Abstract. This paper is devoted to the derivation and analysis of the Frozen Gaussian Approximation (FGA) for the Dirac equation in the semi-classical regime. Unlike the strictly hyperbolic system studied in [J. Lu and X. Yang, Comm. Pure Appl. Math., 65, 759–789, 2012], the Dirac equation possesses eigenfunction spaces of multiplicity two, which demands more delicate expansions for deriving the amplitude equations in FGA. Moreover, we prove that the nonrelativistic limit of the FGA for the Dirac equation is the FGA of the Schrödinger equation, which shows that the nonrelativistic limit is asymptotically preserved after one applies FGA as the semiclassical approximation. Numerical experiments including Klein-Paradox are presented to illustrate the method, and confirm part of the analytical results.

AMS subject classifications.

Notations

- $i$: imaginary unit
- $\varepsilon$: semiclassical parameter
- $\hat{\alpha}, \hat{\beta}_j$: Dirac matrices
- $V$ (or $A$): scalar (or vector) potential
- boldface Greek alphabets (lower and upper cases) such as $\psi^\varepsilon$ and $\Upsilon$: vectors in $\mathbb{C}^4$
- boldface English alphabets (lower and upper cases) such as $Q$ and $x$: vectors in $\mathbb{R}^3$
- $\partial_u B = \{ \partial_u B_j \}_{j,k}$

1. Introduction. This paper is devoted to the derivation and analysis of the Frozen Gaussian Approximation (FGA) for the linear Dirac equation modeling quantum particles subject to a classical electromagnetic field. The Dirac equation is a linear with constant coefficient, Hermitian 4-equation hyperbolic system, with two pairs of double eigenvalues $\pm c$, where $c$ denotes the speed of light. Physically, this equation models a relativistic quantum wave equation for half-spin particles, such as fermions (e.g. electrons) [33]. There is growing interest in Physics for the study of this equation in particular for modeling heavy-ion collisions [30, 18, 2], for pair production using strong laser fields [11, 10, 16], or for modeling Graphene [21]. These active research fields in Physics, have motivated recent computational works [2, 34]. Let us mention [22, 14, 15], where an embarrassingly parallel quantum lattice Boltzmann methods were developed and applied to the simulation of the interaction of relativistic electron with an intense external electric field. For similar purposes, efficient spectral and finite element methods were developed such as the ones presented in [35, 1, 28, 31, 27, 29, 7, 3]. Galerkin methods with balanced basis functions is proposed in [17] for solving the time dependent Dirac equation (TDDDE). Graphene-related simulations using similar techniques are also proposed in [13, 12]. Regarding to the numerical approximation of the TDDDE in the non-relativistic regime, there exists an extended literature; see for instance [6, 4, 5]. The approximation of the Dirac equation in the semi-classical regime has also recently brought some attention, in particular in [36], where a Gaussian beam-based method is proposed based on adiabatic approximation.

In this work, the Dirac equation will be approximated in the semi-classical regime, using the celebrated Frozen Gaussian Approximation (FGA). The latter was originally developed by Herman-Kluk (HK) [20] for the Schrödinger equation in the semi-classical regime. The mathematical analysis was then proposed in [32] showing the accuracy and efficiency of this ansatz in particular when the initial data is localized in phase space. HK formalism was later developed of several types of partial differential equations, such as wave equations [24], linear hyperbolic systems of conservation laws [26], elastic wave equations and seismic tomography [8, 9, 19]. Some applications and analysis on the Schrödinger equations were also proposed in [23, 37]. Unlike the aforementioned equations studied using FGA, the Dirac equation possesses two eigenfunction spaces of multiplicity two, which demands more delicate expansions for deriving the amplitude equations in the FGA formulation. As a deeper investigation, we also prove that the nonrelativistic limit of
the FGA for the Dirac equation is the FGA for the Schrödinger equation, which shows that the nonrelativistic limit is asymptotically preserved after one applies FGA as the semi-classical approximation. In the end, we present several numerical experiments including Klein Paradox to illustrate the method, and confirm part of the analytical results.

Recall first that, in the quantum regime, the Dirac equation reads

$$i \partial_t \psi(t, x) = \hat{H}(t, x) \psi(t, x),$$

where

$$\hat{H} = \alpha \cdot [c p - e A(t, x)] + \beta mc^2 + \mathbb{I}_4 (V_c(t, x) + V(x)),$$

and

$$\alpha_\gamma = \begin{bmatrix} 0 & \sigma_\gamma \\ \sigma_\gamma & 0 \end{bmatrix}, \quad \beta = \begin{bmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{bmatrix}.$$

The $\sigma_\gamma$’s are the usual $2 \times 2$ Pauli matrices defined as

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \text{and} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

while $\mathbb{I}_2$ is the $2 \times 2$ unit matrix. The momentum operator is denoted $p = -i \nabla$. The speed of light $c$ and fermion mass $m$ are kept explicit in Eq. (2), allowing to easily adapt the method to natural or atomic units (a.u.). In (1), $e$ is the electric charge (with $e = -|e|$ for an electron), $\mathbb{I}_4$ is the $4 \times 4$ unit matrix and $\alpha = (\alpha_\gamma)_{\gamma=1,\ldots,4}$, $\beta$ are the Dirac matrices. This equation models a relativistic electron of mass $m$ subject to an interaction potential $V_c$ and electromagnetic field $V(x, A(t, x))$, and for fixed time $t$, $\psi(t, x) \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ is the coordinate $(x = (x, y, z))$ dependent four-spinor. We denote by $\langle \cdot, \cdot \rangle$ the $L^2(\mathbb{R}^3, \mathbb{C}^4)$-inner product. In principle, the Dirac equation must be coupled to Maxwell’s equations, modeling the evolution of the electromagnetic field [22]. In the following, the coupling is neglected, and we then assume that the EM propagates as in vacuum.

2. Frozen Gaussian Approximation for the Dirac equation. This section is devoted to the construction of the FGA for the Dirac equation in the semi-classical regime. We first recall some basic facts about Frozen Gaussian Approximations (FGA) for evolution equations in the semi-classical regime. We then derive the FGA for the field-particle Dirac equation in the relativistic regime. For $\varepsilon > 0$, we reformulate the Dirac equation as follows:

$$i \varepsilon \partial_t \psi^\varepsilon(t, x) = \left(-i \varepsilon \hat{\alpha} \cdot \nabla - \hat{\alpha} \cdot A(x) + m\delta_0 c^2 + V(x) \right) \psi^\varepsilon(t, x),$$

$$\psi^\varepsilon(0, x) = \varphi_0^\varepsilon(x) = \omega_1(x) \exp\left(\frac{i}{\varepsilon} S_1(x) \right).$$

Here $\psi^\varepsilon = (\psi_1^\varepsilon, \psi_2^\varepsilon, \psi_3^\varepsilon, \psi_4^\varepsilon)^T \in \mathbb{C}^4$ is the spinor. In the following, we will assume that $m = 1$, corresponding to the mass of the electron in atomic unit.

2.1. Characteristic fields. The symbol of the Dirac operator which is studied in this paper reads

$$D(q, p) := \hat{\alpha} \cdot (pc - A(q)) + m\delta_0 c^2 + V(q) = \hat{\alpha} \cdot pc + B(q),$$

where we have denoted

$$B(q) := -\hat{\alpha} \cdot A(q) + m\delta_0 c^2 + V(q) \mathbb{I}_4.$$

We easily show that $D$ is a Hermitian matrix, and it has two double (real) eigenvalues

$$h_{\pm}(q, p) = \pm \lambda(q, p) + V(q), \quad \text{where} \quad \lambda(q, p) = \sqrt{|pc - A(q)|^2 + c^4},$$

$$\text{and} \quad \mathbb{I}_4.$$
Denote the corresponding eigenvectors as \( \mathbf{Y}_m, m = \pm 1, \pm 2 \), and let \( u = pc - A(q) \), then

\[
\begin{align*}
\mathbf{Y}_{+1} &= \frac{1}{r_+} \begin{pmatrix} u_3 \\ u_1 + iu_2 \\ \sqrt{|u|^2 + c^4 - c^2} \end{pmatrix}, \\
\mathbf{Y}_{+2} &= \frac{1}{r_+} \begin{pmatrix} u_1 - iu_2 \\ -u_3 \\ \sqrt{|u|^2 + c^4 - c^2} \end{pmatrix}, \\
\mathbf{Y}_{-1} &= \frac{1}{r_-} \begin{pmatrix} -u_3 \\ -u_1 - iu_2 \\ \sqrt{|u|^2 + c^4 - c^2} \end{pmatrix}, \\
\mathbf{Y}_{-2} &= \frac{1}{r_-} \begin{pmatrix} u_3 \\ -u_1 + iu_2 \\ \sqrt{|u|^2 + c^4 + c^2} \end{pmatrix},
\end{align*}
\]

where \( r_\pm = \sqrt{2 - |u|^2 + c^4 \mp \sqrt{|u|^2 + c^4}} \). Other details can be found in Appendix.

2.2. Derivation of the FGA. Using the eigenvector of the Dirac operator symbol, we can now define the FGA for the Dirac equation, which reads as follows

\[
\psi^\text{f}(t, x) = \frac{1}{(2\pi)^{9/2}} \sum_m \int_{\mathbb{R}^9} \left( a_m(t, q, p) + \varepsilon \beta_m(t, q, p) \right) \times \exp \left( \frac{i}{\varepsilon} \Phi_m(t, x, y, q, p) \right) v_m(y, q, p) \, dy \, dq \, dp,
\]

where

\[
\Phi_m(t, x, y, q, p) = S(t, q, p) + \frac{i}{2} |x - Q_m(t, q, p)|^2 + P_m \cdot (x - Q_m(t, q, p)) + \frac{i}{2} |y - q|^2 - p \cdot (y - q),
\]

\[
a_m(t, q, p) = a_m(t, q, p) Y_m(Q_m, P_m),
\]

\[
v_m(y, q, p) = Y_m(q, p) \cdot \psi^\text{f}_m(y).
\]

In this subsection, we respectively derive the evolution equations respectively 1) for the Gaussian profiles \( Q \) and momentum functions \( P \), then 2) for the action function \( S \), and finally 3) for the FGA amplitude \( a \). For the sake of simplicity, we consider one branch (e.g., "+" branch) and drop the subscription without causing any confusion. Let \( \hbar \) be the eigenvalue and \( \mathbf{Y}_1 \) and \( \mathbf{Y}_2 \) be the corresponding eigenvectors.

1. Gaussian profile \( Q \) and momentum function \( P \), evolution equation. As for any FGA, the bi-center \( Q \) and \( P \) simply satisfy the Hamiltonian flow:

\[
\begin{align*}
\frac{dQ}{dt} &= \partial_P h(Q, P), \quad Q(0, q, p) = q, \\
\frac{dP}{dt} &= -\partial_Q h(Q, P), \quad P(0, q, p) = p.
\end{align*}
\]

We then determine the evolution equation for the action function.

