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# FROZEN GAUSSIAN APPROXIMATION FOR THE DIRAC EQUATION IN SEMICLASSICAL REGIME*

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**Abstract.** This paper focuses on the derivation and analysis of the frozen Gaussian approximation (FGA) for the Dirac equation in the semiclassical regime. Unlike the strictly hyperbolic system studied in [J. Lu and X. Yang, *Comm. Pure Appl. Math.*, 65 (2012), pp. 759–789], 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 the Klein paradox are presented to illustrate the method and confirm part of the analytical results.

**Key words.** Dirac equation, semiclassical analysis, frozen Gaussian approximation

**AMS subject classifications.** 65M12, 65M06, 65M15

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## Notations

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

## 1. Introduction.

This paper focuses on 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 a 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) [34]. There is growing interest in physics for the study of this equation in particular for modeling heavy-ion collisions [31, 20, 2], for pair production using strong laser fields [13, 12, 18], or for modeling Graphene [23]. These active research fields in physics have motived recent computational works [2, 35]. Let us mention

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[24, 16, 17], where embarassingly parallel quantum lattice Boltzmann methods were developed and applied to the simulation of the interaction of a 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 [36, 1, 32, 29, 30, 8, 3]. Galerkin methods with balanced basis functions are proposed in [19] for solving the time-dependent Dirac equation (TDDE). Graphene-related simulations using similar techniques are also proposed in [15, 14]. Regarding the numerical approximation of the TDDE in the nonrelativistic regime, there exists an extended literature; see, for instance, [6, 4, 5]. The approximation of the Dirac equation in the semiclassical regime has also recently brought some attention, in particular in [37], where a Gaussian beam–based method is proposed based on adiabatic approximation.

In this work, the Dirac equation will be approximated in the semiclassical regime, using the celebrated FGA. The latter was originally developed by Herman–Kluk (HK) [22] for the Schrödinger equation in the semiclassical regime. The mathematical analysis was then proposed in [33] showing the accuracy and efficiency of this ansatz in particular when the initial data are localized in phase space. HK formalism was later developed of several types of partial differential equations, such as wave equations [26], linear hyperbolic systems of conservation laws [28], elastic wave equations, and seismic tomography [9, 10, 21]. Some applications and analysis on the Schrödinger equations were also proposed in [25, 38]. 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 semiclasscial approximation. In the end, we present several numerical experiments, including the Klein paradox, to illustrate the method and confirm part of the analytical results.

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

$$\mathrm{i}\partial_t \psi(t,\boldsymbol{x}) = \hat{\boldsymbol{H}}\psi(t,\boldsymbol{x}), \tag{1}$$

where

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

and for $\gamma = x, y, z$

$$\alpha_\gamma = \begin{bmatrix} 0 & \sigma_\gamma \\ \sigma_\gamma & 0 \end{bmatrix}, \quad \beta = \begin{bmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{bmatrix}. \tag{3}$$

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

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \quad \text{and} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{4}$$

while $\mathbb{I}_2$ is the $2\times 2$ unit matrix. The momemtum operator is denoted $\boldsymbol{p} = -\mathrm{i}\boldsymbol{\nabla}$. The speed of light $c$ and fermion mass $m$ are kept explicit in (2), allowing one 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 $\boldsymbol{\alpha} = (\alpha_\gamma)_{\gamma=x,y,z}, \beta$ are the Dirac matrices. This equation models a relativistic electron of mass $m$ subject to an interaction potential $V_c(\boldsymbol{x})$ and electromagnetic field $V(t,\boldsymbol{x}), \boldsymbol{A}(t,\boldsymbol{x})$, and where for fixed time $t$, $\psi(t,\boldsymbol{x}) \in L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ is the coordinate ($\boldsymbol{x}=(x,y,z)$) dependent four-spinor. We denote by $\langle\, ,\, \rangle$ 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 [24]. In the following, the coupling is neglected, and we then assume that the EM propagates as in vacuum.

**2. FGA for the Dirac equation.** This section is devoted to the construction of the FGA for the Dirac equation in the semiclassical regime. We first recall some basic facts about FGA for evolution equations in the semiclassical regime. We then derive the FGA for the field-particle Dirac equation in the relativistic regime. In the following, we consider a time-independent electromagnetic field. For $\varepsilon > 0$, we reformulate the Dirac equation as follows:

$$\mathrm{i}\varepsilon\partial_t\boldsymbol{\psi}^\varepsilon(t,\boldsymbol{x}) = \big(-\mathrm{i}c\varepsilon\hat{\boldsymbol{\alpha}}\cdot\nabla - \hat{\boldsymbol{\alpha}}\cdot\boldsymbol{A}(\boldsymbol{x}) + m\beta c^2 + V(\boldsymbol{x})\big)\boldsymbol{\psi}^\varepsilon(t,\boldsymbol{x}) \tag{5}$$

$$\boldsymbol{\psi}^\varepsilon(0,\boldsymbol{x}) = \boldsymbol{\varphi}_I^\varepsilon(\boldsymbol{x}) = \boldsymbol{\omega}_I(\boldsymbol{x})\exp\left(\frac{\mathrm{i}}{\varepsilon}S_I(\boldsymbol{x})\right). \tag{6}$$

Here $\boldsymbol{\psi}^\varepsilon = (\psi_1^\varepsilon,\psi_2^\varepsilon,\psi_3^\varepsilon,\psi_4^\varepsilon)^T \in \mathbb{C}^4$ is the spinor, and $S_I$ (resp., $\omega_I$) is the initial phase (resp., amplitude). 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

$$D(\boldsymbol{q},\boldsymbol{p}) := \hat{\boldsymbol{\alpha}}\cdot(\boldsymbol{p}c - \boldsymbol{A}(\boldsymbol{q})) + m\beta c^2 + V(\boldsymbol{q})\mathbb{I}_4 = \hat{\boldsymbol{\alpha}}\cdot\boldsymbol{p}c + B(\boldsymbol{q}), \tag{7}$$

where we have denoted

$$B(\boldsymbol{q}) := -\hat{\boldsymbol{\alpha}}\cdot\boldsymbol{A}(\boldsymbol{q}) + m\beta c^2 + V(\boldsymbol{q})\mathbb{I}_4. \tag{8}$$

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

$$h_\pm(\boldsymbol{q},\boldsymbol{p}) = \pm\lambda(\boldsymbol{q},\boldsymbol{p}) + V(\boldsymbol{q}), \quad \text{where} \quad \lambda(\boldsymbol{q},\boldsymbol{p}) = \sqrt{|\boldsymbol{p}c - \boldsymbol{A}(\boldsymbol{q})|^2 + c^4}. \tag{9}$$

Denote the corresponding eigenvectors as $\boldsymbol{\Upsilon}_m$, $m=\pm1,\pm2$, and let $\boldsymbol{u}=\boldsymbol{p}c-\boldsymbol{A}(\boldsymbol{q})$. Then

$$\begin{aligned}
&\boldsymbol{\Upsilon}_{+1} = \frac{1}{r_+}\begin{pmatrix} u_3 \\ u_1+\mathrm{i}u_2 \\ \sqrt{|\boldsymbol{u}|^2+c^4}-c^2 \\ 0\end{pmatrix}, \quad \boldsymbol{\Upsilon}_{+2} = \frac{1}{r_+}\begin{pmatrix} u_1-\mathrm{i}u_2 \\ -u_3 \\ 0 \\ \sqrt{|\boldsymbol{u}|^2+c^4}-c^2\end{pmatrix}, \\
&\boldsymbol{\Upsilon}_{-1} = \frac{1}{r_-}\begin{pmatrix} -u_3 \\ -u_1-\mathrm{i}u_2 \\ \sqrt{|\boldsymbol{u}|^2+c^4}+c^2 \\ 0\end{pmatrix}, \quad \boldsymbol{\Upsilon}_{-2} = \frac{1}{r_-}\begin{pmatrix} -u_1+\mathrm{i}u_2 \\ u_3 \\ 0 \\ \sqrt{|\boldsymbol{u}|^2+c^4}+c^2\end{pmatrix},
\end{aligned} \tag{10}$$

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

**2.2. Formulation of the FGA.** We first present the formulation of the FGA for the Dirac equation and leave its derivation for the following subsection. The FGA has the following form:

$$\begin{aligned}\boldsymbol{\psi}^{\varepsilon}_{\mathrm{FGA}}(t,\boldsymbol{x}) &= \frac{1}{(2\pi\varepsilon)^{9/2}}\sum_{\pm m}\int_{\mathbb{R}^9}\boldsymbol{a}_{\pm m}(t,\boldsymbol{q},\boldsymbol{p})\exp\left(\frac{\mathrm{i}}{\varepsilon}\Phi_{\pm}(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})\right)v_{\pm m}(\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p},\end{aligned} \tag{11}$$

where

$$\begin{aligned}\Phi_{\pm}(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}) &= S_{\pm}(t,\boldsymbol{q},\boldsymbol{p}) + \frac{\mathrm{i}}{2}\left|\boldsymbol{x}-\boldsymbol{Q}_{\pm}(t,\boldsymbol{q},\boldsymbol{p})\right|^2 + \boldsymbol{P}_{\pm}(t,\boldsymbol{q},\boldsymbol{p})\cdot(\boldsymbol{x}-\boldsymbol{Q}_{\pm}(t,\boldsymbol{q},\boldsymbol{p}))\\ &\quad + \frac{\mathrm{i}}{2}\left|\boldsymbol{y}-\boldsymbol{q}\right|^2 - \boldsymbol{p}\cdot(\boldsymbol{y}-\boldsymbol{q}),\\ \boldsymbol{a}_{\pm m}(t,\boldsymbol{q},\boldsymbol{p}) &= a_{\pm m}(t,\boldsymbol{q},\boldsymbol{p})\,\boldsymbol{\Upsilon}_{\pm m}(\boldsymbol{Q}_{\pm m},\boldsymbol{P}_{\pm m}),\\ v_{\pm m}(\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}) &= \boldsymbol{\Upsilon}_{\pm m}(\boldsymbol{q},\boldsymbol{p})\cdot\boldsymbol{\psi}^{\varepsilon}_{I}(\boldsymbol{y}).\end{aligned} \tag{12}$$

We present the evolution equations, respectively, (1) for the Gaussian profiles $\boldsymbol{Q}$ and momentum functions $\boldsymbol{P}$, (2) for the action function $S$, and (3) for the FGA amplitude $\boldsymbol{a}$. For the sake of simplicity, we consider one branch (e.g., "+" branch) and drop the subscription without causing any confusion.

1. *Gaussian profile $\boldsymbol{Q}$ and momentum function $\boldsymbol{P}$, evolution equation.* As for any FGA, the bi-center $\boldsymbol{Q}$ and $\boldsymbol{P}$ simply satisfy the Hamiltonian flow:

$$\begin{cases}\dfrac{\mathrm{d}\boldsymbol{Q}}{\mathrm{d}t} = \partial_{\boldsymbol{P}}h(\boldsymbol{Q},\boldsymbol{P}), & \boldsymbol{Q}(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{q},\\ \dfrac{\mathrm{d}\boldsymbol{P}}{\mathrm{d}t} = -\partial_{\boldsymbol{Q}}h(\boldsymbol{Q},\boldsymbol{P}), & \boldsymbol{P}(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{p}.\end{cases} \tag{13}$$

   We then determine the evolution equation for the action function.

2. *Action function $S$, evolution equation.*

$$\frac{\mathrm{d}}{\mathrm{d}t}S = \boldsymbol{P}\cdot\partial_t\boldsymbol{Q} - h(\boldsymbol{Q},\boldsymbol{P}), \quad S(0,\boldsymbol{q},\boldsymbol{p}) = 0. \tag{14}$$

3. *Amplitude evolution equation.*

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}a_1\\ a_2\end{pmatrix} = (\mathcal{L}+\mathcal{M}+\mathcal{N})\begin{pmatrix}a_1\\ a_2\end{pmatrix}, \quad a_1(0,\boldsymbol{q},\boldsymbol{p}) = a_2(0,\boldsymbol{q},\boldsymbol{p}) = 2^{d/2}, \tag{15}$$

   where $\mathcal{L}$, $\mathcal{M}$, and $\mathcal{N}$ are $2\times 2$ matrices given by (36) and details are to be stated in the following subsection.

**2.3. Derivation of the FGA.** In order to derive the FGA formulation, we rewrite the solution of the Dirac equation in the following form:

$$\begin{aligned}\boldsymbol{\psi}^{\varepsilon}(t,\boldsymbol{x}) = \frac{1}{(2\pi\varepsilon)^{9/2}}\sum_{\pm m}\int_{\mathbb{R}^9}&\left(\boldsymbol{a}_{\pm m}(t,\boldsymbol{q},\boldsymbol{p}) + \varepsilon\boldsymbol{\beta}_{\pm m}(t,\boldsymbol{q},\boldsymbol{p})\right)\\ &\times\exp\left(\frac{\mathrm{i}}{\varepsilon}\Phi_{\pm}(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})\right)v_{\pm m}(\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p},\end{aligned} \tag{16}$$

where $\Phi_\pm$ and $v_{\pm m}$ as defined in (12). For the sake of simplicity, we consider one branch (e.g., "+" branch) and drop the subscription without causing any confusion. As required in the FGA framework, the bi-center $\boldsymbol{Q}$ and $\boldsymbol{P}$ satisfy the Hamiltonian system (13). Evolution equations for the action function $S$ and amplitude $\boldsymbol{a}$ can be obtained by substituting (16) into the Dirac equation (5), but this is a much more technical step, and it requires additional preliminary calculations. By definition of $\Phi$, we have

$$\partial_t \Phi = \partial_t S - \boldsymbol{P} \cdot \partial_t \boldsymbol{Q} + (\boldsymbol{x} - \boldsymbol{Q}) \cdot \partial_t (\boldsymbol{P} - \mathrm{i}\boldsymbol{Q}) \tag{17}$$

$$\nabla_{\boldsymbol{x}} \Phi = \mathrm{i}(\boldsymbol{x} - \boldsymbol{Q}) + \boldsymbol{P}. \tag{18}$$

Then taking derivatives to (16) gives

(19)

$$\begin{aligned}\partial_t \boldsymbol{\psi}^\varepsilon &= \int \left( \partial_t \boldsymbol{a} + \varepsilon \partial_t \boldsymbol{\beta} + \frac{\mathrm{i}}{\varepsilon} \partial_t \Phi (\boldsymbol{a} + \varepsilon \boldsymbol{\beta}) \right) \mathrm{e}^{\mathrm{i}\Phi/\varepsilon} v \, \mathrm{d}\boldsymbol{y} \, \mathrm{d}\boldsymbol{q} \, \mathrm{d}\boldsymbol{p} \\ &= \int \left( \partial_t \boldsymbol{a} + \frac{\mathrm{i}}{\varepsilon} \left( \partial_t S - \boldsymbol{P} \cdot \partial_t \boldsymbol{Q} + (\boldsymbol{x} - \boldsymbol{Q}) \cdot \partial_t (\boldsymbol{P} - \mathrm{i}\boldsymbol{Q}) \right) \boldsymbol{a} \right) \mathrm{e}^{\mathrm{i}\Phi/\varepsilon} v \, \mathrm{d}\boldsymbol{y} \, \mathrm{d}\boldsymbol{q} \, \mathrm{d}\boldsymbol{p} \\ &\quad + \int \left( \varepsilon \partial_t \boldsymbol{\beta} + \mathrm{i} \left( \partial_t S - \boldsymbol{P} \cdot \partial_t \boldsymbol{Q} + (\boldsymbol{x} - \boldsymbol{Q}) \cdot \partial_t (\boldsymbol{P} - \mathrm{i}\boldsymbol{Q}) \right) \boldsymbol{\beta} \right) \mathrm{e}^{\mathrm{i}\Phi/\varepsilon} v \, \mathrm{d}\boldsymbol{y} \, \mathrm{d}\boldsymbol{q} \, \mathrm{d}\boldsymbol{p}\end{aligned}$$

(20)

$$\nabla_{\boldsymbol{x}} \boldsymbol{\psi}^\varepsilon = \int \frac{\mathrm{i}}{\varepsilon} \left( \mathrm{i}(\boldsymbol{x} - \boldsymbol{Q}) + \boldsymbol{P} \right) (\boldsymbol{a} + \varepsilon \boldsymbol{\beta}) \, \mathrm{e}^{\mathrm{i}\Phi/\varepsilon} v \, \mathrm{d}\boldsymbol{y} \, \mathrm{d}\boldsymbol{q} \, \mathrm{d}\boldsymbol{p}.$$

We now expand $B(\boldsymbol{x})$ about $\boldsymbol{Q}$

$$B(\boldsymbol{x}) = B(\boldsymbol{Q}) + (\boldsymbol{x} - \boldsymbol{Q}) \cdot \partial_{\boldsymbol{Q}} B(\boldsymbol{Q}) + \frac{1}{2} (\boldsymbol{x} - \boldsymbol{Q})^2 : \partial_{\boldsymbol{Q}}^2 B(\boldsymbol{Q}) + \mathcal{O}(\boldsymbol{x} - \boldsymbol{Q})^3. \tag{21}$$

In order to perform the asymptotics, we introduce the following definition.

