{W}_P(t') = \tilde{H}_P(t') - \tilde{H}_P^\infty(t') . \]  

(68)

As in Eq. (55), the asymptotic dependence of the time-dependent interaction has been canceled exactly (in the \( \beta \to 1 \) limit). Likewise, the phase distortion in the asymptotic channel solutions is canceled by the phase transformation defining the short-range representation, and the asymptotic channels are effectively the Dirac plane waves.

Applying the sharp limit of Eq. (68) to Eqs. (69), we obtain the following factored forms for the time-dependent interaction

\[ \lim_{\beta_C \to 1} \tilde{W}_T(t') = \left( I_4 + \tilde{\alpha}_z \right) Z_T \alpha \delta(t' + z') \ln \left[ \frac{(r' + \tilde{b}/2)^2}{(b/2)^2} \right] , \]  

\[ \lim_{\beta_C \to 1} \tilde{W}_P(t') = \left( I_4 - \tilde{\alpha}_z \right) Z_P \alpha \delta(t' - z') \ln \left[ \frac{(r' - \tilde{b}/2)^2}{(b/2)^2} \right] . \]  

(69)

The short-range, two-center Dirac equation, Eq. (66), in the sharp limit (using Eqs. (69)) has recently been used to compute the high-energy limit of the free electron-positron pair-production amplitudes in peripheral relativistic heavy-ion collisions [27–29]. As in the case of the target frame equation considered previously, the amplitudes derived from Eq. (66) and given in Refs. [27–30] correspond to direct reactions only. For the present case in the collider frame, only asymptotic electron states distant from both target and projectile ions are considered [15]. The contribution of other asymptotic channels to the high-energy limit of free-pair production requires further investigation.

IV. GAUGE TRANSFORMATIONS

In discussing the two-center Dirac equation in the target frame, Eq. (1), for relativistic heavy-ion collisions, Baltz and coworkers have regarded the phase transformation, Eq. (50), used here to define the short-range representation, as a gauge transformation [20, 21, 23, 24]. Eichler et al. have also remarked that the phase factors obtained in solving for the asymptotic channel solutions of Eq. (6) and used to obtain a short-range effective interaction can be interpreted as gauge transformations [14, 15]. In this section, we show explicitly that the phase transformation used to define the short-range representation is equivalent to a gauge transformation, and highlight the relatedness of these two viewpoints.

In investigating the phase transformation, Eq. (51), as a gauge transform, it is convenient to write the two-center Dirac equation explicitly in terms of the electromagnetic four-vector interaction \( A^\mu \). Beginning with Eq. (6), we write the electron-projectile interaction Hamiltonian as \( \tilde{H}_P(t) = A_0 - \tilde{\alpha}_z A_z \), where

\[ A_0(r, t) = \frac{-Z_P \alpha \gamma}{r^2 \tilde{b}(r, t)} , \]  

\[ A_z(r, t) = \beta A_0(r, t) , \]  

(70)

so that the two-center Dirac equation is written in the form
We now re-derive the two-center Dirac equation in the short-range representation, Eq. (53), by substituting the phase transformation in Eq. (51) into Eq. (71) and multiplying from the left by $e^{-iNt}$, to obtain

$$\frac{i}{\hbar} \frac{\partial}{\partial t} |\Psi^{(S)}(\vec{r},t)\rangle = \left[\hat{H}_0 + \hat{H}_T + i_4 A^0_0(\vec{r}) - \alpha_z A^z_0(\vec{r})\right] |\Psi^{(S)}(\vec{r},t)\rangle,$$  

(71)

where the components of the four-vector interaction in the short-range representation are

$$A^0_0(\vec{r}, t) \equiv A_0(\vec{r}, t) - \frac{\partial \chi_{P}(z, t)}{\partial t},$$

$$A^z_0(\vec{r}, t) \equiv A_z(\vec{r}, t) + \frac{\partial \chi_{P}(z, t)}{\partial z},$$

(72)

or, more explicitly,

$$A^0_0(\vec{r}, t) = -Z_P \alpha \gamma \left[ \frac{1}{r_{P}(\vec{r}, t)} - \frac{1}{r_{P}^{\infty}(\vec{r}, t)} \right],$$

$$A^z_0(\vec{r}, t) = -Z_P \alpha \gamma \beta \left[ \frac{1}{r_{P}^{\prime}(\vec{r}, t)} - \frac{1}{r_{P}^{\infty}(\vec{r}, t)} \right].$$

(73)

With the interaction written in the form of Eqs. (73), the phase transformation in Eq. (51) clearly accomplishes a gauge transformation.