2. Action function \( S \), evolution equation. In order to derive the evolution equation for the action function \( S \), preliminary computations are needed. By definition of \( \Phi \), we have

\[
\begin{align*}
\partial_t \Phi &= \partial_t S - P \cdot \partial_t Q + (x - Q) \cdot \partial_t (P - iQ), \\
\nabla_x \Phi &= i(x - Q) + P,
\end{align*}
\]
Then taking derivatives to (11) gives
\[
\partial_t \psi^\varepsilon = \int \left( \partial_t a + \varepsilon \partial_t \beta + \frac{i}{\varepsilon} \partial_t \Phi(a + \varepsilon \beta) \right) e^{i\Phi/\varepsilon} v \, dy \, dq \, dp
\]
(18)
\[
= \int \left( \partial_t a + \frac{i}{\varepsilon} \left( \partial_t S - P \cdot \partial_t Q + (x - Q) \cdot \partial_t (P - iQ) \right) a \right) e^{i\Phi/\varepsilon} v \, dy \, dq \, dp
\]
\[
+ \int \left( \varepsilon \partial_t \beta + i \left( \partial_t S - P \cdot \partial_t Q + (x - Q) \cdot \partial_t (P - iQ) \right) \beta \right) e^{i\Phi/\varepsilon} v \, dy \, dq \, dp
\]
(19)
\[
\nabla_x \psi^\varepsilon = \int \frac{i}{\varepsilon} \left( (i(x - Q) + P) (a + \varepsilon \beta) \right) e^{i\Phi/\varepsilon} v \, dy \, dq \, dp
\]
We now expand \( B(x) \) about \( Q \)
\[
B(x) = B(Q) + (x - Q) \cdot \partial_Q B(Q) + \frac{1}{2} (x - Q)^2 : \partial_Q^2 B(Q) + O(x - Q)^3.
\]
Substitute these into (5), to the order of \( \varepsilon^0 \), we get
\[
- \int \left( \partial_t S - P \cdot \partial_t Q \right) a e^{i\Phi/\varepsilon} v \, dy \, dq \, dp = \int \left( c \hat{\alpha} \cdot P + B(Q) \right) a e^{i\Phi/\varepsilon} v \, dy \, dq \, dp.
\]
(21)
As \( a(t, q, p) = a_1(t, q, p) \, \Upsilon_1(Q, P) + a_2(t, q, p) \, \Upsilon_2(Q, P) \), then the above equation holds if the action function \( S \) satisfies the following evolution equation
\[
\partial_t S = P \cdot \partial_t Q - h(Q, P).
\]
(22)

3. **Amplitude evolution equation.** We now construct the evolution equation for \( a \). This is a much more technical step, and it requires an additional definition.

**Definition 2.1.** Two functions \( f \), and \( g \) are said equivalent if
\[
f \sim g \iff \int f e^{i\Phi/\varepsilon} \, dy \, dq \, dp = \int g e^{i\Phi/\varepsilon} \, dy \, dq \, dp.
\]

Based on this definition, we easily show:

**Lemma 1.**
\[
b \cdot (x - Q) \sim -\varepsilon \partial_z(\delta_j Z_{jk}^{-1}), \quad (x - Q) \cdot G(x - Q) \sim \varepsilon \partial_z Q \cdot G_{ij} Z_{jk}^{-1} + \varepsilon^2 ..., \]
(23)
(24)
where Einstein's summation convention has been used, and where
\[
\partial_z = \partial_q - i \partial_p, \quad Z = \partial_z(Q + iP).
\]
(25)

Moreover, \( (x - Q)^a \sim O(\varepsilon^{|a|-1}) \) for \( |a| > 2 \).

To the order of \( \varepsilon^1 \),
\[
\int i \varepsilon \left( \partial_t a + \frac{i}{\varepsilon} (x - Q) \cdot \partial_t (P - iQ) a + i(\partial_t S - P \cdot \partial_t Q) \beta \right) e^{i\Phi/\varepsilon} v \, dy \, dq \, dp
\]
\[
= \int \left( i c \hat{\alpha} \cdot (x - Q) a + (x - Q) \cdot \partial_Q B a + \frac{1}{2} (x - Q)^2 : \partial_Q^2 B a + \varepsilon D \right) e^{i\Phi/\varepsilon} v \, dy \, dq \, dp.
\]
which implies,
\[
\int \left( \partial_t a + \frac{i}{\varepsilon} (x - Q) \cdot \partial_t (Q + iP) a + i(D(Q, P) - h(Q, P)) \beta \right) e^{i\Phi/\varepsilon} v \, dy \, dq \, dp
\]
\[
= \int \left( \frac{c}{\varepsilon} \hat{\alpha} \cdot (x - Q) + \frac{1}{\varepsilon^2} (x - Q) \cdot \partial_Q B + \frac{1}{2\varepsilon}(x - Q)^2 : \partial_Q^2 B \right) a e^{i\Phi/\varepsilon} v \, dy \, dq \, dp.
\]
(26)
Thus
\[
\int \left[ \partial_t a v - \partial_z \left( \partial_t (Q_j + i P_j) Z_{jk}^{-1} a v \right) + i (D(Q, P) - h(Q, P)) a v \right] e^{i \phi/\varepsilon} \, dy \, dq \, dp \\
= \int \left[ -\partial_z \left( c \alpha_j Z_{jk}^{-1} a v \right) + i \partial_z \left( \partial_Q, B Z_{jk}^{-1} a v \right) - \frac{i}{2} \partial_z Q_i \partial_Q, \partial_Q, B Z_{jk}^{-1} a v \right] e^{i \phi/\varepsilon} \, dy \, dq \, dp,
\]
that is
\[
\partial_t a v - \partial_z \left[ \left( \partial_t (Q_j + i P_j) - c \alpha_j + i \partial_Q, B \right) Z_{jk}^{-1} a v \right] + \frac{i}{2} \partial_z Q_i \partial_Q, \partial_Q, B Z_{jk}^{-1} a v \\
\sim i (h(Q, P) - D(Q, P)) a v.
\]

We define for \( n = 1, 2 \),
\[
F_j^n = (\partial_t (Q_j + i P_j) - c \alpha_j + i \partial_Q, B) \mathcal{Y}_n \\
= (\partial P_j h(Q, P) - i \partial_Q, h(Q, P) - c \alpha_j + i \partial_Q, B) \mathcal{Y}_n
\]
(28) then (27) can be written as
\[
\partial_t a v - \partial_z \left[ \left( a_1 F_j^1 + a_2 F_j^2 \right) Z_{jk}^{-1} a v \right] + \frac{i}{2} \partial_z Q_i \partial_Q, \partial_Q, B Z_{jk}^{-1} a v \\
\sim i (h(Q, P) - D(Q, P)) a v.
\]

Solvability for \( \beta \) gives, for \( m = 1, 2 \)
\[
\mathcal{Y}_m \left\{ \partial_t a v - \partial_z \left[ \left( a_1 F_j^1 + a_2 F_j^2 \right) Z_{jk}^{-1} a v \right] + \frac{i}{2} \partial_z Q_i \partial_Q, \partial_Q, B Z_{jk}^{-1} a v \right\} = 0.
\]

Let \( \mathcal{Y} \in \text{Span}\{\mathcal{Y}_1, \mathcal{Y}_2\} \). Since
\[
(c \alpha \cdot P + B(Q)) \mathcal{Y}(Q, P) = h(Q, P) \mathcal{Y}(Q, P),
\]
then
\[
c \alpha_j \mathcal{Y} + (c \alpha \cdot P + B) \partial P_j \mathcal{Y} = \partial P_j h \mathcal{Y} + h \partial P_j \mathcal{Y}, \\
\partial Q_i B \mathcal{Y} + (c \alpha \cdot P + B) \partial Q_j \mathcal{Y} = \partial Q_j h \mathcal{Y} + h \partial Q_j \mathcal{Y},
\]
and thus for \( m = 1, 2 \),
\[
\mathcal{Y}_m \left( c \alpha_j - \partial P_j h \right) \mathcal{Y} = 0, \\
\mathcal{Y}_m \left( \partial Q_i B(Q) - \partial Q_j h \right) \mathcal{Y} = 0.
\]

Thus for \( m, n = 1, 2 \), \( \mathcal{Y}_m F_j^n = 0 \), and
\[
\mathcal{Y}_m \partial_z \left[ a_n F_j^n Z_{jk}^{-1} a v \right] = \mathcal{Y}_m \partial_z a_n F_j^n Z_{jk}^{-1} a v = -\partial_z \mathcal{Y}_m F_j^n Z_{jk}^{-1} a v.
\]

Notice that
\[
\mathcal{Y}_m \partial_t (a_n \mathcal{Y}_n) = \delta_{mn} \partial_t a_n + \mathcal{Y}_m \left( \partial P_j h \partial Q_j \mathcal{Y}_n - \partial Q_j h \partial P_j \mathcal{Y}_n \right) a_n.
\]

Then (30) gives the equation for \( a_m \)
\[
\delta_{mn} \partial_t a_n - \mathcal{Y}_m \left( \partial Q_j h \partial P_j \mathcal{Y}_n - \partial P_j h \partial Q_j \mathcal{Y}_n \right) a_n \\
= -\partial_z \mathcal{Y}_m F_j^n Z_{jk}^{-1} a_n - \frac{i}{2} \mathcal{Y}_m \partial_z Q_i \partial_Q, \partial_Q, B Z_{jk}^{-1} \mathcal{Y}_n a_n.
\]
In the vector form

\[
\frac{d}{dt} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = (\mathcal{L} + \mathcal{M} + \mathcal{N}) \begin{pmatrix} a_1 \\ a_2 \end{pmatrix},
\]

where \( \mathcal{L}, \mathcal{M}, \mathcal{N} \) are 2 \times 2 matrices

\[
\mathcal{L}_{mn} = \frac{i}{2} \mathcal{Y}^\dagger_m \partial_z Q_l \partial Q_j \mathcal{B} Z_{jk}^{-1} \mathcal{Y}_n,
\]

\[
\mathcal{N}_{mn} = \mathcal{Y}^\dagger_m (\partial Q h \cdot \partial p \mathcal{Y}_n - \partial p h \cdot \partial Q \mathcal{Y}_n),
\]

\[
\mathcal{M}_{mn} = -\partial_z \mathcal{Y}^\dagger_m F^n Z_{jk}^{-1}.
\]

This concludes the construction of the FGA.

**Remark 2.1.** It is easy to see that \( \mathcal{L} \) is diagonal by the orthogonality of the eigenvectors.

We now study the structure of the matrix \( \mathcal{M} \) when \( \mathcal{A} \) is null. This will be a fundamental piece of information in order to determine the nonrelativistic limit of the FGA for the Dirac equation. We first show that \( \mathcal{M} \) is diagonal when \( \mathcal{V} \) are null, and then extend the result for non-null potentials.

**Proposition 2.1.** Assume that \( \mathcal{V} \) and \( \mathcal{A} \) are null, then \( \mathcal{M} \) is diagonal.

**Proof.** When there is no potential, it is easy to show that

\[
P(t) = p, \quad Q(t) = q + \frac{p}{\sqrt{|p|^2 + 1}} t,
\]

\[
\partial_z p = -i I, \quad \partial_z q = I - i t \left( \frac{I}{\lambda^{1/2}} - \frac{p \otimes p}{\lambda^{3/2}} \right),
\]

\[
Z = 2 I - i t \left( \frac{I}{\lambda^{1/2}} - \frac{p \otimes p}{\lambda^{3/2}} \right).
\]

Let us set \( T = \frac{it}{2\lambda} \left( I - \frac{p \otimes p}{\lambda^2} \right) \), then \( Z^{-1} = \frac{1}{2} (I + T + T^2 + T^3 + ...) \). Notice now that

\[
\left( I - \frac{p \otimes p}{\lambda^2} \right)^2 = I - 2 \frac{p \otimes p}{\lambda^2} + |p|^2 \frac{p \otimes p}{\lambda^4} = I - c p \otimes p
\]

\[
\left( I - \frac{p \otimes p}{\lambda^2} \right)^n = I - d p \otimes p.
\]

Thus, we can see that there exists a \( c \) such that

\[
Z^{-1} = \frac{1}{2} (I + c_1 (I - d_1 p \otimes p) + c_2 (I - d_2 p \otimes p) + ...).
\]

Since \( \mathcal{Y} \) does not depend on \( Q \), \( \partial_z \mathcal{Y}^n = -i \partial p \mathcal{Y}^n \). For \( m \neq n \),

\[
\mathcal{M}_{mn} = -\partial_z \mathcal{Y}^\dagger_m F^n Z_{jk}^{-1} = -\partial_z \mathcal{Y}^\dagger_m (\partial p h - \partial h \partial p) \mathcal{Y}_n Z_{jk}^{-1}.
\]

