A time splitting spectral method for the Klein-Gordon Maxwell system

Peter Allmer

joint work with Othmar Koch, Hans P. Stimming and Norbert J. Mauser

Research platform MMM and WPI c/o Fak. Math. Univ. Wien

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Wolfgang Pauli Institute Vienna

Content

The Klein-Gordon Maxwell system (KGM)

- We start by presenting the fully coupled Klein-Gordon Maxwell system, all following quantities are functions of time and spatial position where $(t, \boldsymbol{x}) \in \mathbb{R}^d \times \mathbb{R}^+$ with $d \in \{1, 3\}$.

$$
\begin{aligned}
-\tfrac{1}{c^2}\partial_t^2\psi+\Delta\psi+\tfrac{ie}{\hbar c^2}(\partial_t\phi+\phi\partial_t)\psi-\tfrac{ie}{\hbar}(\nabla\cdot\vec{A}+\vec{A}\nabla)\psi+\tfrac{e^2}{\hbar^2}(\tfrac{\phi^2}{c^2}-\vec{A}^2)\psi-\tfrac{m^2c^2}{\hbar^2}\psi&=0, && (1)\\
\tfrac{\hbar e}{mc^2}\left(i\bar{\psi}\partial_t\psi-i\psi\partial_t\bar{\psi}+2\tfrac{e}{\hbar}\bar{\psi}\phi\psi\right)&=\rho, && (2)\\
\tfrac{\hbar e}{m}\left(-i\bar{\psi}\nabla\psi+i\psi\nabla\bar{\psi}-2\tfrac{e}{\hbar}\bar{\psi}\vec{A}\psi\right)&=\vec{J}, && (3)\\
\tfrac{1}{c^2}\partial_t^2\phi-\Delta\phi&=\tfrac{\rho}{\epsilon_0}, && (4)\\
\tfrac{1}{c^2}\partial_t^2\vec{A}-\Delta\vec{A}&=\mu_0\vec{J}=\tfrac{1}{\epsilon_0c^2}\vec{J}. && (5)
\end{aligned}
$$

- We will treat the system as an initial value problem (IVP) with the following set of initial data

$$
\begin{cases}
\psi(0,\boldsymbol{x})=\psi_0, \quad \partial_t\psi(0,\boldsymbol{x})=\psi_1\\
\phi(0,\boldsymbol{x})=\phi_0, \quad \partial_t\phi(0,\boldsymbol{x})=\phi_1,\\
\vec{A}(0,\boldsymbol{x})=\vec{A}_0, \quad \partial_t\vec{A}(0,\boldsymbol{x})=\vec{A}_1.
\end{cases}
\qquad (6)
$$

Electromagnetic gauge

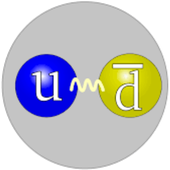
- Due to the gauge freedom in electromagnetism we demand the Lorentz Gauge condition for our electromagnetic potentials ϕ and $\vec{A}$

  $$\partial_t \phi + \nabla \vec{A} = 0. \tag{7}$$

  This yields that the Maxwell equations both become inhomogeneous wave equations.
- We additionally force the initial condition of our system to satisfy (7).

Briefly physical background

- The Klein-Gordon Maxwell system can be boiled down to two ingredients.
  - The Klein-Gordon equation which describes spin-0 particles.
  - The Maxwell equations which describes the interaction with the electromagnetic force.
- What particles can be described by the Klein-Gordon Maxwell system?
  - There is no elementary charged spin-0 particle in the Standard model.
  - But one can consider composed elementary particles!



The Pion (π^+): It has a total spin of 0 (every other meson too) and an electric charge of $e = +1$, it consists of an up quark, an anti-down quark and is held together by gluons.