DEFINITION 2.1. *Two functions $f$ and $g$ are said equivalent if*

$$f \sim g \;\Leftrightarrow\; \int f \mathrm{e}^{\mathrm{i}\Phi/\varepsilon} \, \mathrm{d}\boldsymbol{y} \, \mathrm{d}\boldsymbol{q} \, \mathrm{d}\boldsymbol{p} = \int g \mathrm{e}^{\mathrm{i}\Phi/\varepsilon} \, \mathrm{d}\boldsymbol{y} \, \mathrm{d}\boldsymbol{q} \, \mathrm{d}\boldsymbol{p} \, .$$

And based on this definition, we easily show [27] the following.

LEMMA 1.

$$\boldsymbol{b} \cdot (\boldsymbol{x} - \boldsymbol{Q}) \sim -\varepsilon \partial_{z_k} (b_j Z_{jk}^{-1}) \tag{22}$$

$$(\boldsymbol{x} - \boldsymbol{Q}) \cdot G (\boldsymbol{x} - \boldsymbol{Q}) \sim \varepsilon \partial_{z_k} Q_l G_{lj} Z_{jk}^{-1} + \varepsilon^2 \dots, \tag{23}$$

*where Einstein's summation convention has been used and where*

$$\partial_{\boldsymbol{z}} = \partial_{\boldsymbol{q}} - \mathrm{i}\partial_{\boldsymbol{p}}, \qquad Z = \partial_{\boldsymbol{z}} (\boldsymbol{Q} + \mathrm{i}\boldsymbol{P}). \tag{24}$$

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

Substituting (16) into (5), to the order of $\varepsilon^0$, we get

$$-\int (\partial_t S - \boldsymbol{P} \cdot \partial_t \boldsymbol{Q}) \boldsymbol{a} \, \mathrm{e}^{\mathrm{i}\Phi/\varepsilon} v \, \mathrm{d}\boldsymbol{y} \, \mathrm{d}\boldsymbol{q} \, \mathrm{d}\boldsymbol{p} = \int (c \hat{\boldsymbol{\alpha}} \cdot \boldsymbol{P} + B(\boldsymbol{Q})) \boldsymbol{a} \, \mathrm{e}^{\mathrm{i}\Phi/\varepsilon} v \, \mathrm{d}\boldsymbol{y} \, \mathrm{d}\boldsymbol{q} \, \mathrm{d}\boldsymbol{p}. \tag{25}$$

This equation suggests that $\boldsymbol{a}$ is an eigenvector of $c\hat{\boldsymbol{\alpha}}\cdot\boldsymbol{P}+B(\boldsymbol{Q})$. Then (25) holds if the action function $S$ satisfies the following evolution equation:

$$\partial_t S=\boldsymbol{P}\cdot\partial_t\boldsymbol{Q}-h(\boldsymbol{Q},\boldsymbol{P}). \tag{26}$$

We now construct the evolution equation for $\boldsymbol{a}$. To the order of $\varepsilon^1$,

$$\int \mathrm{i}\varepsilon\left(\partial_t\boldsymbol{a}+\frac{\mathrm{i}}{\varepsilon}(\boldsymbol{x}-\boldsymbol{Q})\cdot\partial_t(\boldsymbol{P}-\mathrm{i}\boldsymbol{Q})\boldsymbol{a}+\mathrm{i}(\partial_t S-\boldsymbol{P}\cdot\partial_t\boldsymbol{Q})\boldsymbol{\beta}\right)\mathrm{e}^{\mathrm{i}\Phi/\varepsilon}v\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}$$
$$=\int\!\!\left(\mathrm{i}c\hat{\boldsymbol{\alpha}}\cdot(\boldsymbol{x}-\boldsymbol{Q})\boldsymbol{a}+(\boldsymbol{x}-\boldsymbol{Q})\cdot\partial_{\boldsymbol{Q}}B\boldsymbol{a}+\frac{1}{2}(\boldsymbol{x}-\boldsymbol{Q})^2:\partial^2_{\boldsymbol{Q}}B\boldsymbol{a}+\varepsilon D\boldsymbol{\beta}\right)\mathrm{e}^{\mathrm{i}\Phi/\varepsilon}v\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p},$$

which implies

$$\begin{aligned}&\int\left(\partial_t\boldsymbol{a}+\frac{1}{\varepsilon}(\boldsymbol{x}-\boldsymbol{Q})\cdot\partial_t(\boldsymbol{Q}+\mathrm{i}\boldsymbol{P})\boldsymbol{a}+\mathrm{i}(D(\boldsymbol{Q},\boldsymbol{P})-h(\boldsymbol{Q},\boldsymbol{P}))\boldsymbol{\beta}\right)\mathrm{e}^{\mathrm{i}\Phi/\varepsilon}v\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}\\&=\int\left(\frac{c}{\varepsilon}\hat{\boldsymbol{\alpha}}\cdot(\boldsymbol{x}-\boldsymbol{Q})+\frac{1}{\mathrm{i}\varepsilon}(\boldsymbol{x}-\boldsymbol{Q})\cdot\partial_{\boldsymbol{Q}}B+\frac{1}{2\mathrm{i}\varepsilon}(\boldsymbol{x}-\boldsymbol{Q})^2:\partial^2_{\boldsymbol{Q}}B\right)\boldsymbol{a}\,\mathrm{e}^{\mathrm{i}\Phi/\varepsilon}v\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}.\end{aligned}\tag{27}$$

Thus,

$$\int\left[\partial_t\boldsymbol{a}v-\partial_{z_k}\left(\partial_t(Q_j+\mathrm{i}P_j)Z^{-1}_{jk}\boldsymbol{a}v\right)+\mathrm{i}(D(\boldsymbol{Q},\boldsymbol{P})-h(\boldsymbol{Q},\boldsymbol{P}))\boldsymbol{\beta}v\right]\mathrm{e}^{\mathrm{i}\Phi/\varepsilon}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}$$
$$=\int\left[-\partial_{z_k}\left(c\hat{\alpha}_jZ^{-1.5}_{jk}\boldsymbol{a}v\right)+\mathrm{i}\partial_{z_k}\left(\partial_{Q_j}BZ^{-1.5}_{jk}\boldsymbol{a}v\right)-\frac{\mathrm{i}}{2}\partial_{z_k}Q_l\,\partial_{Q_l}\partial_{Q_j}B\,Z^{-1}_{jk}\boldsymbol{a}v\right]\mathrm{e}^{\mathrm{i}\Phi/\varepsilon}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p},$$

that is,

$$\begin{aligned}&\partial_t\boldsymbol{a}v-\partial_{z_k}\left[\left(\partial_t(Q_j+\mathrm{i}P_j)-c\hat{\alpha}_j+\mathrm{i}\partial_{Q_j}B\right)Z^{-1}_{jk}\boldsymbol{a}v\right]+\frac{\mathrm{i}}{2}\partial_{z_k}Q_l\,\partial_{Q_l}\partial_{Q_j}B\,Z^{-1}_{jk}\boldsymbol{a}v\\&\sim\ \mathrm{i}(h(\boldsymbol{Q},\boldsymbol{P})-D(\boldsymbol{Q},\boldsymbol{P}))\,\boldsymbol{\beta}\,v.\end{aligned}\tag{28}$$

We define for $n=1,2$,

$$\begin{aligned}\boldsymbol{F}^n_j&=\left(\partial_t(Q_j+\mathrm{i}P_j)-c\hat{\alpha}_j+\mathrm{i}\partial_{Q_j}B\right)\boldsymbol{\Upsilon}_n\\&=\left(\partial_{P_j}h(\boldsymbol{Q},\boldsymbol{P})-\mathrm{i}\partial_{Q_j}h(\boldsymbol{Q},\boldsymbol{P})-c\hat{\alpha}_j+\mathrm{i}\partial_{Q_j}B\right)\boldsymbol{\Upsilon}_n\\&=\left(\partial_{P_j}h(\boldsymbol{Q},\boldsymbol{P})-c\hat{\alpha}_j-\mathrm{i}\partial_{Q_j}h(\boldsymbol{Q},\boldsymbol{P})+\mathrm{i}\partial_{Q_j}B\right)\boldsymbol{\Upsilon}_n.\end{aligned}\tag{29}$$

Then (28) can be written as

$$\begin{aligned}&\partial_t\boldsymbol{a}v-\partial_{z_k}\left[\left(a_1\boldsymbol{F}^1_j+a_2\boldsymbol{F}^2_j\right)Z^{-1}_{jk}v\right]+\frac{\mathrm{i}}{2}\partial_{z_k}Q_l\,\partial_{Q_l}\partial_{Q_j}B\,Z^{-1}_{jk}\boldsymbol{a}v\\&\sim\ \mathrm{i}(h(\boldsymbol{Q},\boldsymbol{P})-D(\boldsymbol{Q},\boldsymbol{P}))\,\boldsymbol{\beta}\,v.\end{aligned}\tag{30}$$

Solvability for $\boldsymbol{\beta}$ gives, for $m=1,2$,

$$\boldsymbol{\Upsilon}^\dagger_m\left\{\partial_t\boldsymbol{a}v-\partial_{z_k}\left[\left(a_1\boldsymbol{F}^1_j+a_2\boldsymbol{F}^2_j\right)Z^{-1}_{jk}v\right]+\frac{\mathrm{i}}{2}\partial_{z_k}Q_l\,\partial_{Q_l}\partial_{Q_j}B\,Z^{-1}_{jk}\boldsymbol{a}v\right\}=0.\tag{31}$$

Let $\boldsymbol{\Upsilon}\in\mathrm{Span}\{\boldsymbol{\Upsilon}_1,\boldsymbol{\Upsilon}_2\}$. Since

$$(c\hat{\boldsymbol{\alpha}}\cdot\boldsymbol{P}+B(\boldsymbol{Q}))\boldsymbol{\Upsilon}(\boldsymbol{Q},\boldsymbol{P})=h(\boldsymbol{Q},\boldsymbol{P})\boldsymbol{\Upsilon}(\boldsymbol{Q},\boldsymbol{P}),$$

then

$$c\hat{\alpha}_j \boldsymbol{\Upsilon} + (c\hat{\boldsymbol{\alpha}} \cdot \boldsymbol{P} + B)\,\partial_{P_j}\boldsymbol{\Upsilon} = \partial_{P_j} h\,\boldsymbol{\Upsilon} + h\,\partial_{P_j}\boldsymbol{\Upsilon},$$
$$\partial_{Q_j} B\,\boldsymbol{\Upsilon} + (c\hat{\boldsymbol{\alpha}} \cdot \boldsymbol{P} + B)\,\partial_{Q_j}\boldsymbol{\Upsilon} = \partial_{Q_j} h\,\boldsymbol{\Upsilon} + h\,\partial_{Q_j}\boldsymbol{\Upsilon},$$

and thus for $m = 1, 2$,

$$\boldsymbol{\Upsilon}_m^\dagger \left(c\hat{\alpha}_j - \partial_{P_j} h\right) \boldsymbol{\Upsilon} = 0,$$
$$\boldsymbol{\Upsilon}_m^\dagger \left(\partial_{Q_j} B(\boldsymbol{Q}) - \partial_{Q_j} h\right) \boldsymbol{\Upsilon} = 0\,.$$

Thus, for $m, n = 1, 2$, $\boldsymbol{\Upsilon}_m^\dagger \boldsymbol{F}_j^n = 0$ and

$$\boldsymbol{\Upsilon}_m^\dagger \partial_{z_k} \left[a_n \boldsymbol{F}_j^n Z_{jk}^{-1} v\right] = \boldsymbol{\Upsilon}_m^\dagger \partial_{z_k} \boldsymbol{F}_j^n Z_{jk}^{-1} a_n\, v = -\partial_{z_k} \boldsymbol{\Upsilon}_m^\dagger \boldsymbol{F}_j^n Z_{jk}^{-1} a_n\, v\ . \tag{32}$$

Notice that

$$\boldsymbol{\Upsilon}_m^\dagger \partial_t (a_n \boldsymbol{\Upsilon}_n) = \delta_{mn} \partial_t a_n + \boldsymbol{\Upsilon}_m^\dagger \left(\partial_{P_j} h \partial_{Q_j} \boldsymbol{\Upsilon}_n - \partial_{Q_j} h \partial_{P_j} \boldsymbol{\Upsilon}_n\right) a_n. \tag{33}$$

Then (31) gives the equation for $a_m$:

$$\begin{aligned} &\delta_{mn}\, \partial_t a_n - \boldsymbol{\Upsilon}_m^\dagger \left(\partial_{Q_j} h \partial_{P_j} \boldsymbol{\Upsilon}_n - \partial_{P_j} h \partial_{Q_j} \boldsymbol{\Upsilon}_n\right) a_n \\ &= -\,\partial_{z_k} \boldsymbol{\Upsilon}_m^\dagger \boldsymbol{F}_j^n Z_{jk}^{-1} a_n - \frac{\mathrm{i}}{2} \boldsymbol{\Upsilon}_m^\dagger \partial_{z_k} Q_l\, \partial_{Q_l} \partial_{Q_j} B\, Z_{jk}^{-1} \boldsymbol{\Upsilon}_n a_n. \end{aligned} \tag{34}$$

In the vector form

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = (\mathcal{L} + \mathcal{M} + \mathcal{N}) \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \tag{35}$$

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

$$\begin{aligned} \mathcal{L}_{mn} &= \frac{\mathrm{i}}{2} \boldsymbol{\Upsilon}_m^\dagger \partial_{z_k} Q_l\, \partial_{Q_l} \partial_{Q_j} B\, Z_{jk}^{-1} \boldsymbol{\Upsilon}_n, \\ \mathcal{N}_{mn} &= \boldsymbol{\Upsilon}_m^\dagger \left(\partial_{\boldsymbol{Q}} h \cdot \partial_{\boldsymbol{P}} \boldsymbol{\Upsilon}_n - \partial_{\boldsymbol{P}} h \cdot \partial_{\boldsymbol{Q}} \boldsymbol{\Upsilon}_n\right), \\ \mathcal{M}_{mn} &= -\partial_{z_k} \boldsymbol{\Upsilon}_m^\dagger \boldsymbol{F}_j^n Z_{jk}^{-1}. \end{aligned} \tag{36}$$

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 $\boldsymbol{A}$ 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 $V$ are null and then extend the result for non-null potentials.