Consider the positive branch and take \( m = 1, n = 2 \),

\[
\mathcal{M}_{12} = \text{Tr} (-\partial_z \mathcal{Y}^\dagger_1 (\partial p h - \partial h \partial p) \mathcal{Y}_2 Z^{-1}),
\]

and

\[
\partial_p \mathcal{Y}^\dagger_1 = \frac{1}{r} \begin{pmatrix} 0 & 1 & P_1/\lambda \\ 0 & -i & P_2/\lambda \\ 1 & 0 & P_3/\lambda \end{pmatrix} - \frac{1}{r} \partial_{pr} \otimes \mathcal{Y}^\dagger_1, = \frac{1}{r} \partial A - \frac{1}{r} \partial_{pr} \otimes \mathcal{Y}^\dagger_1.
\]
Thus this leads to

\[ M_{12} = -\text{Tr} \left( \left( \frac{1}{r} A - \frac{1}{r} \partial_p r \otimes \mathcal{Y}_1 \right) (\partial_p h - \partial h) \mathcal{Y}_2 Z^{-1} \right) \]

\[ = -\text{Tr} \left( \frac{1}{r} A(\partial_p h - \partial h) \mathcal{Y}_2 Z^{-1} \right) + \text{Tr} \left( \frac{1}{r} \partial_p r \otimes \mathcal{Y}_1 (\partial_p h - \partial h) \mathcal{Y}_2 Z^{-1} \right) \]

\[ = -\frac{1}{r} \text{Tr} \left( A(\partial_p h - \partial h) \mathcal{Y}_2 Z^{-1} \right) + 0. \]

\[ (A(\partial_p h - \partial h)) \sqrt{|P|^2 + 1} = \begin{pmatrix} 0 & -P_2 P_3 & P_2^2 - |P|^2 + 1 + 1 \\ P_2 P_3 & 0 & -P_1 P_2 \\ \sqrt{|P|^2 + 1 - P_2^2} - 1 & P_1 P_2 & 0 \end{pmatrix} \]

\[ + i \begin{pmatrix} P_1 P_3 & 0 & \sqrt{|P|^2 + 1 - P_1^2} - 1 \\ 0 & P_1 P_3 & 0 \end{pmatrix}. \]

Thus \( \text{Tr}(A(\partial_p h - \partial h)\mathcal{Y}_2 p \otimes p) = 0 \). Finally, we have \( M_{12} = \text{Tr}(A(\partial_p h - \partial h)\mathcal{Y}_2 Z^{-1}) = 0 \), which concludes the proof. \( \square \)

We now consider the case when \( A \) is null.

**Proposition 2.2.** Assume that \( A \) is null, then \( M \) is diagonal. In addition, \( M_{11} = M_{22} = -\text{Tr}(Z^{-1}\partial_z P \text{Re}(A^{11})) \), where \( \{A^{m n}_j\} = \{\partial_p \mathcal{Y}_m(\partial_p h - c a_j)\mathcal{Y}_n\}_j \).

**Proof.** When the vector potential \( A \) is null, since \( \mathcal{Y} \) does not depend on \( Q \), \( \partial_z \mathcal{Y}_n = -\partial_p \mathcal{Y}_m \mathcal{P} \cdot \partial_p \mathcal{Y}_n \). For \( m \neq n \), \( M_{m n} = -\partial_z \mathcal{Y}_n(\mathcal{P} \mathcal{F}_j Z_j^{-1} = -\partial_z \mathcal{Y}_m(\partial_p h - c a_j)\mathcal{Y}_n Z_j^{-1} = -\text{Tr}(\partial_z \mathcal{P} \cdot \partial_p \mathcal{Y}_m(\partial_p h - c a)\mathcal{Y}_n Z_j^{-1}) \).

Let \( \lambda = \sqrt{c^2 |P|^2 + c^2} \) and \( r = \sqrt{2(\lambda^2 - c^2)} \), then

\[
\partial_p \mathcal{Y}_1(\partial_p h - c a)\mathcal{Y}_1 \frac{r^2 \lambda}{c^2} = \frac{r^2 \lambda}{c^2} \]

\[
= \begin{pmatrix} P_2^2 + P_3^2 + c^2 & -P_2 P_3 & P_2^2 - |P|^2 + 1 + 1 \\ P_2 P_3 & 0 & -P_1 P_2 \\ \sqrt{|P|^2 + 1 - P_2^2} - 1 & P_1 P_2 & 0 \end{pmatrix} \frac{c^2}{\sqrt{|P|^2 + c^2} - 1}
\]

\[+ ic^2 \begin{pmatrix} 0 \sqrt{|cP|^2 + c^2} - c^2 - P_3^2 \\ 0 \end{pmatrix}, \]

\[
\partial_p \mathcal{Y}_2(\partial_p h - c a)\mathcal{Y}_2 \frac{r^2 \lambda}{c^2} = -\partial_p \mathcal{Y}_2(\partial_p h - c a)\mathcal{Y}_1 \frac{r^2 \lambda}{c^2}
\]

\[
= c^2 \begin{pmatrix} 0 & P_2 P_3 & \sqrt{|cP|^2 + c^2} - c^2 - P_2^2 \\ -P_2 P_3 & 0 & P_1 P_2 \\ c^2 - \sqrt{|cP|^2 + c^2} - c^2 - P_2^2 & P_1 P_2 & 0 \end{pmatrix}
\]

\[+ ic^2 \begin{pmatrix} 0 & P_1 P_3 \sqrt{|cP|^2 + c^2} - c^2 - P_1^2 \\ 0 & -P_1 P_3 \end{pmatrix}. \]
Let \( \{A_{jk}^{mn}\} \) be the matrix \( \{\partial P_{m}Y_{n}(\partial P_{j}h - c\hat{a}_{j})Y_{n}\}_{jk} \), and then
\[
\mathcal{M}_{mn} = -2(Z_{jk}^{-1}P_{A_{ij}}^{mn}Z_{jk}) = -(Z_{jk}^{-1}I_{Z_{jk}}P_{A_{ij}}^{mn}) = -\text{Tr}(Z_{jk}^{-1}P_{A_{ij}}^{mn}).
\]

**Lemma 2.** \( Z_{jk}^{-1}P_{A_{ij}}^{mn} \) is symmetric.

As \( A \) is anti-symmetric and \( B \) is symmetric, then \( \text{Tr}(AB) = 0 \). Thus, we can obtain the following
\[
\begin{align*}
(36) & \quad \mathcal{M}_{mn} = -\text{Tr}(Z_{jk}^{-1}P_{A_{ij}}^{mn}) = 0, \quad \text{for } m \neq n \\
(37) & \quad \mathcal{M}_{11} = -\text{Tr}(Z_{jk}^{-1}P_{A_{ij}}^{mn}) = \mathcal{M}_{22}.
\end{align*}
\]

This concludes the proof. □

Notice that when \( c \to \infty \), \( \text{Re}(A^{11}) \to -\frac{1}{2}I \), which implies \( \mathcal{M}_{11} \to \frac{1}{2}\text{Tr}(P_{A_{ij}}^{mn})Z_{jk}^{-1} \).

We now consider the general situation.

**Proposition 2.3.** Assume \( A \) is not null. Then \( \mathcal{M} \) is in general not diagonal, except when \( A \) is only time-dependent. In addition,
\[
\mathcal{M}_{11} = \mathcal{M}_{22} = -\text{Tr}(Z_{jk}^{-1}P_{A_{ij}}^{mn}),
\]
where \( \{A_{jk}^{mn}\} = \{\partial P_{m}Y_{n}(\partial P_{j}h - c\hat{a}_{j})Y_{n}\}_{jk} \).

**Proof.** Let \( U = cP - A(Q) \) and \( \lambda = \sqrt{c^{2}|U|^{2} + c^{4}} \), then from (28),
\[
F_{j}^{n} = (c(\partial U_{j}\lambda - \hat{a}_{j}) + i\partial Q_{j}A \cdot (\partial U_{j}\lambda - \hat{a}_{j}))Y_{n} = (c(\partial U_{j}\lambda - \hat{a}_{j}) + i\partial Q_{j}A \cdot (\partial U_{j}\lambda - \hat{a}_{j})))Y_{n},
\]
which brings
\[
\begin{align*}
\mathcal{M}_{mn} = & \quad -(P_{j}U_{m}^{*}F_{m}^{n}Z_{jk})^{-1} \\
= & \quad -(\partial U_{j}Y_{m}^{*}(c(\partial U_{j}\lambda - \hat{a}_{j}) + i\partial Q_{j}A \cdot (\partial U_{j}\lambda - \hat{a}_{j})))Y_{n}Z_{jk}^{-1} \\
= & \quad -(\partial U_{j}Y_{m}^{*}(c(\partial U_{j}\lambda - \hat{a}_{j}) + i\partial Q_{j}A \cdot (\partial U_{j}\lambda - \hat{a}_{j})))Y_{n}Z_{jk}^{-1} \\
= & \quad -\text{Tr}[Z_{jk}^{-1}(A_{P} - A_{Q}A) \partial U_{m}^{*}(c(\partial U \lambda - \hat{a}) + i\partial Q A \cdot (\partial U \lambda - \hat{a})))Y_{n}Z_{jk}^{-1}] \\
= & \quad -\text{Tr}[Z_{jk}^{-1}(A_{P} - A_{Q}A) \partial U_{m}^{*}(c(\partial U \lambda - \hat{a}) + i\partial Q A \cdot (\partial U \lambda - \hat{a})))Y_{n}].
\end{align*}
\]

Since \( Z = \partial (Q + iP) \),
\[
\begin{align*}
\mathcal{M}_{mn} = & \quad \text{Tr}[icZ_{jk}^{-1}(Z - i\partial Q) + Z_{jk}^{-1}i\partial Q A) \partial U_{m}^{*}(c(\partial U \lambda - \hat{a}) + i\partial Q A \cdot (\partial U \lambda - \hat{a})))Y_{n}] \\
= & \quad \text{Tr}[ic(Z_{jk}^{-1}Z - i\partial Q) + Z_{jk}^{-1}i\partial Q A) \partial U_{m}^{*}(c(\partial U \lambda - \hat{a}) + i\partial Q A \cdot (\partial U \lambda - \hat{a})))Y_{n}] \\
= & \quad \text{Tr}[ic\partial U_{m}^{*}(c(\partial U \lambda - \hat{a}) + i\partial Q A \cdot (\partial U \lambda - \hat{a})))Y_{n}] \\
& \quad - \text{Tr}[icZ_{jk}^{-1}(Z - i\partial Q) - Z_{jk}^{-1}i\partial Q A) \partial U_{m}^{*}(c(\partial U \lambda - \hat{a}) + i\partial Q A \cdot (\partial U \lambda - \hat{a})))Y_{n}],
\end{align*}
\]

which concludes the proof. □
3. Nonrelativistic limit of the FGA for Dirac. In this section, we are interested in the nonrelativistic limit of the Dirac equation in the semi-classical regime. The purpose is to prove that due to the linearity of this equation, we can derive the FGA for the Schrödinger equation in the semi-classical and nonrelativistic regime from the FGA for the Dirac equation. In other words, we show the commutativity of the formal diagram Fig. 1. We will also provide some mathematical properties of the FGA in the nonrelativistic regime. We consider the case of a free particle (no interaction potential) with no external magnetic field \( A \), but subject to an external space-dependent potential. The initial data is

\[
\psi^\varepsilon(0, x) = \omega_I(x) \exp \left( \frac{i}{\varepsilon} S_I(x) \right),
\]

and the FGA reads

\[
\psi^\varepsilon(t, x) = \frac{1}{(2\pi\varepsilon)^{3/2}} \sum_m \int_{\mathbb{R}^3} \left( a_m(t, q, p) + \varepsilon \beta_m(t, q, p) \right) \times \exp \left( \frac{i}{\varepsilon} \Phi_m(t, x, y, q, p) \right) v_m(y, q, p) dy dq dp,
\]

with \( \Phi_m, a_m \) and \( v_m \) defined in (2.6)-(2.8). For the Dirac equation, the center of Gaussian profiles and momentum functions satisfy the Hamiltonian flow:

\[
\begin{align*}
\frac{dQ}{dt} &= \partial_P h(Q, P), & Q(0, q, p) &= q, \\
\frac{dP}{dt} &= -\partial_Q h(Q, P), & P(0, q, p) &= p.
\end{align*}
\]

where one branch \( h = h_+ \) has been selected, and where i) \( h_\pm(q, p) = \pm \lambda(p) + V(q) \) and ii) \( \lambda(p) = \sqrt{p^2 c^2 + c^4} \) with \( p := \|p\|_2 \).