Relation to relativistic quantum plasma

- A plasma is a "hot" phase of matter where the electrons have detached themselves from the nucleis, i.e. it is a huge collection of fermions, but they are spin-$\frac{1}{2}$ particles...
- Usually charged fermions are described by the Dirac-Maxwell system. But the models relative complexity compared to the (scalar) Klein-Gordon Maxwell system is much greater. $\Longrightarrow$ Describe a quantum plasma with Klein-Gordon Maxwell instead.
    - For a laser beam solid - object interaction experiment using Peta-Watt lasers in order to produce the plasma, the main source of nonlinear interactions is via the ponderomotive force, while the electron spin-$\frac{1}{2}$ effect comes in as a perturbation (Eliasson and P. K. Shukla 2011).
    - Or describe plasmas in situations where spin does not matter (Mendonca 2011; Haas, Eliasson, and P. Shukla 2012).

Charge conservation of the system

- Multiply (1) from the left side with $\bar{\psi}$ and subtract the complex conjugated from it, this implies the continuity equation

$$\partial_t \rho + \nabla \cdot \vec{J} = 0. \tag{8}$$

- By virtue of the local conservation law $\partial_t \rho(t, \mathrm{x}) = \nabla \cdot \tilde{\mathrm{J}}(\mathrm{t}, \mathrm{x})\ \forall (\mathrm{t}, \mathrm{x}) \in \mathbb{R} \times \mathbb{R}^3$, we can deduce a global conservation of the charge Q. Therefore we integrate over the whole space and obtain

$$0 = \int_{\mathbb{R}^3} \partial_t \rho(t, \mathrm{x}) - \nabla \cdot \tilde{\mathrm{J}}(\mathrm{t}, \mathrm{x}) = \int_{\mathbb{R}^3} \partial_{\mathrm{t}} \rho(\mathrm{t}, \mathrm{x}) = \partial_{\mathrm{t}} \underbrace{\int_{\mathbb{R}^3} \rho(t, \mathrm{x})}_{=:\mathrm{Q}(\mathrm{t})}.$$

Energy conservation of the system

- The energy functional is given by

$$E(t) = \int_{\mathbb{R}^3} \underbrace{\left| i\epsilon\partial_t\psi - i\phi\psi \right|^2 + \left| i\epsilon\nabla\psi + i\vec{A}\psi \right|^2 + |\psi|^2}_{\text{particle energy density } \epsilon_p} + \underbrace{\frac{1}{2}\left| -\nabla\phi - \partial_t\vec{A} \right|^2 + \frac{1}{2}\left| \nabla \times \vec{A} \right|^2}_{\text{electromagnetic field energy density } \epsilon_f}. \tag{9}$$

- During the time evolution it is conserved as long as there are external forces, i.e.

$$\partial_t\phi_{\mathrm{ext}}(t, \mathsf{x}) = \partial_t\vec{A}_{\mathrm{ext}}(t, \mathsf{x}) = 0.$$

Scaling of the system

- In order to describe the MKG system free of any intrinsic scales we introduce the following practicable length and time scale

$$\bar{x} = \frac{e^2}{m\epsilon_0 c^2}, \quad \bar{t} = \frac{\bar{x}}{c}.$$

- In addition we demand that our fields transform in the following manner:

$$\psi(x,t) \to \bar{x}^{-3/2}\psi(\tilde{x},\tilde{t})$$
$$\phi(x,t) \to c\lambda\phi(\tilde{x},\tilde{t}), \vec{A}(x,t) \to \lambda\vec{A}(\tilde{x},\tilde{t}) \text{ with } \lambda = \frac{mc}{e}$$

.

- After this transformation the equations are free of any intrinsic scale, they only depend on a dimensionless parameter

$$\epsilon = \frac{\hbar\epsilon_0 c}{e^2}.$$

Scaling of the system

We can rewrite the Klein-Gordon Maxwell system in a dimensionless way, where $\tilde{\cdot}$ denotes a dimensionless quantity

$$\epsilon^2\left(-\tilde{\partial}_t^2+\tilde{\Delta}\right)\tilde{\psi}-i\epsilon\left(\tilde{\partial}_t\tilde{\phi}+\tilde{\phi}\tilde{\partial}_t+\tilde{\nabla}\tilde{\vec{A}}+\tilde{\vec{A}}\tilde{\nabla}\right)\tilde{\psi}+\left(\tilde{\phi}^2-\tilde{\vec{A}}^2-1\right)\tilde{\psi}=0, \tag{10}$$