PROPOSITION 2.1. *Assume that $V$ and $\boldsymbol{A}$ are null. Then $\mathcal{M}$ is diagonal.*

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

$$\begin{aligned} &\boldsymbol{P}(t) = \boldsymbol{p}, \qquad \boldsymbol{Q}(t) = \boldsymbol{q} + \frac{\boldsymbol{p}}{\sqrt{|\boldsymbol{p}|^2 + 1}} t, \\ &\partial_{\boldsymbol{z}} \boldsymbol{P} = -\mathrm{i} I, \qquad \partial_{\boldsymbol{z}} \boldsymbol{Q} = I - \mathrm{i}t \left(\frac{I}{\lambda^{1/2}} - \frac{\boldsymbol{p} \otimes \boldsymbol{p}}{\lambda^{3/2}}\right), \\ &Z = 2I - \mathrm{i}t \left(\frac{I}{\lambda^{1/2}} - \frac{\boldsymbol{p} \otimes \boldsymbol{p}}{\lambda^{3/2}}\right). \end{aligned}$$

Let us set $T = \frac{\mathrm{i}t}{2\lambda}\left(I - \frac{\boldsymbol{p}\otimes\boldsymbol{p}}{\lambda^2}\right)$. Then $Z^{-1} = \frac{1}{2}(I + T + T^2 + T^3 + \cdots)$. Notice now that

$$\left(I - \frac{\boldsymbol{p}\otimes\boldsymbol{p}}{\lambda^2}\right)^2 = I - 2\frac{\boldsymbol{p}\otimes\boldsymbol{p}}{\lambda^2} + |\boldsymbol{p}|^2\,\frac{\boldsymbol{p}\otimes\boldsymbol{p}}{\lambda^4}, = I - c\boldsymbol{p}\otimes\boldsymbol{p}$$
$$\left(I - \frac{\boldsymbol{p}\otimes\boldsymbol{p}}{\lambda^2}\right)^n = I - d\boldsymbol{p}\otimes\boldsymbol{p}.$$

Thus, we can see that there exists a $c$ such that

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

Since $\boldsymbol{\Upsilon}$ does not depend on $\boldsymbol{Q}$, $\partial_{\boldsymbol{z}}\boldsymbol{\Upsilon}^n = -\mathrm{i}\partial_{\boldsymbol{P}}\boldsymbol{\Upsilon}^n$. For $m \neq n$,

$$\mathcal{M}_{mn} = -\partial_{z_k}\boldsymbol{\Upsilon}_m^\dagger \boldsymbol{F}_j^n Z_{jk}^{-1} = -\partial_{\boldsymbol{z}}\boldsymbol{\Upsilon}_m^\dagger(\partial_{P_j}h - \hat{a}_j)\boldsymbol{\Upsilon}_n Z_{jk}^{-1}.$$

Consider the positive branch, and take $m = 1$, $n = 2$,

$$\mathcal{M}_{12} = \mathrm{Tr}(-\partial_{\boldsymbol{z}}\boldsymbol{\Upsilon}_1^\dagger(\partial_{\boldsymbol{P}}h - \hat{a})\boldsymbol{\Upsilon}_2 Z^{-1}),$$

and

$$\partial_{\boldsymbol{P}}\boldsymbol{\Upsilon}_1^\dagger = \frac{1}{r}\begin{pmatrix} 0 & 1 & P_1/\lambda & 0 \\ 0 & -\mathrm{i} & P_2/\lambda & 0 \\ 1 & 0 & P_3/\lambda & 0 \end{pmatrix} - \frac{1}{r}\partial_{\boldsymbol{P}}r \otimes \boldsymbol{\Upsilon}_1^\dagger, = \frac{1}{r}A - \frac{1}{r}\partial_{\boldsymbol{P}}r\otimes\boldsymbol{\Upsilon}_1^\dagger.$$

This leads to

$$\begin{aligned}
&\mathcal{M}_{12} \\
&\quad = -\mathrm{Tr}\left(\left(\frac{1}{r}A - \frac{1}{r}\partial_{\boldsymbol{P}}r\otimes\boldsymbol{\Upsilon}_1^\dagger\right)(\partial_{\boldsymbol{P}}h - \hat{a})\boldsymbol{\Upsilon}_2 Z^{-1}\right) \\
&\quad = -\mathrm{Tr}\left(\frac{1}{r}A(\partial_{\boldsymbol{P}}h - \hat{a})\boldsymbol{\Upsilon}_2 Z^{-1}\right) + \mathrm{Tr}\left(\frac{1}{r}\partial_{\boldsymbol{P}}r\otimes\boldsymbol{\Upsilon}_1^\dagger(\partial_{\boldsymbol{P}}h - \hat{a})\boldsymbol{\Upsilon}_2 Z^{-1}\right) \\
&\quad = -\frac{1}{r}\mathrm{Tr}\left(A(\partial_{\boldsymbol{P}}h - \hat{a})\boldsymbol{\Upsilon}_2 Z^{-1}\right) + \boldsymbol{0}, \\
&(A(\partial_{\boldsymbol{P}}h - \hat{a}))\sqrt{|\boldsymbol{P}|^2 + 1} \\
&\quad = \begin{pmatrix} 0 & -P_2 P_3 & P_2^2 - \sqrt{|\boldsymbol{P}|^2+1} + 1 \\ P_2 P_3 & 0 & -P_1 P_2 \\ \sqrt{|\boldsymbol{P}|^2+1} - P_2^2 - 1 & P_1 P_2 & 0 \end{pmatrix} \\
&\qquad + \mathrm{i}\begin{pmatrix} 0 & -P_1 P_3 & P_1 P_2 \\ P_1 P_3 & 0 & \sqrt{|\boldsymbol{P}|^2+1} - P_1^2 - 1 \\ -P_1 P_2 & P_1^2 - \sqrt{|\boldsymbol{P}|^2+1} + 1 & 0 \end{pmatrix}.
\end{aligned}$$

Thus, $\mathrm{Tr}\left(A(\partial_{\boldsymbol{P}}h - \hat{a})\boldsymbol{\Upsilon}_2\boldsymbol{p}\otimes\boldsymbol{p}\right) = 0$. Finally, we have $\mathcal{M}_{12} = \mathrm{Tr}\left(A(\partial_{\boldsymbol{P}}h - \hat{a})\boldsymbol{\Upsilon}_2 Z^{-1}\right) = 0$, which concludes the proof. ∎

We now consider the case when $\boldsymbol{A}$ is null.

PROPOSITION 2.2. *Assume that $\boldsymbol{A}$ is null. Then $\mathcal{M}$ is diagonal. In addition, $\mathcal{M}_{11} = \mathcal{M}_{22} = -\mathrm{Tr}(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{P}Re(A^{11}))$, where $\{A^{mn}_{jk}\} = \{\partial_{P_k}\boldsymbol{\Upsilon}^\dagger_m(\partial_{P_j}h - c\hat{a}_j)\boldsymbol{\Upsilon}_n\}_{jk}$ and, as $c \to \infty$, $\mathcal{M}_{11} \to \frac{1}{2}\mathrm{Tr}\partial_{\boldsymbol{z}}\boldsymbol{P}Z^{-1}$.*

*Proof.* We provide the proof for the "+" branch by mainly using direct computations. Similar arguments can be used for the "−" branch. When the vector potential $\boldsymbol{A}$ is null, since $\boldsymbol{\Upsilon}$ does not depend on $\boldsymbol{Q}$, $\partial_{\boldsymbol{z}}\boldsymbol{\Upsilon}_n = \partial_{\boldsymbol{z}}\boldsymbol{P}\cdot\partial_P\boldsymbol{\Upsilon}_n$. For $m \neq n$, $\mathcal{M}_{mn} = -\partial_{z_k}\boldsymbol{\Upsilon}^\dagger_m\boldsymbol{F}^n_j Z^{-1}_{jk} = -\partial_{z_k}\boldsymbol{\Upsilon}^\dagger_m(\partial_{P_j}h - c\hat{a}_j)\boldsymbol{\Upsilon}_n Z^{-1}_{jk} = -\mathrm{Tr}(\partial_{\boldsymbol{z}}\boldsymbol{P}\cdot\partial_{\boldsymbol{P}}\boldsymbol{\Upsilon}^\dagger_m(\partial_{\boldsymbol{P}}h - c\hat{a})\boldsymbol{\Upsilon}_n Z^{-1})$. Let $\lambda = \sqrt{c^2|\boldsymbol{P}|^2 + c^4}$ and $r = \sqrt{2(\lambda^2 - c^2\lambda)}$. Then we compute

$$
\begin{aligned}
&\partial_{\boldsymbol{P}}\boldsymbol{\Upsilon}^\dagger_1(\partial_{\boldsymbol{P}}h - c\hat{a})\boldsymbol{\Upsilon}_1\\
&\quad= \overline{\partial_{\boldsymbol{P}}\boldsymbol{\Upsilon}^\dagger_2(\partial_{\boldsymbol{P}}h - c\hat{a})\boldsymbol{\Upsilon}_2}\\
&\quad= -\frac{c^4}{2\lambda^3}\begin{pmatrix} P_2^2+P_3^2+c^2 & -P_1P_2 & -P_1P_3\\ -P_1P_2 & P_1^2+P_3^2+c^2 & -P_2P_3\\ -P_1P_3 & -P_2P_3 & P_1^2+P_2^2+c^2\end{pmatrix}\\
&\qquad+\mathrm{i}\frac{c^4}{r^2\lambda}\begin{pmatrix} 0 & c^2-\sqrt{|c\boldsymbol{P}|^2+c^4}+P_3^2 & -P_2P_3\\ \sqrt{|c\boldsymbol{P}|^2+c^4}-c^2-P_3^2 & 0 & P_1P_3\\ P_2P_3 & -P_1P_3 & 0\end{pmatrix}
\end{aligned}
\tag{37}
$$

and

$$
\begin{aligned}
&\partial_{\boldsymbol{P}}\boldsymbol{\Upsilon}^\dagger_1(\partial_{\boldsymbol{P}}h - c\hat{a})\boldsymbol{\Upsilon}_2\\
&\quad= -\partial_{\boldsymbol{P}}\boldsymbol{\Upsilon}^\dagger_2(\partial_{\boldsymbol{P}}h - c\hat{a})\boldsymbol{\Upsilon}_1\\
&\quad= \frac{c^4}{r^2\lambda}\begin{pmatrix} 0 & P_2P_3 & \sqrt{|c\boldsymbol{P}|^2+c^4}-c^2-P_2^2\\ -P_2P_3 & 0 & P_1P_2\\ c^2-\sqrt{|c\boldsymbol{P}|^2+c^4}+P_2^2 & -P_1P_2 & 0\end{pmatrix}\\
&\qquad+\mathrm{i}\frac{c^4}{r^2\lambda}\begin{pmatrix} 0 & P_1P_3 & -P_1P_2\\ -P_1P_3 & 0 & c^2-\sqrt{|c\boldsymbol{P}|^2+c^4}+P_1^2\\ P_1P_2 & \sqrt{|c\boldsymbol{P}|^2+c^4}-c^2-P_1^2 & 0\end{pmatrix}.
\end{aligned}
$$

Let $\{A^{mn}_{jk}\}$ be the matrix $\{\partial_{P_k}\boldsymbol{\Upsilon}^\dagger_m(\partial_{P_j}h - c\hat{a}_j)\boldsymbol{\Upsilon}_n\}_{jk}$. Then

$$
\mathcal{M}_{mn} = -(\partial_{z_k}P_l A^{mn}_{lj}Z^{-1}_{jk}) = -(Z^{-1}_{jk}\partial_{z_k}P_l A^{mn}_{lj}) = -\mathrm{Tr}(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{P}A^{mn}).
$$

It can be showed that, e.g.. as in [21], $Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{P}$ is symmetric. As the trace of the multiplication of a symmetric matrix and an antisymmetric matrix is zero, we can obtain

$$
\mathcal{M}_{mn} = -\,\mathrm{Tr}(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{P}A^{mn}) = 0, \quad \text{for } m \neq n \tag{38}
$$

$$
\mathcal{M}_{11} = -\,\mathrm{Tr}(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{P}\mathrm{Re}(A^{11})) = \mathcal{M}_{22}. \tag{39}
$$

Notice that when $c \to \infty$, a direct computation in (37) shows that $\mathrm{Re}(A^{11}) = -\frac{1}{2}I + O(P^2c^{-2})$, which implies that $\mathcal{M}_{11} \to \frac{1}{2}\mathrm{Tr}\partial_{\boldsymbol{z}}\boldsymbol{P}Z^{-1}$. This concludes the proof. ∎

We now consider the general situation.