3.1. Nonrelativistic limit of the FGA for Dirac equation. We plan to derive a FGA for the Schrödinger equation, by taking the nonrelativistic limit, i.e. \( c \to +\infty \). We will use the \( \sim \)-notation for the FGA in the nonrelativistic limit. We now state an important result of this paper.

**Theorem 3.1.** The nonrelativistic limit of the FGA for the field-free linear Dirac equation is the FGA for the Schrödinger equation.
Proof. First, for \( c \) large

\[
\frac{\partial p h(Q, P)}{\partial t} = \frac{P}{\sqrt{1 + \frac{P^2}{c^2}}} = P \left( 1 - \frac{P^2}{2c^2} + \mathcal{O}(P^4c^{-4}) \right),
\]

where \( P := ||P||_2 \). Then by keeping the leading order terms in (38), we define the Gaussian profiles and momentum centers as solutions to the following Hamiltonian flow, in the semiclassical and nonrelativistic limits:

\[
\begin{cases}
\frac{d\tilde{Q}}{dt} = \tilde{P}, & \tilde{Q}(0, q, p) = q. \\
\frac{d\tilde{P}}{dt} = -\partial_Q V(\tilde{Q}), & \tilde{P}(0, q, p) = p.
\end{cases}
\]

Next, the evolution of the action function

\[
\partial_t S(t, Q, P) = P \cdot \partial_t Q - h(Q, P)
\]

can be rewritten in the nonrelativistic limit, as follows

\[
\partial_t S(t, Q, P) = \frac{P^2}{2} - V(Q) - c^2 + \mathcal{O}(P^2c^{-2}),
\]

where we have used (38), and that

\[
h_{\pm}(Q, P) = \pm c^2 \sqrt{1 + \frac{P^2}{c^2}} + V(Q) = \pm \frac{P^2}{2} + V(Q) \pm c^2 + \mathcal{O}(c^2P^4).
\]

An evolution equation of the action function in the nonrelativistic limit can also be defined as:

\[
\partial_t \tilde{S}(t, \tilde{Q}, \tilde{P}) = c^2 + \frac{P^2}{2} - V(\tilde{Q}).
\]

We now focus on the evolution equation for the amplitude which requires a bit more careful analysis. As \( A \) is assumed null, we can rewrite \( B \) as:

\[
B(x) = \tilde{\beta} + V(Q)\|_0 + (x - Q) \cdot \partial_Q V(Q) + \frac{1}{2}(x - Q)^2 : \partial_Q^2 V(Q) + \mathcal{O}(x - Q)^3.
\]

Next, by taking \( m = n \) in (38), we get for \( n = 1, 2 \)

\[
\begin{align*}
\partial_t a_n &= \mathcal{Y}^\dagger_n (\partial_Q h \partial_P \mathcal{Y} - \partial_P h \partial_Q \mathcal{Y}) a_n \\
&\quad + \mathcal{Y}^\dagger_n \partial_{z_k} \mathcal{F}^n_j Z_{jk}^{-1} \mathcal{Y} \partial_Q a_n - \frac{1}{2} \mathcal{Y}^\dagger_n \partial_{z_k} Q \partial_{z_k} Q_i \partial_{Q_j} V Z_{jk}^{-1} \mathcal{Y} \partial_Q a_n,
\end{align*}
\]

where

\[
\mathcal{F}^n_j = (\partial_P h(Q, P) - c\alpha_j - i\partial_Q h(Q, P) + i\partial_Q V(Q)) \mathcal{Y}.
\]

As \( \mathcal{Y} \) is \( Q \)-independent, \( \partial_{Q_j} \mathcal{Y} = 0 \), so that the second term in the RHS of (41) is also null, and the latter can be rewritten as

\[
\partial_t a_n = \partial_Q \mathcal{Y}^\dagger_n \partial_P \mathcal{Y} \partial_Q a_n + \mathcal{Y}^\dagger_n \partial_{z_k} \mathcal{F}^n_j Z_{jk}^{-1} \mathcal{Y} \partial_Q a_n - \frac{1}{2} \mathcal{Y}^\dagger_n \partial_{z_k} Q_i \partial_{Q_j} V Z_{jk}^{-1} \mathcal{Y} \partial_Q a_n.
\]

Now we make use of the relations (A.8), recalling that \( u = cP \), then \( \partial_P = c\partial_u \), we then get

\[
\partial_t a_n = \partial_Q \mathcal{Y}^\dagger_n \partial_P \mathcal{Y} \partial_Q a_n + \mathcal{Y}^\dagger_n \partial_{z_k} \mathcal{F}^n_j Z_{jk}^{-1} \mathcal{Y} \partial_Q a_n - \frac{1}{2} \mathcal{Y}^\dagger_n \partial_{z_k} Q_i \partial_{Q_j} V Z_{jk}^{-1} \mathcal{Y} \partial_Q a_n.
\]
As we look at the positive branch, we have
\[ r_+(P) = \sqrt{2(P^2c^2 + c^4 - c^2\sqrt{P^2c^2 + c^4})} = c^2\sqrt{2} + \mathcal{O}(P^2c^{-2}), \]
and asymptotically get
\[ \Upsilon^*_n \partial_P \Upsilon_n = \frac{i}{P^2}(P_2, -P_1, 0) + \frac{i}{4c^2}(P_1, P_2, 0). \]

**Case 1.** $V$ is identically null. In this case
\[ \partial_t a_n = \Upsilon^*_n \partial_{zk} F^n_j Z_{jk}^{-1} a_n - \frac{i}{2} \Upsilon^*_n \partial_{zk} Q_l \partial^2_{Q_l Q_j} V Z_{jk}^{-1} \Upsilon_n a_n. \]

Let us focus on the term $\partial_{zk} F^n_j$. We notice that the expression of $F^n_j$ can be simplified into
\[ F^n_j = (\partial_P h(Q, P) - c\alpha_j) \Upsilon_n, \]
so that $\partial_{zk} F^n_j = (\partial_P h(Q, P) - c\alpha_j) \partial_{zk} \Upsilon_n + \Upsilon^*_n \partial_{zk} (\partial_P h(Q, P) \Upsilon_n)$. Now,
\[ \Upsilon^*_n \partial_{zk} F^n_j Z_{jk}^{-1} = \Upsilon^*_n (\partial_{zk} h(Q, P) - \alpha_j) \Upsilon_n Z_{jk}^{-1} + \Upsilon^*_n \partial_{zk} P_j \Upsilon_n Z_{jk}^{-1} \]
\[ = \left( \partial_{zk} \Upsilon_n (\partial_P h(Q, P) - \alpha_j) \Upsilon_n \right) Z_{jk}^{-1} + \Upsilon^*_n \partial_{zk} P_j \Upsilon_n Z_{jk}^{-1}. \]

We make use of the relation
\[ \Upsilon^*_n \partial_{zk} F^n_j Z_{jk}^{-1} = -\partial_{zk} \Upsilon^*_n F^n_j Z_{jk}^{-1} = -\partial_{zk} \Upsilon^*_n (\partial_P h(Q, P) - \alpha_j) \Upsilon_n Z_{jk}^{-1}. \]

Thus
\[ -\partial_{zk} \Upsilon^*_n (\partial_P h(Q, P) - \alpha_j) \Upsilon_n Z_{jk}^{-1} - \left( \partial_{zk} \Upsilon_n (\partial_P h(Q, P) - \alpha_j) \Upsilon_n \right) Z_{jk}^{-1} = \Upsilon^*_n \partial_{zk} P_j \Upsilon_n Z_{jk}^{-1}. \]

Recall that the $\alpha_j$ are hermitian, and that $\partial_{zk} = \partial_{yk} = i\partial_{pk}$, so that
\[ -2\text{Re}\left[ \partial_{zk} \Upsilon^*_n (\partial_P h(Q, P) - \alpha_j) \Upsilon_n Z_{jk}^{-1} \right] = \Upsilon^*_n \partial_{zk} P_j \Upsilon_n Z_{jk}^{-1}. \]

As we have assumed, that $V$ is null, then $P(t) = p, Q(t) = pt + q$, and as a consequence $Z = I(2 - i\tau)$, and $Z_{jk}^{-1} = \delta_{jk}/(2 - i\tau)$. We then deduce that
\[ \text{tr}\left[ \text{Re}\partial_{zk} \Upsilon^*_n (\partial_P h(Q, P) - \alpha_j) \Upsilon_n Z_{jk}^{-1} \right] = \text{tr}\left[ Z_{jk}^{-1} \partial_{zk} P \right]. \]

In order to conclude the proof, we need to show that $\text{tr}\left[ \text{Im}\partial_{zk} \Upsilon^*_n (\partial_P h(Q, P) - \alpha_j) \Upsilon_n Z_{jk}^{-1} \right]$ is at most a $\mathcal{O}(c^{-1})$. After some symbolic computations, we actually show that
\[ \text{tr}\left[ \text{Im}\partial_{zk} \Upsilon^*_n (\partial_P h(Q, P) - \alpha_j) \Upsilon_n Z_{jk}^{-1} \right] = \frac{P^2}{2c} + \mathcal{O}(c^{-2}). \]

In the nonrelativistic limit using (38), we get $\partial_{zk} F^n_j = (P_j - c\alpha_j) \partial_{zk} \Upsilon_n + \partial_{zk} P_j \Upsilon_n + \mathcal{O}(P^2c^{-2})$, then
\[ \Upsilon^*_n \partial_{zk} F^n_j = \frac{1}{2} \Upsilon^*_n \partial_{zk} P_j \Upsilon_n + \mathcal{O}(P^{-1}c^{-1}). \]

We then define the amplitude $\tilde{a}_n$ and its corresponding evolution equation by
\[ \frac{d\tilde{a}_n}{dt} = \frac{1}{2} \partial_{zk} \tilde{P}_j Z_{jk}^{-1} \tilde{a}_n. \]
We deduce from (39), (40), and (43) a nonrelativistic limit of the FGA for Dirac equation consistent with the one for the Schrödinger equation [37], where in particular, the evolution equation for the amplitude reads

\[ \frac{d\tilde{a}}{dt} = \frac{1}{2} \tilde{a} \text{tr}[\left( Z^{-1}(\partial_z \tilde{P}) \right)]. \]

This concludes the proof, when \( V \) is null.

**Case 2. \( V \) is not identically null.** The proof is essentially identical, but now relies on Proposition 2.2. We start from

\[ \frac{d}{dt}(a_1 \Upsilon_1 + a_2 \Upsilon_2) = M(a_1 \Upsilon_1 + a_2 \Upsilon_2). \]

According to Proposition 2.2, \( M \) is diagonal and for \( c \) large, we have established that \( M_{11} = M_{22} \) when \( c \to +\infty \) goes to \( \text{Tr} \partial_z P Z^{-1}/2 \) so that the evolution equation for the amplitude is yet (44). According to Proposition 2.3, the result remains valid for \( t \)-dependent only electric potentials \( A \).

In a bounded domain \( \Omega_t \), non-reflecting conditions are trivially established for the Dirac equation in both relativistic or nonrelativistic regimes. Whenever \( Q(t) \notin \Omega_t \), the contribution of this Gaussian function is simply removed from the reconstruction of \( \psi^\varepsilon \), see [37] for details in the case of the Schrödinger equation.