$$i\epsilon\left(\bar{\tilde{\psi}}\tilde{\partial}_t\tilde{\psi}-\tilde{\psi}\tilde{\partial}_t\bar{\tilde{\psi}}\right)-2\left(\bar{\tilde{\psi}}\tilde{\phi}\tilde{\psi}\right)=\tilde{\rho}, \tag{11}$$

$$-i\epsilon\left(\bar{\tilde{\psi}}\tilde{\nabla}\tilde{\psi}-\tilde{\psi}\tilde{\nabla}\bar{\tilde{\psi}}\right)-2\left(\bar{\tilde{\psi}}\tilde{\vec{A}}\tilde{\psi}\right)=\tilde{\vec{J}}. \tag{12}$$

$$\left(\tilde{\partial}_t^2-\tilde{\Delta}\right)\tilde{\phi}=\tilde{\rho}, \tag{13}$$

$$\left(\tilde{\partial}_t^2-\tilde{\Delta}\right)\tilde{\vec{A}}=\tilde{\vec{J}}. \tag{14}$$

Discretization

- We consider our system on a finite time interval $[0, T]$ in a cubic bounded domain with side length L,

$$\Omega = \left\{ x = (x_1, x_2, x_3) | -\frac{L}{2} \leqslant x_i \leqslant \frac{L}{2}, \quad i = 1, 2, 3 \right\}.$$

  For the discretization we choose $M, N \in \mathbb{N}$ with $i = 1, 2, 3$ and define the spatial mesh in the x_i-direction as $\Delta x_i = L/M$, with

$$x_m = \left(x_{1m_1}, x_{2,m_2}, x_{3,m_3}\right), \quad \text{with} \quad x_{i,m} = -\frac{L}{2} + m\Delta x_i,$$

  and denote the time steps by

$$t_n = n\Delta t, \quad \text{with} \quad 0 \leqslant n \leqslant N.$$

- We impose periodic boundary conditions.

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Notation and conventions

- A compact notation to denote arrays of function values evaluated at each spatial grid point at a certain time $n\Delta t$ is given by ψ^n, ϕ^n and $\vec{A}^n$.
- In the following we will illustrate all numerical schemes in a semi discritized way.
- And note that all spatial derivatives will be implemented as spectral derivatives on the computer.

Operator splitting scheme (OSS)

- We reformulate the electromagnetic KG equation (10) in the framework of Hamiltonian theory (Feshbach and Villars 1958)

$$\boldsymbol{\psi} = \begin{pmatrix} \frac{1}{2}\left(\psi + (i\epsilon\partial_t - \phi)\psi\right) \\ \frac{1}{2}\left(\psi - (i\epsilon\partial_t - \phi)\psi\right) \end{pmatrix}, \tag{15}$$

and find that the corresponding equation reads

$$i\epsilon\partial_t\boldsymbol{\psi} = H\boldsymbol{\psi} := \left(\frac{1}{2}(\tau_3 + i\tau_2)(-i\epsilon\nabla - A)^2 + \mathbb{1}\phi + \tau_3\right)\boldsymbol{\psi}. \tag{16}$$

- For splitting the equation we divide the Hamiltonian as follows

$$\begin{aligned} H = & \underbrace{\tau_3 + \mathbb{1}\phi^n}_{H_1} \underbrace{- \frac{1}{2}(\tau_3 + i\tau_2)\epsilon^2\Delta}_{H_2} \\ & + \underbrace{\frac{1}{2}i\epsilon(\tau_3 + i\tau_2)(\nabla\vec{A} + \vec{A}^n\nabla)}_{H_3} + \underbrace{\frac{1}{2}(\tau_3 + i\tau_2)\left(\vec{A}\right)^2}_{H_4}. \end{aligned} \tag{17}$$