Proposition 2.3. *Assume $\boldsymbol{A}$ is not null. Then $\mathcal{M}$ is in general not diagonal, except when $\boldsymbol{A}$ is only time-dependent.*

*Proof.* Let $\boldsymbol{U} = c\boldsymbol{P} - \boldsymbol{A}(\boldsymbol{Q})$ and $\lambda = \sqrt{c^2 \left|\boldsymbol{U}\right|^2 + c^4}$. Then from (29),

$$\begin{aligned}\boldsymbol{F}_j^n &= \big(c(\partial_{U_j}\lambda - \hat{\alpha}_j) + \mathrm{i}\partial_{Q_j}\boldsymbol{A}\cdot(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}})\big)\boldsymbol{\Upsilon}_n\\ &= \big(c(\partial_{U_j}\lambda - \hat{\alpha}_j) + \mathrm{i}\partial_{Q_j}A_l(\partial_{U_l}\lambda - \hat{\alpha}_l)\big)\boldsymbol{\Upsilon}_n,\end{aligned}$$

which brings

$$\begin{aligned}\mathcal{M}_{mn} &= -\partial_{z_k}\boldsymbol{\Upsilon}_m^\dagger \boldsymbol{F}_j^n Z_{jk}^{-1}\\ &= -\partial_{z_k}\boldsymbol{\Upsilon}_m^\dagger\left(c(\partial_{U_j}\lambda - \hat{\alpha}_j) + \mathrm{i}\partial_{Q_j}A_l(\partial_{U_l}\lambda - \hat{\alpha}_l)\right)\boldsymbol{\Upsilon}_n Z_{jk}^{-1}\\ &= -\partial_{z_k}U_\nu\,\partial_{U_\nu}\boldsymbol{\Upsilon}_m^\dagger\left(c(\partial_{U_j}\lambda - \hat{\alpha}_j) + \mathrm{i}\partial_{Q_j}A_l(\partial_{U_l}\lambda - \hat{\alpha}_l)\right)\boldsymbol{\Upsilon}_n Z_{jk}^{-1}\\ &= -(\partial_{z_k}P_\nu - \partial_{z_k}Q_\mu\,\partial_{Q_\mu}A_\nu)\,\partial_{U_\nu}\boldsymbol{\Upsilon}_m^\dagger\left(c(\partial_{U_j}\lambda - \hat{\alpha}_j) + \mathrm{i}\partial_{Q_j}A_l(\partial_{U_l}\lambda - \hat{\alpha}_l)\right)\boldsymbol{\Upsilon}_n Z_{jk}^{-1}\\ &= -\mathrm{Tr}\left[(\partial_{\boldsymbol{z}}\boldsymbol{P} - \partial_{\boldsymbol{z}}\boldsymbol{Q}\,\partial_{\boldsymbol{Q}}\boldsymbol{A})\,\partial_{\boldsymbol{U}}\boldsymbol{\Upsilon}_m^\dagger\,(c(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}) + \mathrm{i}\partial_{\boldsymbol{Q}}\boldsymbol{A}\cdot(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}))\,\boldsymbol{\Upsilon}_n Z^{-1}\right]\\ &= -\mathrm{Tr}\left[Z^{-1}(\partial_{\boldsymbol{z}}\boldsymbol{P} - \partial_{\boldsymbol{z}}\boldsymbol{Q}\,\partial_{\boldsymbol{Q}}\boldsymbol{A})\,\partial_{\boldsymbol{U}}\boldsymbol{\Upsilon}_m^\dagger\,(c(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}) + \mathrm{i}\partial_{\boldsymbol{Q}}\boldsymbol{A}\cdot(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}))\,\boldsymbol{\Upsilon}_n\right].\end{aligned}$$

Since $Z = \partial_{\boldsymbol{z}}(\boldsymbol{Q} + \mathrm{i}\boldsymbol{P})$,

$$\begin{aligned}&\mathcal{M}_{mn}\\ &= \mathrm{Tr}\left[\left(\mathrm{i}cZ^{-1}(Z - \partial_{\boldsymbol{z}}\boldsymbol{Q}) + Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{Q}\,\partial_{\boldsymbol{Q}}\boldsymbol{A}\right)\,\partial_{\boldsymbol{U}}\boldsymbol{\Upsilon}_m^\dagger\,(c(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}) + \mathrm{i}\partial_{\boldsymbol{Q}}\boldsymbol{A}\cdot(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}))\,\boldsymbol{\Upsilon}_n\right]\\ &= \mathrm{Tr}\left[\left(\mathrm{i}c(\mathbb{I}_3 - Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{Q}) + Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{Q}\,\partial_{\boldsymbol{Q}}\boldsymbol{A}\right)\,\partial_{\boldsymbol{U}}\boldsymbol{\Upsilon}_m^\dagger\,(c(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}) + \mathrm{i}\partial_{\boldsymbol{Q}}\boldsymbol{A}\cdot(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}))\,\boldsymbol{\Upsilon}_n\right]\\ &= \mathrm{Tr}\left[\mathrm{i}c\,\partial_{\boldsymbol{U}}\boldsymbol{\Upsilon}_m^\dagger\,(c(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}) + \mathrm{i}\partial_{\boldsymbol{Q}}\boldsymbol{A}\cdot(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}))\,\boldsymbol{\Upsilon}_n\right]\\ &\quad - \mathrm{Tr}\left[\left(\mathrm{i}cZ^{-1}\partial_{\boldsymbol{z}}\boldsymbol{Q} - Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{Q}\,\partial_{\boldsymbol{Q}}\boldsymbol{A})\right)\partial_{\boldsymbol{U}}\boldsymbol{\Upsilon}_m^\dagger\,(c(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}) + \mathrm{i}\partial_{\boldsymbol{Q}}\boldsymbol{A}\cdot(\partial_{\boldsymbol{U}}\lambda - \hat{\boldsymbol{\alpha}}))\,\boldsymbol{\Upsilon}_n\right],\end{aligned}$$

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 semiclassical regime. It is known (e.g., [7]) that as the speed of light $c \to \infty$, the Dirac equation is convergent to a Schrödinger equation. On the other hand, as the semiclassical parameter $\varepsilon \to 0$, the Dirac and the Schrödinger equations have their FGA, respectively. The purpose of this section is to prove that due to the linearity of this equation, we can derive the FGA for the Schrödinger equation in the semiclassical and nonrelativistic regime from the FGA for the Dirac equation. In other words, we show the commutativity of the formal diagram Figure 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 $\boldsymbol{A}$ but subject to an external space-dependent potential.

We now state one of the main results 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.*

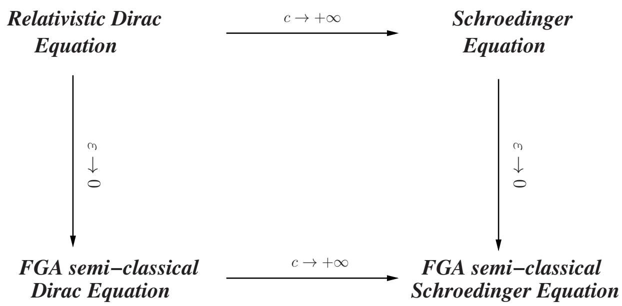



Fig. 1. *Commutation scheme: FGA for Schrödinger from* (1) *semiclassical limit of the nonrelativistic Dirac equation and from* (2) *relativistic limit of the semiclassical limit of the Dirac equation.*

In the remainder of this section, we first review the nonrelativistic limit of the Dirac equation and the FGA for the Schrödinger equation. We then prove Theorem (3.1), and we finally provide some discussion about the FGA in the nonrelativistic regime.

**3.1. Nonrelativistic limit of the Dirac equation.** By setting the vector potential $\boldsymbol{A} \equiv \mathbf{0}$, the Dirac equation reads

$$\mathrm{i}\varepsilon\partial_t\boldsymbol{\psi}^\varepsilon = \left(-\mathrm{i}c\varepsilon\hat{\boldsymbol{\alpha}}\cdot\nabla + \beta c^2 + V\right)\boldsymbol{\psi}^\varepsilon.$$

Here, we fix $\varepsilon$ and let $c \gg 1$. As in, e.g., [7] the derivation of the nonrelativistic limit relies on the reformulation of the Dirac 4-spinor in two 2-spinors. Precisely, for $\boldsymbol{\psi}^\varepsilon = (\psi_1,\psi_2,\psi_3,\psi_4)^T$, we introduce the "upper-large" spinor, $\boldsymbol{\psi}_l = \mathrm{e}^{\mathrm{i}c^2t}(\psi_1,\psi_2)^T$, and the "lower-small" spinor, $\boldsymbol{\psi}_s = \mathrm{e}^{-\mathrm{i}c^2t}(\psi_3,\psi_4)^T$. Notice that two energy shifts $\mathrm{e}^{\mathrm{i}c^2t}$ and $\mathrm{e}^{-\mathrm{i}c^2t}$ are applied in the two 2-spinors, respectively. Substitute $\boldsymbol{\psi}_l$ and $\boldsymbol{\psi}_s$ back to the Dirac equation, and then one obtains equations

$$\mathrm{i}\varepsilon\partial_t\boldsymbol{\psi}_l = -\mathrm{i}c\varepsilon\sigma_k\partial_k\boldsymbol{\psi}_s + V\boldsymbol{\psi}_l \tag{40}$$

$$\mathrm{i}\varepsilon\partial_t\boldsymbol{\psi}_s = -\mathrm{i}c\varepsilon\sigma_k\partial_k\boldsymbol{\psi}_l + V\boldsymbol{\psi}_s - 2c^2\boldsymbol{\psi}_s. \tag{41}$$

From (41), by formal consideration of orders of magnitude, one obtains

$$\boldsymbol{\psi}_s = -\frac{\mathrm{i}}{2c}\varepsilon\sigma_k\partial_k\boldsymbol{\psi}_l + O(c^{-2}),$$

and then by using this in (40), one obtains

$$\mathrm{i}\varepsilon\partial_t\boldsymbol{\psi}_l = -\frac{\varepsilon^2}{2}\sigma_j\sigma_k\partial_j\partial_k\boldsymbol{\psi}_l + V\boldsymbol{\psi}_l = -\frac{\varepsilon^2}{2}\Delta\boldsymbol{\psi}_l + V\boldsymbol{\psi}_l, \tag{42}$$

which is a Schrödinger equation.

**3.2. FGA for the Schrödinger equation.** For the Schrödinger equation, the FGA has been derived and studied in the literature (e.g., [22, 38]), and below we briefly review its formulation. We consider the Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V\psi^\varepsilon \tag{43}$$

in the semiclassical regime ($0 < \varepsilon \ll 1$). The FGA for the Schrödinger equation takes the form of

$$\psi^\varepsilon_{\mathrm{FGA}}(t,\boldsymbol{x}) = \frac{1}{(2\pi\varepsilon)^{9/2}}\int_{\mathbb{R}^9} a\left(t,\boldsymbol{q},\boldsymbol{p}\right)\exp\left(\frac{\mathrm{i}}{\varepsilon}\Phi\left(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}\right)\right)\psi^\varepsilon_I(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}, \tag{44}$$

where

$$\begin{aligned}\Phi &= S\left(t,\boldsymbol{q},\boldsymbol{p}\right) + \frac{\mathrm{i}}{2}\left|\boldsymbol{x}-\boldsymbol{Q}\left(t,\boldsymbol{q},\boldsymbol{p}\right)\right|^2 + \boldsymbol{P}\left(t,\boldsymbol{q},\boldsymbol{p}\right)\cdot\left(\boldsymbol{x}-\boldsymbol{Q}\left(t,\boldsymbol{q},\boldsymbol{p}\right)\right)\\ &\quad + \frac{\mathrm{i}}{2}\left|\boldsymbol{y}-\boldsymbol{q}\right|^2 - \boldsymbol{p}\cdot(\boldsymbol{y}-\boldsymbol{q}).\end{aligned} \tag{45}$$

The evolution equations for the bi-center $\boldsymbol{Q}$ and $\boldsymbol{P}$, action $S$, and FGA amplitude $a$ are

$$\begin{cases}\dfrac{\mathrm{d}\boldsymbol{Q}}{\mathrm{d}t} = \boldsymbol{P}, & \boldsymbol{Q}(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{q},\\ \dfrac{\mathrm{d}\boldsymbol{P}}{\mathrm{d}t} = -\partial_{\boldsymbol{Q}}V(\boldsymbol{Q}), & \boldsymbol{P}(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{p},\\ \dfrac{\mathrm{d}S}{\mathrm{d}t} = \dfrac{|\boldsymbol{P}|^2}{2} - V(\boldsymbol{Q}), & S(0,\boldsymbol{q},\boldsymbol{p}) = 0,\\ \dfrac{\mathrm{d}a}{\mathrm{d}t} = \dfrac{\mathrm{i}}{2}a\mathrm{Tr}\left(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{Q}\partial^2_{\boldsymbol{Q}}V\right) + \dfrac{a}{2}\mathrm{Tr}(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{P}), & a(0,\boldsymbol{q},\boldsymbol{p}) = 2^{d/2}.\end{cases} \tag{46}$$

**3.3. Nonrelativistic limit of the FGA for the Dirac equation.** We plan to derive a FGA for the Schrödinger equation by taking the nonrelativistic limit, i.e., with $c \to +\infty$, of the FGA for the Dirac equation. We will use the $\sim$-notation for the FGA in the nonrelativistic limit.

*Proof of Theorem* 3.1. First, for $c$ large

$$\begin{cases}\partial_{\boldsymbol{P}}h(\boldsymbol{Q},\boldsymbol{P}) = \boldsymbol{P}\dfrac{1}{\sqrt{1+P^2/c^2}} = \boldsymbol{P}\Big(1-\dfrac{P^2}{2c^2}+\mathcal{O}\big(P^4c^{-4}\big)\Big),\\ \partial_{\boldsymbol{Q}}h(\boldsymbol{Q},\boldsymbol{P}) = \partial_{\boldsymbol{Q}}V(\boldsymbol{Q}),\end{cases} \tag{47}$$

where $P := \|\boldsymbol{P}\|_2$. Then by keeping the leading-order terms in (47), we define the Gaussian profiles and momentum centers as solutions to the following Hamiltonian flow in the semiclassical and nonrelativistic limits:

$$\begin{cases}\dfrac{d\widetilde{\boldsymbol{Q}}}{dt} = \widetilde{\boldsymbol{P}}, & \widetilde{\boldsymbol{Q}}(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{q},\\ \dfrac{d\widetilde{\boldsymbol{P}}}{dt} = -\partial_{\boldsymbol{Q}}V(\widetilde{\boldsymbol{Q}}), & \widetilde{\boldsymbol{P}}(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{p}.\end{cases} \tag{48}$$

Next, the evolution of the action function

$$\partial_t S(t,\boldsymbol{Q},\boldsymbol{P}) = \boldsymbol{P}\cdot\partial_t\boldsymbol{Q} - h(\boldsymbol{Q},\boldsymbol{P})$$

can be rewritten in the nonrelativistic limit as follows:

$$\partial_t S(t,\boldsymbol{Q},\boldsymbol{P}) = \frac{P^2}{2} - V(\boldsymbol{Q}) - c^2 + \mathcal{O}\big(P^4 c^{-2}\big),$$

where we have used (47) and that

$$h_\pm(\boldsymbol{Q},\boldsymbol{P}) = \pm c^2\sqrt{1+\frac{P^2}{c^2}} + V(\boldsymbol{Q}) = \pm\frac{P^2}{2} + V(\boldsymbol{Q}) \pm c^2 + \mathcal{O}\big(c^{-2}P^4\big)\,.$$

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

$$\partial_t \widetilde{S}(t,\widetilde{\boldsymbol{Q}},\widetilde{\boldsymbol{P}}) = c^2 + \frac{\widetilde{P}^2}{2} - V(\widetilde{\boldsymbol{Q}})\,. \tag{49}$$