In general, gauge transformations leave physical quantities, such as the S-matrix amplitudes, invariant, whereas other quantities, such as wavefunctions, propagators, and asymptotic channel solutions, may depend on the gauge. Clearly, the invariance of physical quantities relies on an exact formulation. From a practical point of view, however, approximations are often needed. A widely applied method consists in the expansion of the time-dependent wave function in terms of a basis set of channel functions, such that the time dependent Dirac equation (3) is equivalent to an infinite set of coupled equations for the time-dependent expansion coefficients. For practical reasons, this set is truncated at a finite number of states. While the complete set is, of course, invariant under gauge transformations, a finite set usually is not. In fact, a gauge transformation may not only modify the effective interaction, but it also affects the convergence property of the expansion (4). Therefore, both effects should always be considered simultaneously and, actually, can be utilized to speed up convergence (11).

Within an exact treatment, which is our main subject, a distinction has been made in Refs. [20, 22, 23] between gauge transformations which leave the asymptotic channels invariant (or trivially modified) as a result of the gauge function being constant at asymptotic times, and those which modify boundary conditions since the gauge function is not constant asymptotically. Indeed, the gauge transformation considered in defining the short-range representation modifies the asymptotic states since it behaves asymptotically as

$$\lim_{t \to +\infty} \chi_P(z, t) = -\frac{Z_P \alpha}{\beta} \ln \left( \frac{2|z| - \beta t}{b^2} \right),$$

(75)

$$\lim_{t \to +\infty} \chi_P(z, t) = +\frac{Z_P \alpha}{\beta} \ln |2|z| - \beta t|.$$

(76)

Implicit in using the short-range representation (or gauge) in the high-energy limit is that the phase transformation, Eq. (51), defining the representation, exactly cancels the phase distortion of the asymptotic channels induced by the distant projectile ion (see Eq. (20)). As a result, the asymptotic channel solutions for direct reactions in the short-range representation are the undistorted, single-center atomic states, $|\psi_j(\vec{r}, t)\rangle$. In other words, by using undistorted atomic states as asymptotic channels in the short-range representation, as was done in Ref. [20], one is, in effect, using the factored form for the asymptotic channel solutions, Eq. (20), of Eichler and coworkers.

V. CONCLUSIONS

A primary goal of this work was to place on a clear and firm theoretical foundation the “Sharp Dirac equation”, i.e. the two-center Dirac equation(s), in both the target and the collider frames, in the short-range representation, in the extreme relativistic (sharp) limit. The reason this is of primary importance is that the short relativistic limit of the two-center Dirac equation in the short-range representation for heavy-ion collisions simplifies remarkably, and allows for closed form solutions for pair-production amplitudes in this limit.

With these goals in mind, we have described the relationship between asymptotic solutions to the two-center, time-dependent Dirac equation for a single electron in peripheral relativistic heavy-ion collisions, and phase (or gauge) transformations designed to remove the long-range asymptotic interaction from the equation of motion. Direct reactions are central to the discussion. “Charge-transfer” mechanisms for pair production [13, 43] have been omitted here, and should be subsequently considered in the high-energy limit.

We have shown that the asymptotic channel solutions factorize into a space-time dependent phase and an eigenstate of the appropriate time-independent Hamiltonian, in the limit $\beta \to 1$. For collision velocities less than the speed of light, this factorization is approximate with accuracy of the order $1/\gamma^2$. We have also shown that as a result of this factorization a gauge transformation may be performed to a new representation in which the asymptotic dynamics are included in the states. In this representation, the asymptotic interaction between the electron and a distant ion is of short-range form, and
the asymptotic solutions are undistorted, stationary solutions of a time-independent Hamiltonian. Under such conditions, a formally correct formulation of scattering theory may be constructed. In addition, this short-range representation has advantages for the convergence of numerical calculations [13,14,36,37,41].