### 3.2. FGA for Klein-Gordon and nonrelativistic.

A balance-type approach is usually used to derive the nonrelativistic limit of the Klein-Gordon equation. For the sake of simplicity, we assume below that \( A(Q) = 0 \) and \( V(Q) = 0 \). We set \( \psi^\varepsilon = (\phi^\varepsilon, \chi^\varepsilon)^T \) which satisfies

\[
\begin{cases}
1 \varepsilon \partial_t \phi^\varepsilon = -i \varepsilon c \sigma \cdot p \chi^\varepsilon + \beta \varepsilon mc^2 \phi^\varepsilon, \\
1 \varepsilon \partial_t \chi^\varepsilon = -i \varepsilon c \sigma \cdot p \phi^\varepsilon + \beta \varepsilon mc^2 \chi^\varepsilon.
\end{cases}
\]

As \( V \) is null, \( \phi^\varepsilon \) (as well as \( \chi^\varepsilon \)) naturally satisfies the Klein-Gordon equation.

\[ \varepsilon^2 \partial_t^2 \phi^\varepsilon = (c^2 \varepsilon^2 \Delta + m^2 c^4 \mathbb{I}_2) \phi^\varepsilon. \]

Using similar elimination process, the FGA for Klein-Gordon can be directly constructed from the FGA for Dirac. In this goal, we could construct “from scratch” the FGA for Klein-Gordon, and will to that independently, it can be deduced from the one for the potential-free Dirac equation.

We now set \( a_m = (a^{(1)}_m, a^{(2)}_m)^T \), with \( a^{(1)}_m = a_m \Upsilon^{(1)}_m \), and \( \Upsilon_m = (\Upsilon^{(1)}_m, \Upsilon^{(2)}_m)^T \). Under the above assumptions, in the evolution equation for \( a \) only involves the matrix \( M \) which simply reads for \( (m, n) \in \{1, 2\}^2 \)

\[ M_{mn} = -\partial_{z_k} \Upsilon^\dagger_n (\partial_P h(Q, P)). \]

The amplitude equation, as for the Dirac equation then reads

\[ \frac{da_n}{dt} = \tilde{M} a_n, \]

where we have set \( \tilde{M} = M_{11} = M_{22} = \text{tr} \left[ \partial_z \Upsilon^\dagger_n (\partial_P h - \hat{a}) \Upsilon_n Z^{-1} \right] \). Considering again the positive branch

\[ \frac{d}{dt}(a_1 \Upsilon_1 + a_2 \Upsilon_2) = \tilde{M}(a_1 \Upsilon_1 + a_2 \Upsilon_2), \]

direct calculations show that the FGA for Klein-Gordon coincides with the one for Dirac assuming \( V \) null. It was proven in Section 2, that when \( c \) goes to infinity, \( M \) tends to \( \text{tr} [\partial_z P Z^{-1}] / 2 \) which is the amplitude equation for the potential-free Schrödinger equation. As a consequence, one deduces that the nonrelativistic limit of the FGA for Klein-Gordon is the FGA for Schrödinger.
3.3. Mathematical properties in nonrelativistic regime. We present some mathematical properties of the FGA in the nonrelativistic regime. We recall [33] that for smooth external and interaction potential, the Dirac operator is self-adjoint on $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$, while for Kato’s potentials singular at $x = 0$, the Dirac operator is self-adjoint on $C_0^\infty(\mathbb{R}^3 - \{0\}; \mathbb{C}^4)$. It is also well known that the Dirac operator is an unitary operator.

We first discuss the preservation of the $\ell^2$-norm in time. Start from $\psi^\varepsilon(0, \cdot)$ in $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$, and assume that

$$\|\psi^\varepsilon_j\|_2^2 := \sum_{j=1}^4 \int_{\mathbb{R}^3} |\psi^\varepsilon_j(0, x)|^2 \, dx$$

Recall that the dispersion relation for the Dirac operator is self-adjoint on $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$ potential, the Dirac operator is self-adjoint on $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$. As $\psi^\varepsilon$ is the FBI transform (which is a $\varepsilon$-unitary operator) for some smooth cutoff function $\chi_\delta$ defined in [25] and $D^\varepsilon_{0,1}$ is the FGA at order 1 and time $t = 0$. Next,

$$\|\psi^\varepsilon(t, \cdot)\|_2^2 = \frac{1}{(2\pi \varepsilon)^9} \sum_m \int_{\mathbb{R}^3} \int_{\mathbb{R}^4} a_m(t, p, q) v_m(y) e^{i \psi^\varepsilon(t, x, y, p) / \varepsilon} \, dy \, dp \, dx.$$

Recall that $v_m(y, q, p) = \mathcal{Y}_m(q, p) \cdot \psi^\varepsilon_j(y)$. Now [25] as $\|\mathcal{F}^\varepsilon f\|_{L^2(\mathbb{R}^3; \mathbb{C}^4)} = \|f\|_{L^2(\mathbb{R}^3; \mathbb{C}^4)}$, we get

$$\|\psi^\varepsilon(t, \cdot)\|_{L^2(\mathbb{R}^3; \mathbb{C}^4)}^2 = \|\psi^\varepsilon_j\|_{L^2(\mathbb{R}^3; \mathbb{C}^4)}^2 + O(\varepsilon^{-2}).$$

Notice that it is proven (in a more general form) in [25], that denoting $\mathcal{H}_t$ (resp. $\mathcal{H}_t^{\varepsilon, 1}$) a strictly hyperbolic (resp. corresponding FGA at order 1) propagator, the following estimate holds for any $T > 0$ and $m = 0$,

$$\max_{0 \leq t \leq T} \|\mathcal{H}_t \psi^\varepsilon_j - \mathcal{H}_t^{\varepsilon, 1} \psi^\varepsilon_j\|_{L^2(\mathbb{R}^3; \mathbb{C}^4)} \leq C_T \varepsilon,$$

where $\|\psi^\varepsilon_j\|_{L^2(\mathbb{R}^3; \mathbb{C}^4)} = 1$.

We next discuss the numerical dispersion issues, refered in the physics literature as Fermion doubling, which is responsible for the generation of spurious states [14]. Recall that the dispersion relation for the Dirac equation reads $E_k = \pm c^2 \sqrt{\mu^2 + c^4}$ ($m$ is taken equal to 1). Although, it is a problem usually treated at the discrete level, it must also be explored at the continuous level for FGA.

**Proposition 3.1.** Assume that $A$ and $V$ are null. The nonrelativistic FGA for Dirac is non-dispersive up to a $O(\varepsilon^{-2})$.

**Proof.** As $A$ and $V$ are assumed to be null, $P = p$ is constant, and from time 0 to $t$

$$Q(t, q, p) = q \pm t \frac{p}{\sqrt{1 + p^2/c^2}}.$$

The action function reads

$$S(t, Q, P) = S(0, Q, P) + \frac{t^2}{\sqrt{1 + p^2/c^2}}.$$

and

$$P_m \cdot (x - Q_m(t, q, p)) = p_m \cdot (x - q_m) \pm t \frac{p_m}{\sqrt{1 + p^2/c^2}}$$

$$= p_m \cdot (x - Q_m(0, q, p)) \pm t \frac{p_m^2}{\sqrt{1 + p^2/c^2}}.$$
That is, for $c$ large

$$
\Phi_m(t, x, y, q, p) = \Phi_m(0, x, y, q, p) \mp \frac{p_m^2 + c^2}{\sqrt{1 + p_m^2/c^2} t} = \Phi_m(0, x, y, q, p) \mp (p_m^2 + c^2)t + O(p_m^2c^{-2}).
$$

Recall that (3.19) degenerates into $da/dt = Ma$, with

$$
\mathcal{M}_{nn} = -\partial_x \mathcal{Y}_n \mathcal{F}_j^\dagger \mathcal{Z}_{jk}^{-1},
$$

and where $\mathcal{M}$ is diagonal, according to Proposition 2.1. In addition, for $V$, and $c$ large $Z$ is diagonal and reads

$$
Z_{jk} = (\partial_y - i\partial_p)(Q_k + iP_k) = 2\delta_{jk} \pm i\left( \frac{p_jp_kc^4}{(p^2c^2 + c^4)^{3/2}} - \frac{c^2\delta_{jk}}{\sqrt{p^2c^2 + c^4}} \right) t = 2\delta_{jk} \pm i\frac{c^2\delta_{jk}}{\sqrt{p^2c^2 + c^4}} + O(c^{-2}).
$$

As a consequence, denoting $\tilde{a} = (\tilde{a}_1, \tilde{a}_2)^T$,

$$
\frac{d\tilde{a}_n}{dt} = \frac{1}{2} \partial_z \mathcal{F}_j Z_{jk}^{-1} \tilde{a}_n = \frac{3}{2(t + 2i)} \tilde{a}_n,
$$

as $a_n(t, q, p) = (2i + t)^{3/2}a_n(0, q, p)$. We deduce that the dispersion relation is satisfied by the FGA for $c$ and $\varepsilon^{-1}$ large enough, that is

$$
\text{Arg} \left( a(t, q, p) \exp \left( \frac{1}{\varepsilon} \Phi_m(t, x, y, q, p) \right) \right) = \text{Arg} \left( (2i + t)^{3/2} \exp \left( \frac{1}{\varepsilon} \Phi_m(0, x, y, q, p) \right) \right) \mp p_m^2c^2t + O(p_m^2c^{-2}t).
$$

Notice that the $(2i + t)^{3/2}$ is a low frequency term, so that at the continuous level and $\varepsilon$ small enough, the dispersion relation is satisfied up to a $O(p^2c^{-2})$ term. $\square$

4. Relativistic regime. We propose in this section some analytical results related to FGA in the relativistic regime. We are in particular interested in the relevance of the FGA in multiscale regimes.

4.1. Error analysis. For fixed $c$, the order-$K$ FGA error is estimated in [25] for strictly hyperbolic systems, while since the Dirac equation is not strictly hyperbolic for $d > 1$ and is not homogeneous, the same proof in [25] can not directly apply to the Dirac equation. However, following the same type of arguments in [25], one may conjecture that the error estimate remains valid. That is,

**Conjecture 4.1.** Assume that $\psi_f \in L^2(\mathbb{R}^d)$, we get the following error estimate for the order-$K$ FGA:

$$
\max_{0 \leq t \leq T} \| \mathcal{H}_t \psi_f^\varepsilon - \mathcal{H}_t^{\varepsilon_1,\delta} \psi_f^\varepsilon \|_{L^2(\mathbb{R}^d; C^s)} \leq C_{T,K} \| \psi_f^\varepsilon \| \varepsilon^K,
$$

for some for some $C_{T,K} > 0$.

The rigorous proof to the conjecture is lengthy and technically involved, and thus we shall leave it as a future work. According to [25], if $m = 0$, the constant $C_{T,K}$ is linear in $c$, while $C_{T,K}$ is quadratic in $c$ for $m \neq 0$. In other words, $K$ should be taken large enough or $\varepsilon$ small enough, such that $c^2\varepsilon^K$ is small. This error estimates tells us that in the relativistic limit, either $K$ should be taken very large or $\varepsilon$ must be small enough to get an accurate FGA. This important problem is addressed in the following subsection dedicated to the relevance of the FGA depending on the relative values of $c$ and $\varepsilon$. 


4.2. Multiscale FGA in relativistic regime. In the relativistic regime, the mass-term ($\beta mc^2$) gives rise to the so-called *sitterbewegung* effect which corresponds to a fluctuation of the electron position with a frequency of $2mc^2$. In order to accurately capture this effect, the time step of a numerical solver must be taken smaller than $1/mc^2$ corresponding physically to the zepto-second regime ($10^{-21}$ second). More specifically, as numerically $c \approx 137$ a.u., then $1/c^2 \approx 5.3 \times 10^{-5}$. We discuss this question for FGAs in the relativistic regime in presence of an external electromagnetic field. The eigenvalues are of the form $\lambda(q, p) = \pm c\sqrt{|p - A(q)/c|^2 + c^2}$. We consider 3 cases $c\varepsilon \ll 1$, $c\varepsilon = O(1)$ and $c\varepsilon \gg 1$. Initially the FGA was derived in $(t, x)$-variable from the Dirac equation, by introducing the $(t', x')$-variables, by setting $t' = t\varepsilon$ and $x' = \varepsilon x$. Basically, the FGA as derived above is accurate if $c\varepsilon \ll 1$. In particular, the scaling $x' = \varepsilon x$ makes sense if the initial state, the external or interaction potentials possess high wavenumbers. We will assume below that $\varepsilon = c^{-1/a}$ with $a > 0$ and discuss the relevance of the FGA depending on the value of $a$. The term $c\hat{\alpha} \cdot (x - Q)/\varepsilon$ behaves as $\varepsilon^{-a}$, and is same order or dominant against the other $\varepsilon^{-1}$ term, and $\hat{\beta}_0c^2$ is of order $\varepsilon^{-2a}$.