We now focus on the evolution equation for the amplitude, which requires a bit more careful analysis. Recall the amplitude equation (35). We can obtain

$$\frac{\mathrm{d}a_m}{\mathrm{d}t}\boldsymbol{\Upsilon}_m = \left(\mathcal{L}_{mn} + \mathcal{M}_{mn} + \mathcal{N}_{mn}\right) a_n \boldsymbol{\Upsilon}_m\,, \tag{50}$$

where Einstein's summation convention has been used. We then look at the three terms on the right-hand side of the above equation, respectively. When $\boldsymbol{A}\equiv\boldsymbol{0}$, from (36) and Proposition 2.2, we obtain

$$\begin{aligned}
\mathcal{L}_{mn} &= \frac{\mathrm{i}}{2}\boldsymbol{\Upsilon}_m^\dagger\partial_{z_k}Q_l\,\partial_{Q_l}\partial_{Q_j}B\,Z_{jk}^{-1}\boldsymbol{\Upsilon}_n = \frac{\mathrm{i}}{2}\boldsymbol{\Upsilon}_m^\dagger\partial_{z_k}Q_l\,\partial_{Q_l}\partial_{Q_j}V\,Z_{jk}^{-1}\boldsymbol{\Upsilon}_n\\
&= \frac{\mathrm{i}}{2}\delta_{mn}\partial_{z_k}Q_l\,\partial_{Q_l}\partial_{Q_j}V\,Z_{jk}^{-1} = \frac{\mathrm{i}}{2}\delta_{mn}\mathrm{Tr}\left(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{Q}\partial_{\boldsymbol{Q}}^2 V\right),\\
\mathcal{N}_{mn} &= \boldsymbol{\Upsilon}_m^\dagger\left(\partial_{\boldsymbol{Q}}h\cdot\partial_{\boldsymbol{P}}\boldsymbol{\Upsilon}_n - \partial_{\boldsymbol{P}}h\cdot\partial_{\boldsymbol{Q}}\boldsymbol{\Upsilon}_n\right) = \boldsymbol{\Upsilon}_m^\dagger\left(-\frac{\mathrm{d}\boldsymbol{P}}{\mathrm{d}t}\cdot\partial_{\boldsymbol{P}}\boldsymbol{\Upsilon}_n - \frac{\mathrm{d}\boldsymbol{Q}}{\mathrm{d}t}\cdot\partial_{\boldsymbol{Q}}\boldsymbol{\Upsilon}_n\right)\\
&= -\boldsymbol{\Upsilon}_m^\dagger\frac{\mathrm{d}\boldsymbol{\Upsilon}_n}{\mathrm{d}t},\\
\mathcal{M}_{mn} &= -\partial_{z_k}\boldsymbol{\Upsilon}_m^\dagger\boldsymbol{F}_j^n Z_{jk}^{-1} = \delta_{mn}\frac{1}{2}\mathrm{Tr}(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{P}) + O(P^2c^{-2}).
\end{aligned}$$

Substitute the above into (50) and obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}(a_m\boldsymbol{\Upsilon}_m) = \left(\frac{\mathrm{i}}{2}\mathrm{Tr}\left(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{Q}\partial_{\boldsymbol{Q}}^2V\right) + \frac{1}{2}\mathrm{Tr}(Z^{-1}\partial_{\boldsymbol{z}}\boldsymbol{P})\right)a_m\boldsymbol{\Upsilon}_m + O(P^2c^{-2}).$$

Thus, in the nonrelativistic limit the amplitude vector $\tilde{\boldsymbol{a}}$ satisfies

$$\frac{\mathrm{d}\tilde{\boldsymbol{a}}}{\mathrm{d}t} = \left(\frac{\mathrm{i}}{2}\mathrm{Tr}\left(Z^{-1}\partial_{\boldsymbol{z}}\tilde{\boldsymbol{Q}}\partial_{\boldsymbol{Q}}^2V\right) + \frac{1}{2}\mathrm{Tr}(Z^{-1}\partial_{\boldsymbol{z}}\tilde{\boldsymbol{P}})\right)\tilde{\boldsymbol{a}}. \tag{51}$$ ∎

*Remark* 3.1. In a bounded domain $\Omega_\varepsilon$, nonreflecting conditions are trivially established for the Dirac equation in both relativistic and nonrelativistic regimes. Whenever $\boldsymbol{Q}(t)\notin\Omega_\varepsilon$, the contribution of this Gaussian function is simply removed from the reconstruction of $\boldsymbol{\psi}^\varepsilon$; see [38] for details in the case of the Schrödinger equation.

**3.4. 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 $\boldsymbol{A}(\boldsymbol{Q}) = \boldsymbol{0}$ and $V(\boldsymbol{Q}) = 0$. We set $\boldsymbol{\psi}^\varepsilon = \big(\boldsymbol{\phi}^\varepsilon, \boldsymbol{\chi}^\varepsilon\big)^T$, which satisfies

$$\left\{\begin{array}{l} \mathrm{i}\varepsilon\partial_t\boldsymbol{\phi}^\varepsilon = -\mathrm{i}c\varepsilon\boldsymbol{\sigma}\cdot\boldsymbol{p}\boldsymbol{\chi}^\varepsilon + \beta mc^2\boldsymbol{\phi}^\varepsilon, \\ \mathrm{i}\varepsilon\partial_t\boldsymbol{\chi}^\varepsilon = -\mathrm{i}c\varepsilon\boldsymbol{\sigma}\cdot\boldsymbol{p}\boldsymbol{\phi}^\varepsilon + \beta mc^2\boldsymbol{\chi}^\varepsilon . \end{array}\right.$$

As $V$ is null, $\boldsymbol{\phi}^\varepsilon$ (as well as $\boldsymbol{\chi}^\varepsilon$) naturally satisfies the Klein–Gordon equation:

$$\varepsilon^2\partial_t^2\boldsymbol{\phi}^\varepsilon = \big(c^2\varepsilon^2\triangle + m^2c^4\mathbb{I}_2\big)\boldsymbol{\phi}^\varepsilon .$$

Using a similar elimation 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, or it can be deduced from the one for the potential-free Dirac equation.

We now set $\boldsymbol{a}_m = (\boldsymbol{a}_m^{(1)}, \boldsymbol{a}_m^{(2)})^T$ with $\boldsymbol{a}_m^{(1,2)} = a_m\boldsymbol{\Upsilon}_m^{(1,2)}$ and $\boldsymbol{\Upsilon}_m = (\boldsymbol{\Upsilon}_m^{(1)}, \boldsymbol{\Upsilon}_m^{(2)})^T$. Under the above assumptions, the matrix $\mathcal{M}$ simply reads for $(m,n) \in \{1,2\}^2$

$$\mathcal{M}_{mn} = -\partial_{z_k}\boldsymbol{\Upsilon}_m^\dagger\big(\partial_{P_j}h(\boldsymbol{Q},\boldsymbol{P})\, .$$

The amplitude equation, as for the Dirac equation, then reads

$$\frac{da_n}{dt} = \widetilde{\mathcal{M}}a_n,$$

where we have set $\widetilde{\mathcal{M}} = \mathcal{M}_{11} = \mathcal{M}_{22} = \mathrm{tr}\big[\partial_{\boldsymbol{z}}\boldsymbol{\Upsilon}_n^\dagger\big(\partial_{\boldsymbol{P}}h - \hat{\alpha}\big)\boldsymbol{\Upsilon}_n\boldsymbol{Z}^{-1}\big]$. Considering again the positive branch

$$\frac{d}{dt}\big(a_1\boldsymbol{\Upsilon}_1 + a_2\boldsymbol{\Upsilon}_2\big) = \widetilde{\mathcal{M}}\big(a_1\boldsymbol{\Upsilon}_1 + a_2\boldsymbol{\Upsilon}_2),$$

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, $\mathcal{M}$ tends to $\mathrm{tr}[\partial_{\boldsymbol{z}}\boldsymbol{P}\boldsymbol{Z}^{-1}]/2$, 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.

**3.5. Mathematical properties in nonrelativistic regime.** We present some mathematical properties of the FGA in the nonrelativistic regime. We recall [34] 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 $\boldsymbol{x} = \boldsymbol{0}$, the Dirac operator is self-adjoint on $C_0^\infty(\mathbb{R}^3 - \{\boldsymbol{0}\};\mathbb{C}^4)$. It is also well known that the Dirac operator is a unitary operator.

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

$$\begin{aligned} \|\boldsymbol{\psi}_I^\varepsilon\|_2^2 &:= \sum_{j=1}^4\int_{\mathbb{R}^3}|\boldsymbol{\psi}_j^\varepsilon(0,\boldsymbol{x})|^2d\boldsymbol{x} \\ &= \sum_{m=1}^4\int_{\mathbb{R}^6}\Big|\boldsymbol{a}_m(0,\boldsymbol{q},\boldsymbol{p})\boldsymbol{\Upsilon}_m(\boldsymbol{q},\boldsymbol{p})\cdot\mathcal{F}^\varepsilon\boldsymbol{\psi}_I^\varepsilon(\boldsymbol{q},\boldsymbol{p})\Big|^2\mathrm{d}\boldsymbol{q}\mathrm{d}\boldsymbol{p} \\ &= \sum_{j=1}^4\int_{\mathbb{R}^3}|\omega_{I,j}(\boldsymbol{x})|^2d\boldsymbol{x} + \mathcal{O}(\varepsilon) = 1. \end{aligned}$$

The $\mathcal{O}(\varepsilon)$-term is coming from the first-order term in (2.5). This can be expressed as well as

$$\|\mathcal{D}^{\varepsilon}_{0,1,\delta}\boldsymbol{\psi}^{\varepsilon}_I\|_{L^2(\mathbb{R}^3;\mathbb{C}^4)} = \|\mathcal{F}^{\varepsilon} * (\chi_{\delta}\mathcal{F}^{\varepsilon}\boldsymbol{\psi}^{\varepsilon}_I)\|_{L^2(\mathbb{R}^3;\mathbb{C}^4)},$$

where $\mathcal{F}^{\varepsilon}$ is the FBI transform (which is a $L^2(\mathbb{R}^3)$-unitary operator) for some smooth cutoff function $\chi_{\delta}$ defined in [27] and $\mathcal{D}^{\varepsilon}_{0,1}$ is the FGA at order 1 and time $t = 0$. Next,

$$\|\boldsymbol{\psi}^{\varepsilon}(t,\cdot)\|_2^2 = \frac{1}{(2\pi\varepsilon)^9}\sum_m \int_{\mathbb{R}^3}\Big|\int_{\mathbb{R}^9} \boldsymbol{a}_m(t,\boldsymbol{p},\boldsymbol{q})v_m(\boldsymbol{y})e^{\mathrm{i}\Phi_m(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{p},\boldsymbol{q})/\varepsilon}\mathrm{d}\boldsymbol{y}\mathrm{d}\boldsymbol{q}\mathrm{d}\boldsymbol{p}\Big|^2\mathrm{d}\boldsymbol{x}\,.$$

Recall that $v_m(\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{\Upsilon}_m(\boldsymbol{q},\boldsymbol{p})\cdot\boldsymbol{\psi}^{\varepsilon}_I(\boldsymbol{y})$. Now [27], as $\|\mathcal{F}^{\varepsilon}f\|_{L^2(\mathbb{R}^6;\mathbb{C}^4)} = \|f\|_{L^2(\mathbb{R}^3;\mathbb{C}^4)}$, we get

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

Notice that it is proven (in a more general form) in [27] that denoting $\mathcal{H}_t$ (resp., $\mathcal{H}^{\varepsilon}_{t,1}$) a *strictly* hyperbolic (resp., corresponding FGA at order 1) propagator, the following estimate holds for any $T > 0$ and $m = 0$:

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

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

We next discuss the numerical dispersion issues, referred in the physics literature as Fermion doubling, which is responsible for the generation of spurious states [16]. Recall that the dispersion relation for the Dirac equation reads $E_{\boldsymbol{k}} = \pm c^2 p^2_{\boldsymbol{k}} + c^4$ ($m$ 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* $\boldsymbol{A}$ *and* $V$ *are null. The nonrelativistic FGA for Dirac is nondispersive up to a* $O(c^{-2})$.

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

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

The action function reads

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

and

$$\begin{aligned}\boldsymbol{P}_m\cdot\big(\boldsymbol{x}-\boldsymbol{Q}_m(t,\boldsymbol{q},\boldsymbol{p})\big) &= \boldsymbol{p}_m\cdot\big(\boldsymbol{x}-\boldsymbol{q}_m \mp t\frac{\boldsymbol{p}_m}{\sqrt{1+p^2/c^2}}\big)\\ &= \boldsymbol{P}_m\cdot\big(\boldsymbol{x}-\boldsymbol{Q}_m(0,\boldsymbol{q},\boldsymbol{p})\big) \mp t\frac{p_m^2}{\sqrt{1+p^2/c^2}}\,.\end{aligned}$$

That is, for $c$ large

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

Recall that (3.19) degenerates into $d\boldsymbol{a}/dt = \mathcal{M}\boldsymbol{a}$ with

$$\mathcal{M}_{nn} = -\partial_{z_k}\boldsymbol{\Upsilon}_n^\dagger \boldsymbol{F}_j^n Z_{jk}^{-1}$$

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

$$\begin{aligned} Z_{jk} &= \big(\partial_{q_j} - \mathrm{i}\partial_{p_j}\big)\big(Q_k + \mathrm{i}P_k\big) \\ &= 2\delta_{jk} \pm \mathrm{i}\left(\frac{p_j p_k c^4}{\big(p^2c^2 + c^4\big)^{3/2}} - \frac{c^2\delta_{jk}}{\sqrt{p^2c^2+c^4}}\right)t \\ &= 2\delta_{jk} \mp \mathrm{i}\frac{c^2\delta_{jk}}{\sqrt{p^2c^2+c^4}}t + \mathcal{O}(c^{-2}) . \end{aligned}$$

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

$$\frac{d\widetilde{a}_n}{dt} = \frac{1}{2}\partial_{z_k}\widetilde{\boldsymbol{P}}_j Z_{jk}^{-1}\widetilde{a}_n = \frac{3}{2(t+2\mathrm{i})}\widetilde{a}_n$$

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

$$\begin{aligned} \mathrm{Arg}\Big(\boldsymbol{a}(t,\boldsymbol{q},\boldsymbol{p})\exp\Big(\frac{\mathrm{i}}{\varepsilon}\Phi_m(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})\Big)\Big) &= \mathrm{Arg}\Big((2\mathrm{i}+t)^{3/2}\exp\Big(\frac{\mathrm{i}}{\varepsilon}\Phi_m(0,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})\Big)\Big) \\ &\quad \mp p_m^2c^2t + \mathcal{O}(p_m^2c^{-2}t) . \end{aligned}$$

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

## 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 [27] for strictly hyperbolic systems, while since the Dirac equation is not strictly hyperbolic for $d > 1$ and is not homogeneous, the same proof in [27] cannot directly apply to the Dirac equation. However, following the same type of arguments in [27], one may conjecture that the error estimate remains valid.