The factorization of the asymptotic solutions in the \( \beta \to 1 \) limit also provides a significant simplification in the dynamics. A further simplification is achieved if the magnitude of the transverse coordinate, \( \tau_{\perp} \), and the impact parameter, \( b \), are constrained to be much smaller than \( \gamma \). In this limit, the time-dependent interaction factors into a logarithmic function of the transverse coordinate, and a Dirac-delta function of a light-front variable, \( \tau_{\perp} = (z \pm t)/2 \), describing an electromagnetic shock on the lightfront [23,24]. The identification of the separable form has allowed for the closed-form solution of amplitudes for electron-positron pair production in the high-energy limit of heavy-ion collisions [25,26].

We have also made a connection with the previous pioneering work of Eichler et al. on the Coulomb-boundary conditions. We have elucidated and discussed the relatedness of the Coulomb-boundary approach and what Baltz and coworkers have recently accomplished via the machinery of gauge-transformations. We have shown that in the high energy limit, these two approaches are in agreement, and differ mostly in their language.

The replacement strategy previously developed by Eichler and coworkers was designed to remove the long-range part by a gauge or phase transformation. This treatment is fully symmetric with respect to the target and projectile frame, has the correct nonrelativistic limit and has been successful in a number of calculations. We note however, that there is no unique way to derive "replacements". When the purpose is to have a good basis-set for numerical calculation, a replacement procedure is a useful and adequate approximation. On the other hand, if one is treating the problem in a formal approach, as was recently done for the high-energy collision limit in Refs. [26,27], the rigorous definition of the short-range representation as presented here is of significant importance.

In regard to using the factored solution as an accurate, but approximate, asymptotic channel solution for calculation of high-energy collision phenomena, one should keep in mind that the factored solution, e.g. the phase factor times a single-center eigenstate, is an exact solution to the two-center Dirac equation for asymptotically large times, only in the limit \( \beta \to 1 \). For large, but finite \( \gamma \), the factored solution is an approximate solution to the asymptotic Dirac equation accurate to order \( 1/\gamma^2 \). Hence, choosing between factors of \( \beta \) in the argument of the phase is largely a matter of personal taste.

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APPENDIX A: ASYMPTOTIC ELECTRON-ION DISTANCE

In this appendix, we discuss the asymptotic limit of the electron-projectile distance needed to describe the interaction of an electron with a projectile ion at asymptotic times \( |t| \to \infty \). The electron-projectile distance in the projectile’s rest frame,

\[
r''_p = \sqrt{(r''_p)^2 + (z'')^2}, \quad (A1)
\]

is represented in terms of the target-frame coordinates as

\[
r''_p(\tilde{r}, t) = \sqrt{(\tilde{r}_{\perp} - \tilde{b})^2 + \gamma^2(z - \beta t)^2}, \quad (A2)
\]

where \( \{r''_{\perp}, z'', t''\} \) and \( \{\tilde{r}_{\perp}, z, t\} \) are the space-time coordinates of the electron in the projectile frame and in the target frame, respectively, which are related by an inhomogeneous Lorentz transformation as in Eqs. (1). We would like to obtain an asymptotic (i.e. \( |t| \to \infty \)) limit for \( r''_p \) when the internuclear separation \( R'' \),

\[
R''(t'') = \sqrt{b^2 + \beta^2(t'')^2}, \quad (A3)
\]

is large compared to the separations between the electron and the target.