**Case 1.** $\varepsilon = c^{-1/a}$ with $0 < a < 1/2$. First, we notice that the computation of the Gaussian and momentum functions do not impose any $c$-related constraints on the time step, as this system explicitly reads:

$$
\begin{align*}
\frac{dQ}{dt} &= \pm \frac{(P - A(Q)/c)}{\sqrt{1 + |P - A(Q)/c|^2}}, \quad Q(0, q, p) = q, \\
\frac{dP}{dt} &= -\partial_Q V(Q) + \frac{(P_t(Q) - A_t(Q)/c)a_Q A_t(Q)}{\sqrt{1 + |P - A(Q)/c|^2}}, \quad P(0, q, p) = p.
\end{align*}
$$

Next, the action function reads

$$
\partial_t S(t, Q, P) = \frac{P \cdot (P - A(Q)/c)}{\sqrt{1 + |P - A(Q)/c|^2}} - c^2 \left(\sqrt{|P + A(Q)|^2/c^4 + 1} - 1\right).
$$

In order to solve this equation, we can proceed as follows. We first determine $S$ solution to

$$
\partial_t S(t, Q, P) = \frac{P \cdot (P - A(Q)/c)}{\sqrt{1 + |P - A(Q)/c|^2}} - c^2 \left(\sqrt{|P + A(Q)|^2/c^4 + 1} - 1\right),
$$

from which we have removed the stiff-term $c^2$ from the action function equation. Then, we get $S(t, Q, P) = c^2t + S(t, Q, P)$. The overall FGA should be then constructed as in (2.6-2.8) except that $\Phi_m$ is rewritten as

$$
\Psi_m(t, x, y, q, p) = S(t, q, p) + \frac{i}{2} |x - Q_m(t, q, p)|^2 + P_m \cdot (x - Q_m(t, q, p)) + \frac{i}{2} |y - q|^2 - p \cdot (y - q),
$$

$$
\Phi_m(t, x, y, q, p) = \Psi_m(t, x, y, q, p) + c^2t.
$$

Let us now focus on the evolution equation for the amplitude. The latter involves $\mathcal{L}$, $\mathcal{M}$ and $\mathcal{N}$ as defined in (3.19). From (45), we have deduced that the computation of $Q$ and $P$ is not restricted by $c^2$, so that the same conclusion holds for $Z^{-1}$. Recall that the eigenvectors are normalized. Let us start with $\mathcal{L}$

$$
\mathcal{L}_{mn} = \frac{i}{2} \Upsilon_m^\dagger \partial_2 Q_l \partial_Q \partial_Q \partial_Q B Z^{-1}_{jk} \Upsilon_n,
$$

where $B = -\hat{\alpha} \cdot A + c^2\hat{\beta}_0 + V_{\parallel 4}$. As the mass term $c^2\hat{\beta}_0$ is an order 0 operator, the computation of $\partial Q B(Q)$ is also free from $c^2$-constraints. The same conclusion holds for $\mathcal{N}$. Regarding to $\mathcal{M}$, the main term to study is $F^m_j$ which is the sum of several terms including $c\hat{\alpha}_j$, while the other terms are $O(1)$ in $c$. However,

$$
\partial_2 \Upsilon_m = \partial_2 Q_j \partial_Q \Upsilon_m + \partial_2 P_j \partial_P \Upsilon_m,
$$

15
This highly oscillating phase does not impose any restriction on the computation of the amplitude $a$ which is then $a(\varepsilon)$.

The rest of the algorithm is identical to the one described in Section 1.

Case 2. $\varepsilon = O(c^{-2})$. In this case, the $\hat{\beta}_0 c^2$-term is the only term in $O(\varepsilon^{-1})$ in $B$ (8), then $D$, (7). This naturally modifies the construction of the FGA. As a consequence the double eigenvalues to $D$ becomes

$$h_{\pm}(q, p) = \pm|cp - A(q)| + V(q).$$

The eigenvectors have to be recomputed accordingly, denoting again $u = cp - A(q)$ and $r = \sqrt{2}|u|$, we have

$$\Upsilon_{\pm 1} = \frac{1}{r} \begin{pmatrix} \pm u_3 \\ \pm (u_1 + i u_2) \\ |u| \\ 0 \end{pmatrix}, \quad \Upsilon_{\pm 2} = \frac{1}{r} \begin{pmatrix} \pm (u_1 - i u_2) \\ \mp u_3 \\ 0 \\ |u| \end{pmatrix}. $$

The rest of the algorithm is identical to the one described in Section 1.

Case 3. $\varepsilon = O(c^{-1})$. In this case, the FGA must in principle be re-derived from scratch. Indeed, the $\hat{\beta}_0 c^2$-term is now a $O(\varepsilon^{-2})$ (8), and the term $c\hat{\alpha} \cdot p$ term behaves as $\hat{\alpha} \cdot p / \varepsilon$. Moreover,

$$\frac{c}{\varepsilon} \hat{\alpha} \cdot (x - Q) = -\partial_{x_k} (\hat{\alpha}_j Z_{jk}^{-1} a v),$$

which is then a $\varepsilon^{-2}$ term and should be removed from the previous expression of $F^n_j$, that is,

$$F^n_j = (\partial_p h(Q, P) - i \partial_Q h(Q, P) + i \partial_{Q_j} B(Q)) \Upsilon_n,$$

then from the evolution equation for $a$. Now $\hat{\alpha}_j \Upsilon_n = \partial_p h \Upsilon_n$, so that

$$-\partial_{x_k} (\hat{\alpha}_j Z_{jk}^{-1} a v) = -\partial_{x_k} (\partial_p h Z_{jk}^{-1} a v) = -\partial_{x_k} (\partial_p h Z_{jk}^{-1} a_1 \Upsilon_1 v) - \partial_{x_k} (\partial_p h Z_{jk}^{-1} a_2 \Upsilon_2 v),$$

and from (3.16)

$$-\partial_{x_k} (\partial_p h Z_{jk}^{-1} a_1 \Upsilon_1 v) = -\Upsilon_2 \partial_{x_k} \Upsilon_2 \partial_p h Z_{jk}^{-1} a_1 \Upsilon_1 v,$$

$$-\partial_{x_k} (\partial_p h Z_{jk}^{-1} a_2 \Upsilon_2 v) = -\Upsilon_1 \partial_{x_k} \Upsilon_1 \partial_p h Z_{jk}^{-1} a_2 \Upsilon_2 v.$$

Then the action function equation still reads, as $\Upsilon_{2,1} \Upsilon_{1,2} = 0$,

$$\partial_i S = P \cdot Q - h(Q, P).$$

The term $c^2 \hat{\beta}_0$ now behaves $\hat{\beta}_0 \varepsilon^{-2}$, and we can argue that the nonrelativistic limit should be considered in the first place.

Case 4. $\varepsilon < O(c^{-1})$. In this case all the $c$-terms would have to be “removed” from the FGA construction, as they would correspond to high order terms and would then have to be treated independently. In this case and as above, we should instead take the nonrelativistic limit.
5. Numerical experiments. This section is devoted to numerical experiments to illustrate the accuracy and relevance of the FGA for the Dirac equation.

5.1. A simple accuracy FGA test. We set $A \equiv 0$ and $V \equiv 0$ in the Dirac equation (5), and set the initial condition (6) as

\[ \omega_I(x) = \left( \exp \left( -A |x - x_0|^2 \right), 0, 0, 0 \right)^T, \]  
and $S_I(x) = p_0 \cdot x,$

with $A = 32$, $x_0 = (1, 1, 1)$, and $p_0 = (1, 0, 0)$. We compute the solutions using FGA for different $\varepsilon$’s and compare them with the reference solutions computed by Fourier spectral method. In this first set, we set $c = 1$, which allows in particular, for a removal of the computational difficulty due to the very small time-scale $(1/c^2)$ coming from the $\beta_0 c^2$-term. The solutions with $\varepsilon = 2^{-7}$ are shown in Fig 2, and the relative $L^2$ errors are listed in Table 1 illustrating the accuracy of the FGA.

![Fig. 2](image)

(a) FGA solution  
(b) Reference solution

**Table 1**  
The $L^2$-errors at $t = 0.2$.

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$2^{-4}$</th>
<th>$2^{-5}$</th>
<th>$2^{-6}$</th>
<th>$2^{-7}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$|\psi^\varepsilon - \hat{\psi}_{FGA}|_2$</td>
<td>$2.63 \times 10^{-2}$</td>
<td>$7.62 \times 10^{-3}$</td>
<td>$4.21 \times 10^{-3}$</td>
<td>$3.19 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

**Remark 5.1.** Let us remark that an partially explicit solution can be constructed for specific initial data:

$\psi(0, x, z) = \mathcal{N}[1, 0, 0, 0]^T \times e^{-((x-0.5)^2+(z-1)^2)/4\Delta^2}.$

The corresponding Fourier transform is given by

$\hat{\psi}(0, p_x, p_z) = 4\pi \Delta^2 \mathcal{N}[1, 0, 0, 0]^T \times e^{-\Delta^2 p^2},$

where $p^2 = p_x^2 + p_z^2$. The solution to

$\imath \partial_t \hat{\psi}(t, p_x, p_z) = (c\mathbf{\alpha} \cdot p + \beta c^2 / \varepsilon) \hat{\psi}(t, p_x, p_z),$

is given by

$\hat{\psi}(t, p_x, p_z) = \exp \left[ - \imath c\mathbf{\alpha} \cdot p t - \imath \beta c^2 t / \varepsilon \right] \hat{\psi}(0, p_x, p_z)$

$= \left[ \mathbb{I}_4 \cos(E\varepsilon t) - \imath \frac{c\mathbf{\alpha} \cdot p \mathbf{e} z + \beta c^2}{\varepsilon E\varepsilon} \sin(E\varepsilon t) \right] \hat{\psi}(0, p_x, p_z),$
with $E_{c} = \sqrt{p^{2}c^{2} + c^{4}/\varepsilon^{2}}$. We set $p'_{x} := \varepsilon p_{x}$ and $p'_{z} := \varepsilon p_{z}$, $t' := t/\varepsilon$, $p' := \sqrt{(p'_{x})^{2} + (p'_{z})^{2}}$, $E' = \sqrt{(p')^{2}c^{2} + c^{4}}$ and $\Delta' := \Delta/\varepsilon$, then

$$
(47) \quad \tilde{\psi}(t, p'_{z}/\varepsilon, p'_{z}/\varepsilon) = 4\pi \Delta' \left[ I_{1}(\cos(E't')) - i \frac{c\hat{c}}{E'} \sin(E't') \right] N[1, 0, 0, 0]^{T} \times e^{-(\Delta'p')^{2}},
$$

so that, denoting $x' = x\varepsilon$, $z' = z\varepsilon$ and $r' = \sqrt{(x')^{2} + (y')^{2}}$,

$$
\left\{
\begin{array}{ll}
\psi_{1}(t', x', z') & = 2N(\Delta')^{2} \int_{0}^{\infty} p'e^{-(\Delta'p')^{2}} J_{0}(p'\varepsilon) \left( \cos(E't') - i \frac{c^{2}}{E'} \sin(E't') \right) dp', \\
\psi_{2}(t', x', z') & = 0, \\
\psi_{3}(t', x', z') & = -2N(\Delta')^{2} \sin(\theta) \int_{0}^{\infty} p'e^{-(\Delta'p')^{2}} J_{1}(p'\varepsilon) \frac{cp'}{E'} \sin(E't') dp', \\
\psi_{4}(t', x', z') & = -2N(\Delta')^{2} \sin(\theta) \int_{0}^{\infty} p'e^{-(\Delta'p')^{2}} J_{1}(p'\varepsilon) \frac{cp'}{E'} \sin(E't') dp',
\end{array}
\right.
$$

where $J_{0,1}$ are the zeroth and first order Bessel functions, $\theta = \tan^{-1}(z'/x')$. For instance taking $r' = 0$, using the Erfi-function, we get

$$
\psi_{1}(t', 0, 0) = N \left[ 1 - \sqrt{\pi} \frac{\varepsilon ct'}{2\Delta} \exp \left( -\left( \frac{\varepsilon ct'}{2\Delta} \right)^{2} \right) \right].
$$