CONJECTURE 4.1. *Assume that $\boldsymbol{\psi}_I \in L^2(\mathbb{R}^d)$. We get the error estimate for the order-K FGA,*

$$\max_{0\le t\le T}\|\mathcal{H}_t\boldsymbol{\psi}_I^\varepsilon - \mathcal{H}_{t,1,\delta}^\varepsilon\boldsymbol{\psi}_I^\varepsilon\|_{L^2(\mathbb{R}^3;\mathbb{C}^4)} \le C_{T,K}\|\boldsymbol{\psi}_I\|\varepsilon^K,$$

*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 [27], 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/and $\varepsilon$ 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 ($\widehat{\beta}mc^2$) gives rise to the so-called *zitterbewegung* 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 the presence of an external electromagnetic field. The eigenvalues are of the form $\lambda(\boldsymbol{q},\boldsymbol{p}) = \pm c\sqrt{\left|\boldsymbol{p}-\boldsymbol{A}(\boldsymbol{q})/c\right|^2 + c^2}$. We consider three cases, $c\varepsilon \ll 1$, $c\varepsilon = \mathcal{O}(1)$, and $c\varepsilon \gg 1$. Initially the FGA was derived in the $(t,\boldsymbol{x})$-variable from the Dirac equation by introducing the $(t',\boldsymbol{x}')$-variables and by setting $t' = t\varepsilon$ and $\boldsymbol{x}' = \varepsilon\boldsymbol{x}$. Basically, the FGA as derived above is accurate if $c\varepsilon \ll 1$. In particular, the scaling $\boldsymbol{x}' = \varepsilon\boldsymbol{x}$ makes sense if the initial state and 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 $c\widehat{\boldsymbol{\alpha}}\cdot(\boldsymbol{x}-\boldsymbol{Q})/\varepsilon$ behaves as $\varepsilon^{-a}$ and is same order or dominant against the other $\varepsilon^{-1}$ term, and $\widehat{\beta}_0 c^2$ 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:

$$
(52)\quad \begin{cases} \dfrac{d\boldsymbol{Q}}{dt} = \pm\dfrac{\big(\boldsymbol{P}-\boldsymbol{A}(\boldsymbol{Q})/c\big)}{\sqrt{1+|\boldsymbol{P}-\boldsymbol{A}(\boldsymbol{Q})/c|^2}}, & \boldsymbol{Q}(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{q},\\[2mm] \dfrac{d\boldsymbol{P}}{dt} = -\partial_{\boldsymbol{Q}}V(\boldsymbol{Q}) \mp \dfrac{\big(P_l(\boldsymbol{Q})-A_l(\boldsymbol{Q})/c\big)\partial_{\boldsymbol{Q}}A_l(\boldsymbol{Q})}{\sqrt{1+|\boldsymbol{P}-\boldsymbol{A}(\boldsymbol{Q})/c|^2}}, & \boldsymbol{P}(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{p}. \end{cases}
$$

Next, the action function reads

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

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

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

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

$$
\begin{aligned}
\Psi_m(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}) &= \mathcal{S}(t,\boldsymbol{q},\boldsymbol{p}) + \frac{\mathrm{i}}{2}|\boldsymbol{x}-\boldsymbol{Q}_m(t,\boldsymbol{q},\boldsymbol{p})|^2 + \boldsymbol{P}_m\cdot\big(\boldsymbol{x}-\boldsymbol{Q}_m(t,\boldsymbol{q},\boldsymbol{p})\big)\\
&\quad + \frac{\mathrm{i}}{2}|\boldsymbol{y}-\boldsymbol{q}|^2 - \boldsymbol{p}\cdot(\boldsymbol{y}-\boldsymbol{q}),\\
\Phi_m(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}) &= \Psi_m(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}) + c^2 t\,.
\end{aligned}
$$

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 (52), we have deduced that the computation of

$\boldsymbol{Q}$ and $\boldsymbol{P}$ 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 $\mathcal{L}$

$$\mathcal{L}_{mn} = \frac{\mathrm{i}}{2}\boldsymbol{\Upsilon}_m^\dagger \partial_{z_k} Q_l \partial_{Q_l} \partial_{Q_j} B Z_{jk}^{-1} \boldsymbol{\Upsilon}_n,$$

where $B = -\widehat{\boldsymbol{\alpha}} \cdot \boldsymbol{A} + c^2\widehat{\beta}_0 + V\mathbb{I}_4$. As the mass term $c^2\widehat{\beta}_0$ is an order 0 operator, the computation of $\partial^2_{\boldsymbol{Q}} B(\boldsymbol{Q})$ is also free from $c^2$-constraints. The same conclusion holds for $\mathcal{N}$. Regarding $\mathcal{M}$, the main term to study is $\boldsymbol{F}_j^n$, which is the sum of several terms including $c\widehat{\alpha}_j$, while the other terms are $\mathcal{O}(1)$ in $c$. However,

$$\partial_{z_k} \boldsymbol{\Upsilon}_m = \partial_{z_k} Q_j \partial_{Q_j} \boldsymbol{\Upsilon}_m + \partial_{z_k} P_j \partial_{P_j} \boldsymbol{\Upsilon}_m$$

and

$$\boldsymbol{F}_j^n = \Big(\frac{P_j - A_j(\boldsymbol{Q})/c}{\sqrt{1 + |\boldsymbol{P} - \boldsymbol{A}(\boldsymbol{Q})/c|^2}} - c\widehat{\alpha}_j\Big)\boldsymbol{\Upsilon}_n\,.$$

The conclusion is that the main multiscale constraint is in the reconstruction of the phase of the FGA:

$$\boldsymbol{\psi}^\varepsilon(t,\cdot) = \frac{e^{\mathrm{i}c^2 t/\varepsilon}}{(2\pi\varepsilon)^9}\sum_m \int_{\mathbb{R}^3}\int_{\mathbb{R}^9} \boldsymbol{a}_m(t,\boldsymbol{p},\boldsymbol{q}) v_m(\boldsymbol{y}) e^{\mathrm{i}\Psi_m(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{p},\boldsymbol{q})/\varepsilon} \mathrm{d}\boldsymbol{y}\mathrm{d}\boldsymbol{q}\mathrm{d}\boldsymbol{p}\mathrm{d}\boldsymbol{x}\,.$$

This highly oscillating phase does not impose any restriction on the computation of the amplitude $a$, the shifted phase $\mathcal{S}$, or the Hamiltonian flow. In this first case, the FGA is kept unaltered.

*Case* 2. $\varepsilon = \mathcal{O}(c^{-2})$. In this case, the $\widehat{\beta}_0 c^2$-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

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

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

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

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

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

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

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

$$\boldsymbol{F}_j^n = \big(\partial_{P_j} h(\boldsymbol{Q},\boldsymbol{P}) - \mathrm{i}\partial_{Q_j} h(\boldsymbol{Q},\boldsymbol{P}) + \mathrm{i}\partial_{Q_j} B(\boldsymbol{Q})\big)\boldsymbol{\Upsilon}_n,$$

then from the evolution equation for $\boldsymbol{a}$. Now $\widehat{\alpha}_j \boldsymbol{\Upsilon}_n = \partial_{P_j} h \boldsymbol{\Upsilon}_n$, so that

$$\begin{aligned} -\partial_{z_k}\left(\widehat{\alpha}_j Z_{jk}^{-1}\boldsymbol{a}v\right) &= -\partial_{z_k}\left(\partial_{P_j} h Z_{jk}^{-1}\boldsymbol{a}v\right) \\ &= -\partial_{z_k}\left(\partial_{P_j} h Z_{jk}^{-1} a_1 \boldsymbol{\Upsilon}_1 v\right) - \partial_{z_k}\left(\partial_{P_j} h Z_{jk}^{-1} a_2 \boldsymbol{\Upsilon}_2 v\right), \end{aligned}$$

and from (3.16)

$$-\partial_{z_k}\left(\partial_{P_j} h Z_{jk}^{-1} a_1 \boldsymbol{\Upsilon}_1 v\right) = -\boldsymbol{\Upsilon}_2 \partial_{z_k} \boldsymbol{\Upsilon}_2^\dagger \partial_{P_j} h Z_{jk}^{-1} a_1 \boldsymbol{\Upsilon}_1 v,$$

$$-\partial_{z_k}\left(\partial_{P_j} h Z_{jk}^{-1} a_2 \boldsymbol{\Upsilon}_2 v\right) = -\boldsymbol{\Upsilon}_1 \partial_{z_k} \boldsymbol{\Upsilon}_1^\dagger \partial_{P_j} h Z_{jk}^{-1} a_2 \boldsymbol{\Upsilon}_2 v\,.$$

Then the action function equation still reads, as $\boldsymbol{\Upsilon}_{2,1}^\dagger \boldsymbol{\Upsilon}_{1,2} = 0$,

$$\partial_t S = \boldsymbol{P}\cdot\boldsymbol{Q} - h(\boldsymbol{Q},\boldsymbol{P})\,.$$

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

*Case* 4. $\varepsilon < \mathcal{O}(c^{-1})$. 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.

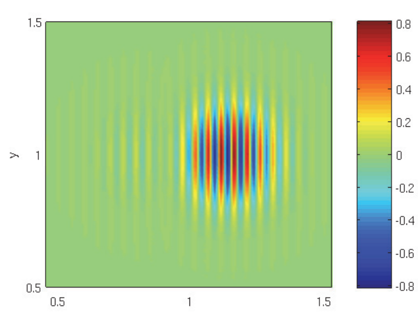
This section is devoted to numerical experiments to illustrate the accuracy and relevance of the FGA for the Dirac equation.

### 5.1. A simple accuracy FGA test.

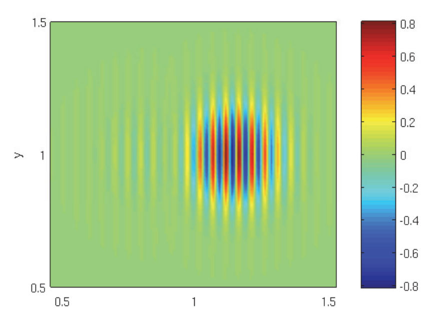
We set $A \equiv 0$ and $V \equiv 0$ in the Dirac equation (5) and set the initial condition (6) as

$$\boldsymbol{\omega}_I(\boldsymbol{x}) = \left(\exp\left(-\mu\,|\boldsymbol{x}-\boldsymbol{x}_0|^2\right), 0, 0, 0\right)^T \quad \text{and} \quad S_I(x) = \boldsymbol{p}_0\cdot\boldsymbol{x} \tag{53}$$

with $\mu = 32$, $\boldsymbol{x}_0 = (1,1,1)$, and $\boldsymbol{p}_0 = (1,0,0)$. We compute the solutions using FGA for different $\varepsilon$'s and compare them with the reference solutions computed by the 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 Figure 2, and the relative $L^2$ errors are listed in Table 1 illustrating the accuracy of the FGA.




(a) FGA solution




(b) Reference solution

Fig. 2.

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

| $\varepsilon$ | $2^{-4}$ | $2^{-5}$ | $2^{-6}$ | $2^{-7}$ |
|---|---|---|---|---|
| $\\|\boldsymbol{\psi}^\varepsilon - \boldsymbol{\psi}^\varepsilon_{FGA}\\|_2$ | $2.63 \times 10^{-2}$ | $7.62 \times 10^{-3}$ | $4.21 \times 10^{-3}$ | $3.19 \times 10^{-3}$ |

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

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

The corresponding Fourier transform is given by

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

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

$$\mathrm{i}\partial_t\widehat{\boldsymbol{\psi}}(t, p_x, p_z) = \big(c\widehat{\boldsymbol{\alpha}} \cdot \boldsymbol{p} + \beta c^2/\varepsilon\big)\widehat{\boldsymbol{\psi}}(t, p_x, p_z)$$

is given by

$$\begin{aligned}\widehat{\boldsymbol{\psi}}(t, p_x, p_z) &= \exp\big[-\mathrm{i}c\widehat{\boldsymbol{\alpha}} \cdot \boldsymbol{p}t - \mathrm{i}\widehat{\beta}c^2 t/\varepsilon\big]\widehat{\boldsymbol{\psi}}(0, p_x, p_z)\\ &= \Big[\mathbb{I}_4\cos(E_\varepsilon t) - \mathrm{i}\frac{c\widehat{\boldsymbol{\alpha}} \cdot \boldsymbol{p}\varepsilon + \widehat{\beta}c^2}{\varepsilon E_\varepsilon}\sin(E_\varepsilon t)\Big]\widehat{\boldsymbol{\psi}}(0, p_x, p_z)\end{aligned}$$

with $E_\varepsilon = \sqrt{p^2c^2 + c^4/\varepsilon^2}$. We set $p'_x := \varepsilon p_x$ and $p'_z := \varepsilon p_z$, $t' := t/\varepsilon$, $p' := \sqrt{(p'_x)^2 + (p'_z)^2}$, $E' = \sqrt{(p')^2c^2 + c^4}$, and $\Delta' := \Delta/\varepsilon$. Then

(54)
$$\begin{aligned}&\widehat{\boldsymbol{\psi}}\big(t, p'_x/\varepsilon, p'_z/\varepsilon\big)\\ &\quad= 4\pi\Delta^2\Big[\mathbb{I}_4\cos(E't') - \mathrm{i}\frac{c\widehat{\boldsymbol{\alpha}} \cdot \boldsymbol{p}' + \widehat{\beta}c^2}{E'}\sin(E't')\Big]\mathcal{N}[1, 0, 0, 0]^T \times e^{-(\Delta' p')^2},\end{aligned}$$

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

$$\begin{cases} \psi_1(t', x', z') = 2\mathcal{N}(\Delta')^2 \int_0^\infty p' e^{-(\Delta' p')^2} J_0(p'r)\big(\cos(E't') - \mathrm{i}\dfrac{c^2}{E'}\sin(E't')\big)dp',\\ \psi_2(t',' x', z') = 0,\\ \psi_3(t', x', z') = -2\mathcal{N}(\Delta')^2\sin(\theta) \int_0^\infty p' e^{-(\Delta' p')^2} J_1(p'r)\dfrac{cp'}{E'}\sin(E't')\big)dp',\\ \psi_4(t', x', z') = -2\mathcal{N}(\Delta')^2\sin(\theta) \int_0^\infty p' e^{-(\Delta' p')^2} J_1(p'r)\dfrac{cp'}{E'}\sin(E't')\big)dp', \end{cases}$$

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

$$\boldsymbol{\psi}_1(t', 0, 0) = \mathcal{N}\Big[1 - \sqrt{\pi}\frac{\varepsilon ct'}{2\Delta}\exp\Big(-\Big(\frac{\varepsilon ct'}{2\Delta}\Big)^2\Big)\mathrm{Erfi}\Big(\frac{\varepsilon ct'}{2\Delta}\Big)\Big].$$

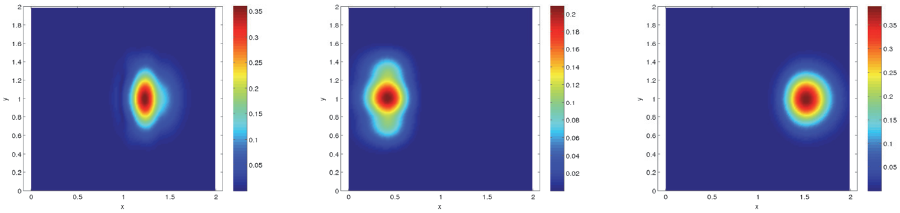


FIG. 3. *Barrier potential (Left) $V_0 = 0.2$ corresponding to an almost null reflection. (Middle) $V_0 = 1$ corresponding to a total reflection. (Right) No-potential.*

**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

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

where $k := \sqrt{k_x^2 + k_y^2 + k_z^2}$ and the barrier potential is defined as

$$V(x, y, z) = \frac{V_0}{2}\Big(1 + \tanh\big(\frac{x}{L_V}\big)\Big)\,. \tag{55}$$

In the semiclassical regime, the wavepacket should be totally reflected if $V_0/\varepsilon > E_\varepsilon - c^2/\varepsilon$, while it should be totally transmitted otherwise. Notice that we do not expect the Klein paradox to occur in this regime; see the next subsection. We consider both situation in a three-dimensional simulation on a spatial domain $[0, 2]^3$ of a wavepacket defined by

$$\begin{aligned}\boldsymbol{\psi}&(0, x, y)\\ &= \mathcal{N}[1, 0, 0, 0]^T \times \exp\big(-\big((x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2\big)/4\Delta^2\big)\exp(\mathrm{i}k_x x),\end{aligned}$$

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 $E_\varepsilon = \sqrt{1.25}/\varepsilon$, when $V_0 =$ (resp., $V_0 = 0$). The time step is taken equal to $\Delta t = 10^{-2}$ As expected, total transmission (resp., reflection) occurs (Figure 3 (left) (resp., (middle)), when $V_0/\varepsilon < E_\varepsilon - 1/\varepsilon$ (resp., $V_0/\varepsilon > E_\varepsilon - 1$). We also report in Figure 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 for different 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 Theorem 3.1). We represent the first component $\psi_1$ of the FGA solution with Cauchy data

$$\begin{aligned}\boldsymbol{\psi}&(0, x, y, z)\\ &= \mathcal{N}[1, 0, 0, 0]^T \times \exp\big(-\big((x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2\big)/4\Delta^2\big)\exp(\mathrm{i}k_x x),\end{aligned}$$

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 Figure 4. As numerically observed in 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.