We now discuss the problem of the asymptotic electron-projectile separation in two different versions.

\[\text{a. Internuclear separation}\]

Following the arguments given in Refs. [9,12], we substitute the internuclear separation \( R'' \) for the asymptotic electron-projectile separation, which should be a good approximation for very large positive or negative times. Formally, this corresponds to taking

\[
\tilde{r}_{\perp} \to 0, \quad z \to 0 \quad (A4)
\]

in the target frame. Once this replacement is performed, we consider \( R'' \) as a parameter of the system describing the internuclear motion and no longer the position of the electron, that is, we leave the Lorentz transformation,

\[
t'' = \gamma(t - \beta z), \quad (A5)
\]
relating the projectile-frame time to the target-frame time for an arbitrary electron position, intact. This constitutes an inconsistency, if the position of the target nucleus with respect to the projectile nucleus is interpreted as an electronic position with the coordinates \( \mathbf{A} \). In this respect, the replacement \( \vec{r}'_p \to R'' \) with \( R'' \) given by Eqs. (A3) and (A5), i.e.,

\[
\vec{r}'_p \to \sqrt{b^2 + \gamma^2 (\beta^2 z - \beta t)^2} \quad (A6)
\]

is not the formally derivable asymptotic limit. According to Eq. (A4), formal consistency can only be achieved by replacing \( \vec{r}'_p \to \gamma t \), i.e.

\[
\vec{r}'_p \to \sqrt{b^2 + \gamma^2 \beta^2 t^2} \quad (A7)
\]

However, Eq. (A7) is not useful for our purpose, because the \( z \)-dependence is required to describe the magnetic component of the electromagnetic interaction at asymptotic times for large \( \gamma \). In the nonrelativistic limit \( \beta^2 \ll 1, \gamma \approx 1 \), when \( t'' \approx t \), no inconsistency occurs, and Eqs. (A3) or (A5) immediately lead to the usual and successfully applied replacement \( \mathbf{x} \)

\[
\vec{r}'_p \to R = \sqrt{b^2 + \beta^2 t^2} \quad (A8)
\]

b. Longitudinal electron-projectile separation

To obtain a formally rigorous \( z \) dependence for the asymptotic limit of the electron-projectile distance \( r''_p \) for an electron near to the target but distant from the projectile, one should not use \( \vec{r}'_p \to R'' \), but should maintain the dependence on the \( z \) coordinate, that is, retain the exact longitudinal electron-projectile distance. Even if \( |z| \ll \beta |t| \) in the laboratory at asymptotic times, we do not set it to zero. This means that instead of Eq. (A4), we take

\[
\vec{r}'_\perp \to 0 \quad (A9)
\]

while \( z \) is retained. This procedure guarantees that Lorentz transformations can be consistently applied. The resulting, formally correct asymptotic limit of the electron-projectile distance is

\[
\lim_{|t| \to \infty} r''_p (\vec{r}', t) = r''_\infty (\vec{r}', t) = \sqrt{b^2 + \gamma^2 (z - \beta t)^2} \quad (A10)
\]

This, no doubt, is a better approximation to Eq. (A2) than \( \vec{r}'_p \to R'' \). In order to compare it with Eq. (A6), we may write

\[
\lim_{|t| \to \infty} r''_p (\vec{r}', t) = \sqrt{b^2 + \gamma^2 (\gamma^{-2} + \beta^2) z - \beta t^2} \quad (A11)
\]

Note that, compared to Eq. (A6), an additional term with \( 1/\gamma^2 \) appears. This term reflects the difference between taking the longitudinal electron-projectile separation and the internuclear separation. One sees this difference more explicitly by considering the ratio \( r''_p/R'' \) in the limit \( \gamma \gg 1 \), \( |z| \ll \beta |t| \), and \( b \ll \gamma |t| \). Keeping terms proportional to \( z/t \), we obtain

\[
\frac{r''_p}{R''} \approx 1 - \frac{z}{\gamma^2 t} \quad (A12)
\]

Indeed, for very large values of \( \gamma \), the target atom as seen from the projectile shrinks to a disk, so that the electronic \( z \)-coordinate almost coincides with the \( z = 0 \) coordinate of an electron located at the target nucleus.