5.2. Barrier potential. This test is devoted to the propagation of a wavepacket toward a smooth barrier potential. We denote the energy of a wavepacket with wavenumber $(k_{x}, k_{y}, k_{z})$, by

$$
E_{c} = \sqrt{k^{2}c^{2} + c^{4}/\varepsilon},
$$

where $k := \sqrt{k_{x}^{2} + k_{y}^{2} + k_{z}^{2}}$ and the barrier potential is defined as

$$
(48) \quad V(x, y, z) = \frac{V_{0}}{2} \left( 1 + \tanh \left( \frac{x}{L_{v}} \right) \right).
$$

In the semi-classical regime, the wavepacket should be totally reflected if $V_{0}/\varepsilon > E_{c} - c^{2}/\varepsilon$, while it should be totally transmitted otherwise. Notice that we do not expect Klein paradox to occur in this regime, see next subsection. We consider both situation in a 3-d simulation on a spatial domain $[0, 2]^{3}$, of a wavepacket defined by

$$
\psi(0, x, y, z) = N[1, 0, 0, 0]^{T} \times \exp \left( - \left( (x - x_{0})^{2} + (y - y_{0})^{2} + (z - z_{0})^{2} \right)/4\Delta^{2} \right) \exp(ik_{x}x),
$$

where $x_{0} = 0.5$, $y_{0} = z_{0} = 1$, $k_{x} = 0.5$ and $\Delta = 4\sqrt{2}$. In this test we take $c = 1$, $L_{v} = 0.2$. We report the modulus of the first component $\psi_{1}$ of the FGA solution at time $T = 1.5$, with $\varepsilon = 2^{-6}$, corresponding to wavepacket energy equal to $E_{c} = \sqrt{1.25}/\varepsilon$, when $V_{0} = (\text{resp. } V_{0} = 0)$. The time step is taken equal to $\Delta t = 10^{-2}$ As expected, total transmission (resp. reflection) occurs Fig. 3 (Left) (resp. (Middle)), when $V_{0}/\varepsilon < E_{c} - 1/\varepsilon$ (resp. $V_{0}/\varepsilon > E_{c} - 1$). We also report in Fig. 3 (Right) the FGA without potential, that is $V_{0} = 0$.

5.3. Nonrelavistic limit. This test is dedicated to the computation of the FGA making vary values of $c$. We compare the FGA solution, with $\varepsilon = 2^{-7}$, from $c$ small to $c$ large, and observe in particular that the FGA is convergent when $c$ goes to infinity (to the FGA for Schrödinger, see Theo. 3.1). We represent the first component $\psi_{1}$ of the FGA solution, with Cauchy data

$$
\psi(0, x, y, z) = N[1, 0, 0, 0]^{T} \times \exp \left( - \left( (x - x_{0})^{2} + (y - y_{0})^{2} + (z - z_{0})^{2} \right)/4\Delta^{2} \right) \exp(ik_{x}x),
$$

where $x_{0} = y_{0} = z_{0} = 1$, $k_{x} = 0.5$, and $\Delta = 4$. We report the solution for $c = 0.1, 0.5, 1, 5, 10, 10000$ in Fig. 4. As numerically observed on this example, for $c$ large enough, the FGA solution becomes independent of $c$, and corresponds to the FGA solution for the Schrödinger equation, according to Theorem 3.1.
5.4. **Klein Paradox.** The Klein paradox refers to the partial transmission of an electronic wavepacket through a potential energy barrier higher than the kinetic energy $E_p$ of an incoming electron [7]. We will perform two series of tests in 1-d and 2-d. We show in particular, that the direct FGA does not allow to capture this quantum effect.

5.4.1. **One-dimensional tests.** The electronic kinetic energy is given here by

$$E_{k_x}^{(e)} = \sqrt{c^2 k_x^2 + c^4 / \varepsilon}.$$  

In order to apply the FGA, we regularize the barrier potential as follows

$$V(x) = \frac{V_0}{2} \left( 1 + \tanh \left( \frac{x}{L_V} \right) \right),$$

where $L_V$ is a small parameter characterizing the gradient of the potential. In theory, transmission occurs when $V_0 / \varepsilon > E_{k_x}^{(e)} + 2c^2 / \varepsilon$. The transmission $T$ and reflection $R$ coefficients for a barrier potential located...
at 0, are respectively given by
\[
\mathcal{T} = \frac{\int_{\mathbb{R}_+} \psi^* \psi}{\int_{\mathbb{R}_-} \psi^* \psi}, \quad \mathcal{R} = \frac{\int_{\mathbb{R}_-} \psi^* \psi}{\int_{\mathbb{R}_-} \psi^* \psi},
\]
where
\[
\mathcal{T} = -\frac{\sinh(\pi k^{(e)} L_V) \sinh(\pi \kappa^{(e)} L_V)}{\sinh(\pi V_0/\varepsilon + k^{(e)} + \kappa^{(e)}) L_V/2) \sinh(\pi (V_0/\varepsilon - k^{(e)} - \kappa^{(e)}) L_V/2)},
\] (49)
and
\[
k^{(e)} = \frac{1}{\varepsilon} \sqrt{\left(E^{(e)} - V_0/\varepsilon\right)^2 - c^4/\varepsilon^2}, \quad \kappa^{(e)} = -\frac{1}{\varepsilon} \sqrt{\left(E^{(e)} - V_0/\varepsilon\right)^2 - c^4/\varepsilon^2}.
\]

As a preliminary test, we perform a test in the quantum regime using a method described in [14]. We assume that \(\varepsilon = 1/8\), which is close to a semi-classical regime. The spatial domain is \([-20, 20]\), \(L_V = 10^{-4}\), and \(V_0 = 5 \times 10^4\). The time step is given by \(\Delta t = 2.23 \times 10^{-5}\) and space step \(\Delta x = 1.53 \times 10^{-4}\), corresponding to \(N = 262144\) grid points. The initial data is a Gaussian centered at \(x_0 = -5\) and is given by
\[
\psi(0, x) = [1, 0, 0, C]^T \times \exp\left(-\frac{\left(x - x_0\right)^2}{4 \Delta^2}\right) \exp(\imath k_x x),
\]
with width \(\Delta = 1\), wavenumber \(k_x/\varepsilon = 500\) and
\[
C = \frac{c k_x}{c^2 + \sqrt{c^4 + 2 k_x^2}}.
\]
The theoretical transmission coefficient is given by \(\mathcal{T} = 0.322\), while the numerical one is given by \(\mathcal{T}_n = 0.327\). At total of \(8 \times 10^4\) time iterations is necessary to perform this computation, corresponding to \(\approx 2160.9\) seconds (on 16 processors), which is relatively very resource demanding for a such a simple test.

5.4.2. Two-dimensional tests. We here consider a quantum and semi-classical regime simulation.

**Quantum regime.** We assume that \(\varepsilon = 1\), \(c \approx 137.0359895\). The spatial domain is \([-1, 1] \times [-2, 2]\), \(L_V = 10^{-4}\),
\[
V(x, z) = \frac{V_0}{2} \left(1 + \tanh\left(\frac{z}{L_V}\right)\right),
\]
with \(V_0 = 4.64 \times 10^4\). The time step is given by \(\Delta t = 2.85 \times 10^{-5}\) and space step \(\Delta x = \Delta z = 2 \times 10^{-5}\). The initial data is a Gaussian centered at \((x_0, z_0) = (0, -1.0)\) and is given by
\[
\psi(0, x, z) = [1, 0, 0, C]^T \times \exp\left(-\frac{\left((x - x_0)^2 + (z - z_0)^2\right)}{4 \Delta^2}\right) \exp(\imath k_x x),
\] (50)
with width \(\Delta = 0.2\), wavenumber \(k_x = 200\) and
\[
C = \frac{c k_x}{c^2 + \sqrt{c^4 + 2 k_x^2}}.
\]
Then \(E^{(e)}_{k_x} = 3.3224 \times 10^3\) and \(\kappa^{(e)} = 133.9374\). The transmission coefficient which is computed numerically is given by \(\mathcal{T}_n \approx 0.661\) and the theoretical one is \(\mathcal{T} = 0.65\). The computation is performed on 8 processors with a total of 12304 seconds.

**Semi-classical regime.** We consider the initial condition (50), with \(\Delta = 1/64\), \(x_0 = z_0 = 1\), and \(k_x = 0.5\). We assume that \(\varepsilon = 2^{-7}\) and \(c = 1\). The barrier potential is defined by (48) with \(L_v = 0.2\), and \(V_0 = 4\), and as a consequence \(V_0/\varepsilon > E_x + 2c^2/\varepsilon\). In the quantum regime, the transmission coefficient gives \(\tau \approx 0.485\), when \(L_v\) small enough. In the semi-classical limit, we numerically report the FGA wavepacket at time \(T = 1\). The wavepacket is totally reflected illustrating the inability for the direct FGA, which is a semi-classical solution, to simulate the Klein paradox which is a quantum effect. A special treatment must be implemented in order to allow the transmission.
6. **Direct spectral method.** The computational domain is \([-a_x, a_x] \times [-a_y, a_y] \times [-a_z, a_z]\), where \(a_x > 0\), \(a_y > 0\) and \(a_z > 0\). We denote the grid-point set by

\[D_{N_x,N_y,N_z} = \left\{ x_{k_1,k_2,k_3} = (x_{k_1}, y_{k_2}, z_{k_3}) \right\}_{(k_1,k_2,k_3) \in O_{N_x,N_y,N_z}},\]

where

\[O_{N_x,N_y,N_z} = \{ (k_1, k_2, k_3) \in \mathbb{N}^3 : k_1 = 0, \cdots , N_x - 1 ; k_2 = 0, \cdots , N_y - 1 ; k_3 = 0, \cdots , N_z - 1 \}.\]

Then, we define the space steps as

\[h_x = x_{k_1+1} - x_{k_1} = 2a_x/N_x,\]
\[h_y = y_{k_2+1} - y_{k_2} = 2a_y/N_y,\]
\[h_z = z_{k_3+1} - z_{k_3} = 2a_z/N_z.\]
The matrices \( \Pi \) are defined as follows.

\[
\Pi_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix}, \quad \Pi_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & -i & 0 \\ 1 & 0 & 0 & 1 \\ -i & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix}, \quad \Pi_z = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}.
\]

A first or second order splitting method is used in combination with the Fast Fourier Transform. The first order splitting reads as follows. We denote by \( \alpha_\gamma = \Pi_z \Lambda_\gamma \Pi_y^T \), for \( \nu = x, y, z \) and where

\[
\Lambda_\gamma = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.
\]

This step is performed exactly, up to the approximation of \( A \) (resp. \( V \)) by their projection \( A_h \) (resp. \( V_h \)) on a finite difference grid.