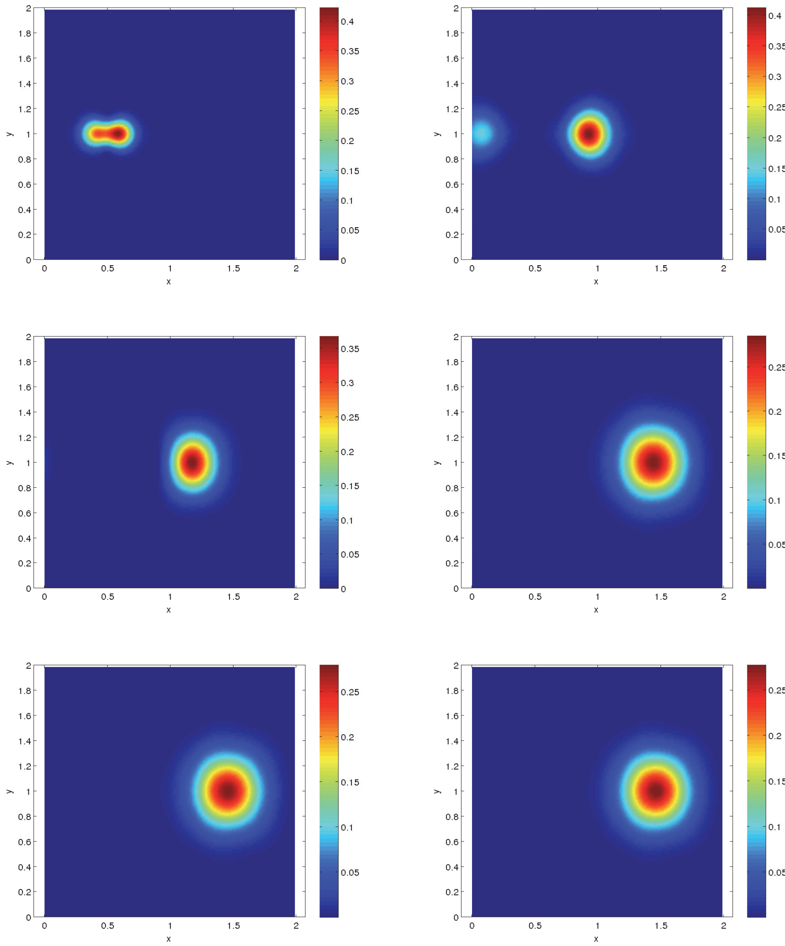


FIG. 4. *Modulus of first component. For c, respectively, equal to* 0.1, 0.5, 1, 5, 10, 10000.

**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 [8]. We will perform two series of tests in one and two dimensions. We show in particular that the direct FGA does *not* allow to capture this quantum effect.

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

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

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

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

where $L_V$ is a small parameter characterizing the gradient of the potential. In theory, transmission occurs when $V_0/\varepsilon > E_{k_x}^{(\varepsilon)} + 2c^2/\varepsilon$. The transmission $\mathcal{T}$ and reflection $\mathcal{R}$

coefficients for a barrier potential located at 0 are, respectively, given by

$$\mathcal{T} = \frac{\int_{\mathbb{R}_+} \boldsymbol{\psi}^\dagger \boldsymbol{\psi}}{\int_{\mathbb{R}} \boldsymbol{\psi}^\dagger \boldsymbol{\psi}}, \qquad \mathcal{R} = \frac{\int_{\mathbb{R}_-} \boldsymbol{\psi}^\dagger \boldsymbol{\psi}}{\int_{\mathbb{R}} \boldsymbol{\psi}^\dagger \boldsymbol{\psi}},$$

where

$$\mathcal{T} = -\frac{\sinh(\pi k^{(\varepsilon)} L_V)\sinh(\pi \kappa^{(\varepsilon)} L_V)}{\sinh\big(\pi(V_0/c\varepsilon + k^{(\varepsilon)} + \kappa^{(\varepsilon)})L_V/2\big)\sinh\big(\pi(V_0/c\varepsilon - k^{(\varepsilon)} - \kappa^{(\varepsilon)})L_V/2\big)} \tag{56}$$

and

$$k^{(\varepsilon)} = \frac{1}{c}\sqrt{(E^{(\varepsilon)}_{k_x} - V_0/\varepsilon)^2 - c^4/\varepsilon^2}, \qquad \kappa^{(\varepsilon)} = -\frac{1}{c}\sqrt{\big(E^{(\varepsilon)} - V_0/\varepsilon\big)^2 - c^4/\varepsilon^2}\,.$$

As a preliminary test, we report in Figure 5, a test in the quantum regime using a method described in [16]. We assume that $\varepsilon = 1/8$, which is close to a semiclassical regime. The spatial domain is $[-20, 20]$, $L_V = 10^{-4}$, and $V_0 = 5\times 10^4$. The time step is given by $\Delta t = 2.23\times 10^{-6}$ 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

$$\boldsymbol{\psi}(0, x) = [1, 0, 0, C]^T \times \exp\big(-(x - x_0)^2/4\Delta^2\big)\exp(\mathrm{i}k_x x)$$

with width $\Delta = 1$, wavenumber $k_x/\varepsilon = 500$, and

$$C = \frac{ck_x}{c^2 + \sqrt{c^4 + 2k_x^2}}.$$

The theoretical transmission coefficient is given by $\mathcal{T} = 0.322$, while the numerical one is given by $\mathcal{T}_h = 0.327$. At total of $8\times 10^4$ time iterations is necessary to performed this computation, corresponding to $\approx 2160.9$ seconds (on 16 processors), which is relatively very resource demanding for a such a simple test.

**5.4.1. Two-dimensional tests.** We here consider a quantum and semiclassical regime simulation.

**5.5. Quantum regime.** We assume that $\varepsilon = 1$, $c \approx 137.0359895$. The spatial domain is $[-1, 1]\times[-2, 2]$, $L_V = 10^{-4}$,

$$V(x, z) = \frac{V_0}{2}\Big(1 + \tanh\big(\frac{z}{L_V}\big)\Big),$$

with $V_0 = 4.64\times 10^4$. The time step is given by $\Delta t = 2.85\times 10^{-5}$ and the space step by $\Delta x = \Delta z = 2\times 10^{-3}$. The initial data is a Gaussian centered at $(x_0, z_0) = (0, -1.0)$ and is given by

$$\boldsymbol{\psi}(0, x, z) = [1, 0, 0, C]^T \times \exp\big(-((x - x_0)^2 + (z - z_0))^2/4\Delta^2\big)\exp(\mathrm{i}k_x x) \tag{57}$$

with width $\Delta = 0.2$, wavenumber $k_x = 200$, and

$$C = \frac{ck_x}{c^2 + \sqrt{c^4 + 2k_x^2}}.$$

Then $E^{(\varepsilon)}_{k_x} = 3.3224\times 10^3$ and $\kappa^{(\varepsilon)} = 133.9374$. The transmission coefficient, which

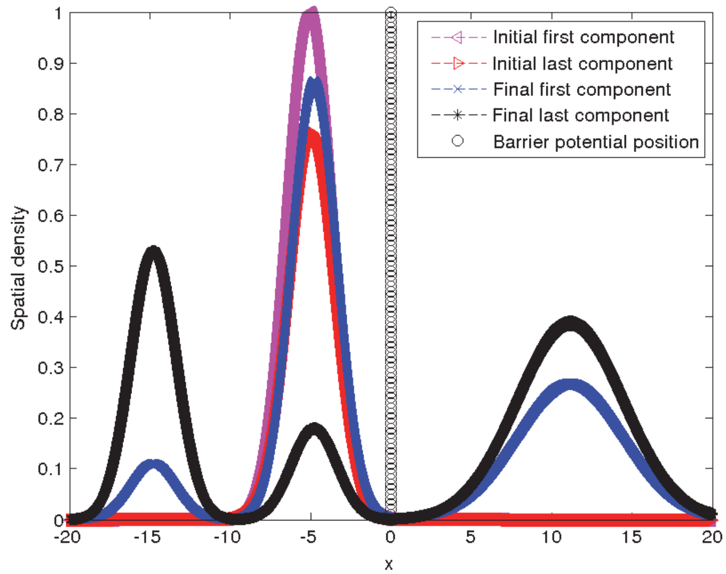



FIG. 5. *Klein paradox in one dimension in quantum regime* ($\varepsilon = 1/8$). *First and fourth spinor component: initial data and final time is* $T = 0.22$.

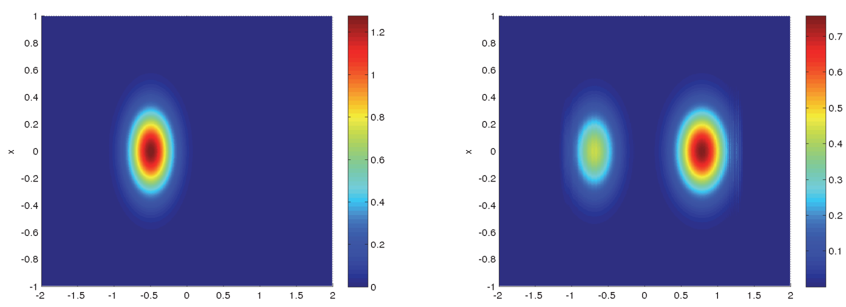


FIG. 6. *Klein paradox in two dimensions in quantum regime* ($\varepsilon = 1$). *Density* $\sum_{i=1}^{4} |\boldsymbol{\psi}_i|^2$*: initial data (left) and final time is* $T = 0.0171$ *(right).*

is computed numerically, is given by $\mathcal{T}_h \approx 0.661$, and the theoretical one is $\mathcal{T} = 0.65$. The computation is performed on eight processors with a total of 1230.4 seconds.

**Semiclassical regime.** We consider the initial condition (57) 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 (55) with $L_v = 0.2$ and $V_0 = 4$, and as a consequence $V_0/\varepsilon > E_\varepsilon + 2c^2/\varepsilon$. In the quantum regime, the transmission coefficient gives $\tau \approx 0.485$ when $L_v$ small enough. In the semiclassical 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 semiclassical solution, to simulate the Klein paradox, which is a quantum effect. A special treatment must be implemented in order to allow the transmission.

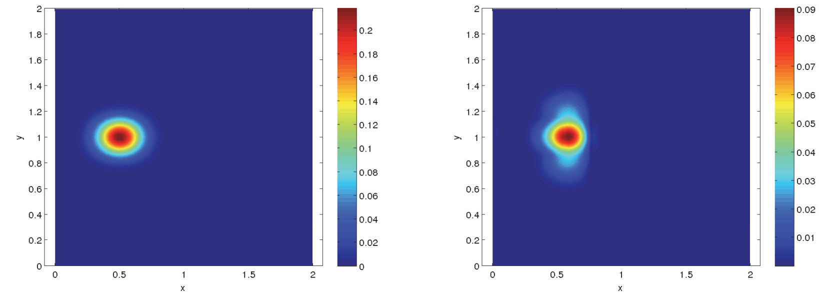


FIG. 7. *Klein paradox in two dimensions in quantum regime* ($\varepsilon = 2^{-7}$). *Density* $|\boldsymbol{\psi}_1|^2$*: initial data (left) and final time is* $T = 1$ *(right).*

**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

$$\mathcal{D}_{N_x,N_y,N_z} = \big\{\boldsymbol{x}_{k_1,k_2,k_3} = (x_{k_1}, y_{k_2}, z_{k_3})\big\}_{(k_1,k_2,k_3)\in\mathcal{O}_{N_xN_yN_z}},$$

where

$$\mathcal{O}_{N_xN_yN_z} = \big\{(k_1,k_2,k_3) \in \mathbb{N}^3, :\; k_1 = 0,\dots,N_x-1;\; k_2 = 0,\dots,N_y-1;\; k_3 = 0,\dots,N_z-1\big\}.$$

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 corresponding discrete wavenumbers are defined by $\boldsymbol{\xi} := (\xi_p, \xi_q, \xi_r)$, where $\xi_p = p\pi/a_x$ with $p \in \{-N_x/2,\dots,N_x/2-1\}$, $\xi_q = q\pi/a_y$ with $q \in \{-N_y/2,\dots,N_y/2-1\}$ and $\xi_r = r\pi/a_z$ with $r \in \{-N_z/2,\dots,N_z/2-1\}$. We denote next by $\alpha_\gamma = \Pi_\gamma\Lambda_\gamma\Pi_\gamma^\dagger$ for $\nu = x, y, z$ and where

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

The matrices $\Pi_\gamma$ are defined as follows:

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

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 $t_{n^*} := t_n + \Delta t$.

Naturally, in order to capture the high frequencies $\Delta t$ must be chosen smaller than $c^2/\varepsilon$, naturally motivating the use of computational method in the semiclassical limit. We denote by $\boldsymbol{\psi}_h^n$ the approximate spinor at time $t_N$.

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

$$\boldsymbol{\psi}_h^{n_1} = \exp\Big( - \mathrm{i}\Delta t\big(\beta c^2/\varepsilon + V_h/\varepsilon - \boldsymbol{\alpha}\cdot\mathbf{A}_h\big)\Big)\boldsymbol{\psi}_h^n.$$

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

2. Second step: integration of the generalized transport equation in Fourier space. One sets $\boldsymbol{\phi}_h^{n_1} := \Pi_x^\dagger \boldsymbol{\psi}_h^{n_1}$ and solves

$$\partial_t \phi + \Lambda_x \partial_x \phi = 0$$

   from time $t_n$ to $t_{n_2} = t_n + \Delta t$, basically by discretizing in space: $\phi(t_{n+1},\cdot) = \mathcal{F}_x^{-1}(e^{-\mathrm{i}\xi\Delta t\Lambda_x}\mathcal{F}_x(\phi(t_n,\cdot)))$, where $\mathcal{F}_x$ is the Fourier transform in the $x$-direction, that is, for $\ell = 1,\dots,4$ such that $\phi^\ell$ denotes the $\ell$th component of $\phi$. We denote $\boldsymbol{\phi}_h^{(\ell),n_1}$, the $\ell$th component $\boldsymbol{\phi}_h$ at time $n_1$,

$$\boldsymbol{\phi}_h^{(\ell),n_2} = \frac{1}{N_x}\sum_{p=-N_x/2}^{N_x/2-1}\Big(e^{-\mathrm{i}\xi_p\Delta t\lambda_\ell^{(x)}}\sum_{k_1=0}^{N_x-1}\boldsymbol{\phi}_{h,k_1}^{(\ell),n_1}e^{-\mathrm{i}\xi_p(x_{k_1}+a_x)}\Big)e^{\mathrm{i}\xi_p(x+a_{x_j})},$$

   where $\lambda_\ell^{(x)}$ is the $\ell$th eigenvalues of $\Lambda_x$.