We have discussed two different approaches for identifying the asymptotic electron-projectile separation. The first is based on a substitution by the internuclear separation, which implies a formal inconsistency if interpreted as a true electronic separation instead of a parameter describing the projectile motion. However, it appears physically reasonable and has the correct nonrelativistic limit. The second is formally rigorously derivable by keeping the longitudinal electronic coordinate and hence encounters no problems when applying Lorentz transformations in a straightforward fashion. Both approaches differ in a term of the order of \( 1/\gamma^2 \) in the asymptotic electron-projectile separation and agree for \( \beta \to 1 \). As discussed in Sec. II A and in Appendix B, discrepancies of this order propagate into the factored forms of the asymptotic channel solutions and the asymptotic interaction when they are applied for large, but finite, \( \gamma \).

APPENDIX B: PHASE CHOICES FOR ASYMPTOTIC CHANNELS

In Sec. II A, we have discussed two versions, Eqs. (11) and (17), for separating asymptotic wave functions by introducing the phases (12) and (18), respectively. These phases, differing only in factors \( \beta^2 \), arise from different choices for the asymptotic electron-ion distance (see Appendix A). For our present purposes, choosing among these different phase arguments is largely a matter of personal taste since only in the \( \gamma \to \infty \) limit does the asymptotic interaction vanish exactly in the short-range representation. For large finite values of \( \gamma \), terms of the order of \( 1/\gamma^2 \) remain. In order to illustrate the consequences of phase choices, consider yet another product ansatz for the solution of the asymptotic two-center Dirac equation in the target frame,

\[
|\Phi_T^\infty (\vec{r}', t)\rangle = e^{-i \Lambda_P (z, t)} |\psi_T (\vec{r}', t)\rangle , \quad (B1)
\]

where

\[
\Lambda_P (z, t) \equiv Z_P \alpha \beta \ln \left[ \gamma (z - \beta t) + \sqrt{b^2 + \gamma^2 (z - \beta t)^2} \right] \quad (B2)
\]

Substituting this ansatz into Eq. (13), multiplying from the left by \( e^{i \Lambda_T (z, t)} \), and collecting like terms gives
\[ \frac{\partial}{\partial t}\psi_T(\vec{r}, t) = \left[ \hat{H}_0 + \hat{H}_T - \left( \frac{1}{\gamma^2} \right) \frac{Z_p \alpha \gamma I_4}{\beta^2 + \gamma^2(z - \beta t)^2} \right] \psi_T(\vec{r}, t). \]  

(B3)

With the phase choice in Eq. (B2), the vector component of the asymptotic electron-projectile interaction is canceled exactly, and the remaining scalar component is of order $1/\gamma^2$. In contrast, with the phase choice made in Eq. (18), which differs from Eq. (B2) only by a factor of $\beta^2$, the scalar component cancels exactly, and the vector component is of order $1/\gamma^2$.

One may always perform a gauge transformation such that a single component (or a single linear combination of components) of the four-vector electromagnetic interaction is exactly zero for all times. Such a gauge condition is known as an axial gauge (see Refs. [31,32]). The novelty of the short-range representation in the $\beta \to 1$ limit is that in it the full, asymptotic interaction (both scalar and vector components) is zero.

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FIG. 1. Coordinate systems for a relativistic collision between two ions. The position of the target ion, with charge $Z_T$, is the origin of the unprimed coordinates. The position of the projectile ion, with charge $Z_P$, is the origin of the doubly primed coordinates. The projectile moves with constant velocity $\beta$ parallel to the $z$ axis on a trajectory with impact parameter $\vec{b}$. The electron $e^-$ has the coordinate $\vec{r}_T$ with respect to the target frame and $\vec{r}_P''$ with respect to the projectile frame.

FIG. 2. Coordinate systems for a relativistic collision between to ions similar to Fig. 1 except that the collider (or center-of-velocity) frame is shown in addition. The electron has the coordinates $\vec{r}_C'$ with respect to the collider frame. The projectile and target ions have the collider-frame coordinates, $\vec{R}_P'$, and $\vec{R}_T'$, respectively.
Figure 1, Wells et al.
Figure 2, Wells et al.