1. First step: integration of the source from \( t_n \) to \( t_{n_1} = t_n + \Delta t \).

\[
\psi^{n_1}_h = \exp \left( -i \Delta t (\beta c^2 / \varepsilon + V_h / \varepsilon - \alpha \cdot A_h) \right) \psi^n_h.
\]

2. Second step: integration of the generalized transport equation in Fourier space. One sets \( \phi^{n_1}_h := \Pi_x^T \psi^{n_1}_h \), and solve

\[
\partial_t \phi + A_x \partial_x \phi = 0,
\]

from time \( t_n \) to \( t_{n_2} = t_n + \Delta t \), basically by discretizing in space: \( \phi(t_{n+1}, \cdot) = F_x^{-1} \left( e^{-i \xi \Delta t} A_x F_x (\phi(t_n, \cdot)) \right) \), where \( F_x \) is the Fourier transform in the \( x \)-direction that is for \( \ell = 1, \ldots, 4 \), such that \( \phi^{\ell} \) denotes the \( \ell \)th component of \( \phi \). We denote \( \phi^{(\ell),n_1}_h \), the \( \ell \)th component \( \phi_h \) at time \( n_1 \).

\[
\phi^{(\ell),n_2}_h = \frac{1}{N_x} \sum_{p=-N_x/2}^{N_x/2-1} \left( e^{-i \xi \Delta t} A_x^{(\ell)} \sum_{k_1=0}^{N_x-1} \phi^{(\ell),n_1}_h, e^{-i \xi p (x_{k_1} + a_x)} \right) e^{i \xi p (x+a_x)},
\]
where $\lambda^{(z)}$ is the $\ell$th eigenvalues of $A_x$.

3. Similarly one computes, from $t_n$ to $t_{n+1} = t_n + \Delta t$

$$
\phi^{(\ell),n+1}_h = \frac{1}{N_y} \sum_{y=-N_y/2}^{N_y/2-1} \left( e^{-i\xi_y \Delta t \lambda^{(n)}_x} \sum_{k_2=0}^{N_z-1} \phi^{(\ell),n}_h \mathcal{A} \left( e^{-i\xi_y(y_{k_2}+a_y)} \right) \right) \left( e^{i\xi_y(y+a_y)} \right),
$$

where $\phi^{n}_h = \Pi_y \phi^{n}_h$ and finally

$$
\phi^{(\ell),n+1}_h = \frac{1}{N_z} \sum_{z=-N_z/2}^{N_z/2-1} \left( e^{-i\xi_z \Delta t \lambda^{(n)}_x} \sum_{k_3=0}^{N_z-1} \phi^{(\ell),n}_h \mathcal{A} \left( e^{-i\xi_z(z_{k_3}+a_z)} \right) \right) \left( e^{i\xi_z(z+a_z)} \right),
$$

where $\phi^{n}_h = \Pi_z \phi^{n}_h$. Finally $\psi^{n+1}_h = \Pi_z \phi^{n+1}_h$.

Alternatively, it is possible to directly apply 3d FFTs. By construction, the $\ell_2$-norm is naturally conserved.

7. Conclusion. This paper derives and analyzes the frozen Gaussian approximation (FGA) for the linear Dirac equation in the semi-classical limit. Strong connections of the FGA for Dirac and Klein-Gordon equations with the Schrödinger equation are established in the non-relativistic limit. Important physical properties, such as numerical dispersion, are also mathematically analyzed and illustrated by numerical experiments. In future works, FGA for the Dirac equation will be used to solve realistic strong fields problems in quantum relativistic physics.

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Appendix A. Eigenvalues and eigenvectors.

A.1. Eigenvectors computation. In order to determine $\mathcal{M}$ and $\mathcal{N}$ in (34), we need to explicitly construct $\partial h$ and $\partial \mathcal{Y}$. First notice

$$
\partial Q_h = \pm \frac{c(P_c-A_j)\partial Q_A}{\sqrt{|P_c-A(Q)|^2+c^4}} + \partial Q V, \quad \partial p h = \pm \frac{(P_c-A)}{\sqrt{|P_c-A(Q)|^2+c^4}},
$$

$$
\partial P_j \partial Q_h = \pm \frac{(P_c-A_j)(P_c-A) \cdot \partial Q_k A}{\left( |P_c-A(Q)|^2+c^4 \right)^{3/2}} \pm \frac{c \partial Q_j A}{\sqrt{|P_c-A(Q)|^2+c^4}},
$$

$$
\partial P_j \partial P_h = \pm \frac{c(P_c-A_j)(P_c-A_k)}{\left( |P-A(Q)|^2+c^4 \right)^{3/2}} \pm \frac{c \delta_{jk}}{\sqrt{|P_c-A(Q)|^2+c^4}},
$$

$$
\partial Q_j \partial Q_h = \pm \frac{(P_c-A) \cdot \partial Q_j A (P_c-A) \cdot \partial Q_k A}{\left( |P_c-A(Q)|^2+c^4 \right)^{3/2}} + \partial Q_j \partial Q_k V,
$$

$$
\partial Q_j \partial P_h = \pm \frac{\partial Q_j A \cdot \partial Q_k A - (P_c-A) \cdot \partial Q_j A}{\sqrt{|P_c-A(Q)|^2+c^4}} + \partial Q_j \partial Q_k V.
$$

Hence

$$
\partial \mathcal{Y} = \partial \mathcal{Y}_1 = \partial \mathcal{Y}_2.
$$

Let $\lambda = \sqrt{|u|^2+c^4}$, and $u = P_c - A(Q)$. We now determine the positive and negative branches.

A.2. Positive branch. The corresponding eigenvectors read

$$
\mathcal{Y}_1 = \frac{1}{r} \begin{pmatrix}
\frac{u_3}{|u|^2+c^4-c^2} \\
\frac{u_1+iu_2}{|u|^2+c^4-c^2} \\
0
\end{pmatrix}, \quad \mathcal{Y}_2 = \frac{1}{r} \begin{pmatrix}
\frac{u_1-iv_2}{|u|^2+c^4-c^2} \\
\frac{-u_2}{|u|^2+c^4-c^2} \\
0
\end{pmatrix},
$$
where \( r = \sqrt{2 \left( |u|^2 + c^4 - c^2 \sqrt{|u|^2 + c^4} \right)} \), and \( u = P c - A(Q) \). We have

\[
\partial_u \mathcal{Y}_1 = \frac{1}{r} \begin{pmatrix}
0 & 1 & u_1 / \lambda & 0 \\
0 & i & u_2 / \lambda & 0 \\
1 & 0 & u_3 / \lambda & 0
\end{pmatrix} - \frac{1}{r} \partial_u r \otimes \mathcal{Y}_1,
\]

\[
\partial_u \mathcal{Y}_2 = \frac{1}{r} \begin{pmatrix}
1 & 0 & 0 & u_1 / \lambda \\
-i & 0 & 0 & u_2 / \lambda \\
0 & -1 & 0 & u_3 / \lambda
\end{pmatrix} - \frac{1}{r} \partial_u r \otimes \mathcal{Y}_2,
\]

and

\[
\partial_u r = -\frac{1}{r} \left( \frac{1}{\sqrt{|u|^2 + c^4}} - 2 \right) u.
\]

Thus

\[
\mathcal{Y}_1^\dagger \partial_u \mathcal{Y}_1 = \frac{i}{r^2} (-u_2, u_1, 0), \\
\mathcal{Y}_2^\dagger \partial_u \mathcal{Y}_2 = \frac{i}{r^2} (u_2, -u_1, 0),
\]

\[
\mathcal{Y}_2^\dagger \partial_u \mathcal{Y}_1 = \frac{1}{r^2} (-u_3, -iu_3, u_1 + iu_2), \\
\mathcal{Y}_1^\dagger \partial_u \mathcal{Y}_2 = \frac{1}{r^2} (u_3, -iu_3, -u_1 + iu_2).
\]

We define the following Berry connection matrices:

\[
\mathcal{B} = \frac{1}{r^2} \begin{bmatrix}
-iu_2 & u_3 \\
-u_3 & iu_2
\end{bmatrix}, \begin{bmatrix}
u_1 & -iu_3 \\
-iu_3 & -iu_1
\end{bmatrix}, \begin{bmatrix}0 & -u_1 + iu_2 \\
u_1 + iu_2 & 0
\end{bmatrix}.
\]

**A.3. Negative branch.** The corresponding eigenvectors read

\[
\mathcal{Y}_1 = \frac{1}{r} \begin{pmatrix}
-u_3 \\
-u_1 - iu_2 \\
0
\end{pmatrix}, \quad \mathcal{Y}_2 = \frac{1}{r} \begin{pmatrix}
u_1 \\
-0 \end{pmatrix},
\]

where \( r = \sqrt{2 \left( |u|^2 + c^4 - c^2 \sqrt{|u|^2 + c^4} \right)} \).

\[
\partial_u \mathcal{Y}_1 = \frac{1}{r} \begin{pmatrix}
0 & -1 & u_1 / \lambda & 0 \\
0 & -i & u_2 / \lambda & 0 \\
-1 & 0 & u_3 / \lambda & 0
\end{pmatrix} - \frac{1}{r} \partial_u r \otimes \mathcal{Y}_1,
\]

\[
\partial_u \mathcal{Y}_2 = \frac{1}{r} \begin{pmatrix}
-1 & 0 & 0 & u_1 / \lambda \\
i & 0 & 0 & u_2 / \lambda \\
0 & 1 & 0 & u_3 / \lambda
\end{pmatrix} - \frac{1}{r} \partial_u r \otimes \mathcal{Y}_2,
\]

\[
\partial_u r = \frac{1}{r} \left( \frac{1}{\sqrt{|u|^2 + c^4}} + 2 \right) u.
\]
Thus

\[
\begin{align*}
\textbf{Y}_1^\dagger \partial_u \textbf{Y}_1 &= \frac{i}{r^2} (-u_2, \quad u_1, \quad 0), \\
\textbf{Y}_2^\dagger \partial_u \textbf{Y}_2 &= \frac{i}{r^2} ( \quad u_2, \quad -u_1, \quad 0), \\
\textbf{Y}_1^\dagger \partial_u \textbf{Y}_1 &= \frac{1}{r^2} (-u_3, \quad -iu_3, \quad u_1 + iu_2), \\
\textbf{Y}_2^\dagger \partial_u \textbf{Y}_2 &= \frac{1}{r^2} ( \quad u_3, \quad -iu_3, \quad -u_1 + iu_2).
\end{align*}
\]

We define the following Berry connection matrices:

\[
\mathcal{B} = \frac{1}{r^2} \begin{pmatrix} -iu_2 & u_3 \\ -u_3 & iu_2 \end{pmatrix} - i \begin{pmatrix} 0 & -u_1 + iu_2 \\ u_1 + iu_2 & 0 \end{pmatrix}.
\]

We conclude this appendix, by providing some working values, necessary to determine the non-relativistic limit of the FGA.

A.4. Intermediate values. Denoting again \( r = \sqrt{2(p^2c^2 + c^4 - c^2\sqrt{p^2c^2 + c^4})} \), and for the positive branch

\[
\begin{align*}
\partial_{p_1} \textbf{Y}_1 &= \frac{1}{r} \begin{pmatrix} 0 & c \\ p_1c^2 & \sqrt{p^2c^2 + c^4} \end{pmatrix} - \frac{\partial_{p_1} r}{r^2} \textbf{Y}_1, \\
\partial_{p_2} \textbf{Y}_1 &= \frac{1}{r} \begin{pmatrix} 0 & 1c \\ p_2c^2 & \sqrt{p^2c^2 + c^4} \end{pmatrix} - \frac{\partial_{p_2} r}{r^2} \textbf{Y}_1, \\
\partial_{p_3} \textbf{Y}_1 &= \frac{1}{r} \begin{pmatrix} c & 0 \\ p_3c^2 & \sqrt{p^2c^2 + c^4} \end{pmatrix} - \frac{\partial_{p_3} r}{r^2} \textbf{Y}_1.
\end{align*}
\]

\[
\begin{align*}
\partial_{p_1} \textbf{Y}_2 &= \frac{1}{r} \begin{pmatrix} 0 & 0 \\ p_1c^2 & \sqrt{p^2c^2 + c^4} \end{pmatrix} - \frac{\partial_{p_1} r}{r^2} \textbf{Y}_2, \\
\partial_{p_2} \textbf{Y}_2 &= \frac{1}{r} \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p^2c^2 + c^4} \end{pmatrix} - \frac{\partial_{p_2} r}{r^2} \textbf{Y}_2, \\
\partial_{p_3} \textbf{Y}_2 &= \frac{1}{r} \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p^2c^2 + c^4} \end{pmatrix} - \frac{\partial_{p_3} r}{r^2} \textbf{Y}_2.
\end{align*}
\]

REFERENCES