3. Similarly one computes from $t_n$ to $t_{n_3} = t_n + \Delta t$

$$\boldsymbol{\phi}_h^{(\ell),n_3} = \frac{1}{N_y}\sum_{q=-N_y/2}^{N_y/2-1}\Big(e^{-\mathrm{i}\xi_q\Delta t\lambda_\ell^{(y)}}\sum_{k_2=0}^{N_y-1}\boldsymbol{\phi}_{h,k_2}^{(\ell),n_2^*}e^{-\mathrm{i}\xi_q(y_{k_2}+a_y)}\Big)e^{\mathrm{i}\xi_q(y+a_{y_j})},$$

   where $\boldsymbol{\phi}_h^{n_2^*} = \Pi_y^\dagger\Pi_x\boldsymbol{\phi}_h^{n_2}$, and finally

$$\boldsymbol{\phi}_h^{(\ell),n+1} = \frac{1}{N_z}\sum_{r=-N_z/2}^{N_z/2-1}\Big(e^{-\mathrm{i}\xi_r\Delta t\lambda_\ell^{(z)}}\sum_{k_3=0}^{N_z-1}\boldsymbol{\phi}_{h,k_3}^{(\ell),n_3^*}e^{-\mathrm{i}\xi_r(z_{k_3}+a_z)}\Big)e^{\mathrm{i}\xi_r(z+a_{z_j})},$$

   where $\boldsymbol{\phi}_h^{n_3^*} = \Pi_z^\dagger\Pi_y\boldsymbol{\phi}_h^{n_3}$. Finally $\boldsymbol{\psi}_h^{n+1} = \Pi_z\boldsymbol{\phi}_n^{n+1}$.

Alternatively, it is possible to directly apply three-dimensional fast Fourier transforms. By construction, the $\ell_2$-norm is naturally conserved.

**7. Conclusion.** This paper derives and analyzes the FGA for the linear Dirac equation in the semiclassical limit. Strong connections of the FGA for Dirac and Klein–Gordon equations with the Schrödinger equation are established in the nonrelativistic 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; combined with the splitting technique used in [11], we also plan to apply the FGA method to study the nonlinear Dirac equation.

## Appendix A. Eigenvalues and eigenvectors.

**A.1. Eigenvectors computation.** In order to determine $\mathcal{M}$ and $\mathcal{N}$ in (35), we need to explicitly construct $\partial h$ and $\partial \boldsymbol{\Upsilon}$. First notice

$$\partial_{\boldsymbol{Q}} h_\pm = \mp \frac{c(P_l c - A_l)\partial_{\boldsymbol{Q}} A_l}{\sqrt{|\boldsymbol{P}c - \boldsymbol{A}(\boldsymbol{Q})|^2 + c^4}} + \partial_{\boldsymbol{Q}} V, \quad \partial_{\boldsymbol{P}} h_\pm = \pm \frac{(\boldsymbol{P}c - \boldsymbol{A}(\boldsymbol{Q}))}{\sqrt{|\boldsymbol{P}c - \boldsymbol{A}(\boldsymbol{Q})|^2 + c^4}}, \tag{58}$$

$$\begin{aligned}
\partial_{P_j}\partial_{Q_k} h_\pm &= \pm \frac{(P_j c - A_j)(\boldsymbol{P}c - \boldsymbol{A})\cdot \partial_{Q_k}\boldsymbol{A}}{\left(|\boldsymbol{P}c - \boldsymbol{A}(\boldsymbol{Q})|^2 + c^4\right)^{3/2}} \mp \frac{c\partial_{Q_k} A_j}{\sqrt{|\boldsymbol{P}c - \boldsymbol{A}(\boldsymbol{Q})|^2 + c^4}},\\
\partial_{P_j}\partial_{P_k} h_\pm &= \mp \frac{c(P_j c - A_j)(P_k c - A_k)}{\left(|\boldsymbol{P} - \boldsymbol{A}(\boldsymbol{Q})|^2 + c^4\right)^{3/2}} \pm \frac{c\delta_{jk}}{\sqrt{|\boldsymbol{P}c - \boldsymbol{A}(\boldsymbol{Q})|^2 + c^4}}\\
\partial_{Q_j}\partial_{Q_k} h_\pm &= \mp \frac{(\boldsymbol{P}c - \boldsymbol{A})\cdot \partial_{Q_j}\boldsymbol{A}\,(\boldsymbol{P}c - \boldsymbol{A})\cdot \partial_{Q_k}\boldsymbol{A}}{\left(|\boldsymbol{P}c - \boldsymbol{A}(\boldsymbol{Q})|^2 + c^4\right)^{3/2}}\\
&\quad \pm \frac{\partial_{Q_j}\boldsymbol{A}\cdot\partial_{Q_k}\boldsymbol{A} - (\boldsymbol{P}c - \boldsymbol{A})\cdot\partial_{Q_j}\partial_{Q_k}\boldsymbol{A}}{\sqrt{|\boldsymbol{P}c - \boldsymbol{A}(\boldsymbol{Q})|^2 + c^4}} + \partial_{Q_j}\partial_{Q_k} V.
\end{aligned} \tag{59}$$

Hence,

$$\partial_{\boldsymbol{z}}\boldsymbol{\Upsilon} = \partial_{\boldsymbol{z}} Q_j \partial_{Q_j}\boldsymbol{\Upsilon} + \partial_{\boldsymbol{z}} P_j \partial_{P_j}\boldsymbol{\Upsilon}. \tag{60}$$

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

**A.2. Positive branch.** The corresponding eigenvectors read

$$\boldsymbol{\Upsilon}_1 = \frac{1}{r}\begin{pmatrix} u_3 \\ u_1 + \mathrm{i}u_2 \\ \sqrt{|\boldsymbol{u}|^2 + c^4} - c^2 \\ 0 \end{pmatrix}, \quad \boldsymbol{\Upsilon}_2 = \frac{1}{r}\begin{pmatrix} u_1 - \mathrm{i}u_2 \\ -u_3 \\ 0 \\ \sqrt{|\boldsymbol{u}|^2 + c^4} - c^2 \end{pmatrix}, \tag{61}$$

where $r = \sqrt{2\left(|\boldsymbol{u}|^2 + c^4 - c^2\sqrt{|\boldsymbol{u}|^2 + c^4}\right)}$ and $\boldsymbol{u} = \boldsymbol{P}c - \boldsymbol{A}(Q)$. We have

$$\partial_{\boldsymbol{u}}\boldsymbol{\Upsilon}_1 = \frac{1}{r}\begin{pmatrix} 0 & 1 & u_1/\lambda & 0 \\ 0 & \mathrm{i} & u_2/\lambda & 0 \\ 1 & 0 & u_3/\lambda & 0 \end{pmatrix} - \frac{1}{r}\partial_{\boldsymbol{u}} r \otimes \boldsymbol{\Upsilon}_1 \tag{62}$$

$$\partial_{\boldsymbol{u}}\boldsymbol{\Upsilon}_2 = \frac{1}{r}\begin{pmatrix} 1 & 0 & 0 & u_1/\lambda \\ -\mathrm{i} & 0 & 0 & u_2/\lambda \\ 0 & -1 & 0 & u_3/\lambda \end{pmatrix} - \frac{1}{r}\partial_{\boldsymbol{u}} r \otimes \boldsymbol{\Upsilon}_2 \tag{63}$$

and

$$\partial_{\boldsymbol{u}} r = -\frac{1}{r}\left(\frac{1}{\sqrt{|\boldsymbol{u}|^2 + c^4}} - 2\right)\boldsymbol{u}. \tag{64}$$

Thus,

$$\begin{aligned}
\boldsymbol{\Upsilon}_1^\dagger \partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_1 &= \frac{\mathrm{i}}{r^2}\left(-u_2, \quad u_1, \quad 0\right), \\
\boldsymbol{\Upsilon}_2^\dagger \partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_2 &= \frac{\mathrm{i}}{r^2}\left(\ u_2, \quad -u_1, \quad 0\right), \\
\boldsymbol{\Upsilon}_2^\dagger \partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_1 &= \frac{1}{r^2}\left(-u_3, \quad -\mathrm{i}u_3, \quad u_1 + \mathrm{i}u_2\right), \\
\boldsymbol{\Upsilon}_1^\dagger \partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_2 &= \frac{1}{r^2}\left(\ u_3, \quad -\mathrm{i}u_3, \quad -u_1 + \mathrm{i}u_2\right).
\end{aligned} \tag{65}$$

We define the following Berry connection matrices:

$$\boldsymbol{\mathcal{B}} = \frac{1}{r^2}\left[\begin{pmatrix} -\mathrm{i}u_2 & u_3 \\ -u_3 & \mathrm{i}u_2 \end{pmatrix}, \begin{pmatrix} \mathrm{i}u_1 & -\mathrm{i}u_3 \\ -\mathrm{i}u_3 & -\mathrm{i}u_1 \end{pmatrix}, \begin{pmatrix} 0 & -u_1 + \mathrm{i}u_2 \\ u_1 + \mathrm{i}u_2 & 0 \end{pmatrix}\right]. \tag{66}$$

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

$$\boldsymbol{\Upsilon}_1 = \frac{1}{r}\begin{pmatrix} -u_3 \\ -u_1 - \mathrm{i}u_2 \\ \sqrt{|\boldsymbol{u}|^2 + c^4} + c^2 \\ 0 \end{pmatrix}, \quad \boldsymbol{\Upsilon}_2 = \frac{1}{r}\begin{pmatrix} -u_1 + \mathrm{i}u_2 \\ u_3 \\ 0 \\ \sqrt{|\boldsymbol{u}|^2 + c^4} + c^2 \end{pmatrix}, \tag{67}$$

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

$$\partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_1 = \frac{1}{r}\begin{pmatrix} 0 & -1 & u_1/\lambda & 0 \\ 0 & -\mathrm{i} & u_2/\lambda & 0 \\ -1 & 0 & u_3/\lambda & 0 \end{pmatrix} - \frac{1}{r}\partial_{\boldsymbol{u}} r \otimes \boldsymbol{\Upsilon}_1 \tag{68}$$

$$\partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_2 = \frac{1}{r}\begin{pmatrix} -1 & 0 & 0 & u_1/\lambda \\ \mathrm{i} & 0 & 0 & u_2/\lambda \\ 0 & 1 & 0 & u_3/\lambda \end{pmatrix} - \frac{1}{r}\partial_{\boldsymbol{u}} r \otimes \boldsymbol{\Upsilon}_2 \tag{69}$$

$$\partial_{\boldsymbol{u}} r = \frac{1}{r}\left(\frac{1}{\sqrt{|\boldsymbol{u}|^2 + c^4}} + 2\right)\boldsymbol{u}. \tag{70}$$

Thus,

$$\begin{aligned}
\boldsymbol{\Upsilon}_1^\dagger \partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_1 &= \frac{\mathrm{i}}{r^2}\left(-u_2, \quad u_1, \quad 0\right), \\
\boldsymbol{\Upsilon}_2^\dagger \partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_2 &= \frac{\mathrm{i}}{r^2}\left(\ u_2, \quad -u_1, \quad 0\right), \\
\boldsymbol{\Upsilon}_2^\dagger \partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_1 &= \frac{1}{r^2}\left(-u_3, \quad -\mathrm{i}u_3, \quad u_1 + \mathrm{i}u_2\right), \\
\boldsymbol{\Upsilon}_1^\dagger \partial_{\boldsymbol{u}} \boldsymbol{\Upsilon}_2 &= \frac{1}{r^2}\left(\ u_3, \quad -\mathrm{i}u_3, \quad -u_1 + \mathrm{i}u_2\right).
\end{aligned} \tag{71}$$

We define the following Berry connection matrices:

$$\boldsymbol{\mathcal{B}} = \frac{1}{r^2}\left[\begin{pmatrix} -\mathrm{i}u_2 & u_3 \\ -u_3 & \mathrm{i}u_2 \end{pmatrix}, \begin{pmatrix} \mathrm{i}u_1 & -\mathrm{i}u_3 \\ -\mathrm{i}u_3 & -\mathrm{i}u_1 \end{pmatrix}, \begin{pmatrix} 0 & -u_1 + \mathrm{i}u_2 \\ u_1 + \mathrm{i}u_2 & 0 \end{pmatrix}\right]. \tag{72}$$

We conclude this appendix, by providing some working values, necessary to determine the nonrelativistic 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

$$\partial_{p_1}\boldsymbol{\Upsilon}_1 = \frac{1}{r}\begin{pmatrix} 0 \\ c \\ \dfrac{p_1c^2}{\sqrt{p^2c^2 + c^4}} \\ 0 \end{pmatrix} - \frac{\partial_{p_1}r}{r^2}\boldsymbol{\Upsilon}_1\,, \quad \partial_{p_1}\boldsymbol{\Upsilon}_2 = \frac{1}{r}\begin{pmatrix} c \\ 0 \\ 0 \\ \dfrac{p_2c^2}{\sqrt{p^2c^2 + c^4}} \end{pmatrix} - \frac{\partial_{p_1}r}{r^2}\boldsymbol{\Upsilon}_2$$

$$\partial_{p_2}\boldsymbol{\Upsilon}_1 = \frac{1}{r}\begin{pmatrix} 0 \\ \mathrm{i}c \\ \dfrac{p_2c^2}{\sqrt{p^2c^2 + c^4}} \\ 0 \end{pmatrix} - \frac{\partial_{p_2}r}{r^2}\boldsymbol{\Upsilon}_1\,, \quad \partial_{p_2}\boldsymbol{\Upsilon}_2 = \frac{1}{r}\begin{pmatrix} -\mathrm{i}c \\ 0 \\ 0 \\ \dfrac{p_2c^2}{\sqrt{p^2c^2 + c^4}} \end{pmatrix} - \frac{\partial_{p_2}r}{r^2}\boldsymbol{\Upsilon}_2$$

$$\partial_{p_3}\boldsymbol{\Upsilon}_1 = \frac{1}{r}\begin{pmatrix} c \\ 0 \\ \dfrac{p_3c^2}{\sqrt{p^2c^2 + c^4}} \\ 0 \end{pmatrix} - \frac{\partial_{p_3}r}{r^2}\boldsymbol{\Upsilon}_1\,, \quad \partial_{p_3}\boldsymbol{\Upsilon}_2 = \frac{1}{r}\begin{pmatrix} 0 \\ -c \\ 0 \\ \dfrac{p_3c^2}{\sqrt{p^2c^2 + c^4}} \end{pmatrix} - \frac{\partial_{p_3}r}{r^2}\boldsymbol{\Upsilon}_2\,.$$

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