Operator splitting scheme (OSS)

- Where τ_i, $i \in \{1,2,3\}$, denoting the three Pauli matrices in their standard representation as skew hermitian 2×2-matrices

  $$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

  which satisfy the usual relations

  $$\begin{aligned} \tau_i \tau_j &= i\epsilon_{i,j,k}\tau_k + \mathbb{1}, \\ [\tau_i, \tau_j] &= 2i\epsilon_{i,j,k}, \\ \{\tau_i, \tau_j\} &= 2\,\mathbb{1}. \end{aligned}$$

- and $\mathbb{1}$ denotes the 2×2 identity matrix.

Operator splitting scheme (OSS)

- The corresponding time evolution operators for the individual parts of the Hamiltonian H are given by

$$U_k = e^{-\frac{i}{\epsilon}\int_t^{t+\Delta t} H_k(x,s)ds}.$$

- Note that H_1 is an diagonal matrix and therefore the matrix exponential U_1 is easy to compute.
- $(\tau_3 + i\tau_2)$ isn't a diagonal matrix but fortunately it is nilpotent of order two. This truncates the exponential sum in the time evolution operator after the second term and they can be expressed exact, yielding

$$\begin{aligned} U_2 &= \mathbb{1} + \frac{1}{2} i(\tau_3 + i\tau_2)\epsilon^2\Delta, \\ U_3 &= \mathbb{1} + \frac{1}{2}(\tau_3 + i\tau_2)(\nabla\vec{A} + \vec{A}\nabla), \\ U_4 &= \mathbb{1} - \frac{1}{2} i\epsilon^{-1}(\tau_3 + i\tau_2)A^2. \end{aligned}$$

Crank-Nicolson scheme (CNS)

- We solve the Maxwell equations (13) and (14) which are of the form

  $$\left(\partial_t^2 - \Delta\right) f(t, \boldsymbol{x}) = F(t, \boldsymbol{x})$$

  with a Crank-Nicolson method.
- The scheme (in time discretization) reads

$$\left(1+\frac{\Delta t^2\,\Delta}{4}\right)\begin{pmatrix}\hat{f}^{n+1}\\ \partial_t \hat{f}^{n+1}\end{pmatrix}=\begin{pmatrix}1-\frac{\Delta t^2\,\Delta}{4} & \Delta t\\ -\Delta t\,\Delta & 1-\frac{\Delta t^2\,\Delta}{4}\end{pmatrix}\begin{pmatrix}\hat{f}^{n}\\ \partial_t \hat{f}^{n}\end{pmatrix}+\begin{pmatrix}\frac{\Delta t^2}{4}\\ \frac{\Delta t}{2}\end{pmatrix}\left(\hat{F}^{n}+\hat{F}^{n+1}\right), \tag{18}$$

Relaxation of the electric potential

- To update the electric potential we need to take care of the implicit occurrence of the potential in ψ due to the definition in (15).
- Therefore we define $\tilde{\rho} := \rho + 2|\psi|^2\phi$ where we approximate

$$\tilde{\rho}^n \approx \frac{\tilde{\rho}^{n+1/2} + \tilde{\rho}^{n-1/2}}{2}.$$

- We replace the source terms in the Maxwell equation for the eclectic potential by

$$\rho^{n+1} + \rho^n := 2\tilde{\rho}^{n+1/2} - 2|\psi^n|^2\phi^n - 2|\psi^{n+1}|^2\phi^{n+1}$$

. Finally we solve the CNS scheme (18) for ϕ^{n+1} according to (Besse 2005).

The algorithm in a nutshell

Algorithm 1: Time propagation using Lorentz gauge

Data: Given: N,
$$\boldsymbol{\psi}^0 = \psi_0, \partial_t \boldsymbol{\psi}^0 = \psi_1, \phi^0 = \phi_0, \partial_t \phi^0 = \phi_1, \vec{A}^0 = \vec{A}_0, \partial_t \vec{A}^0 = \vec{A}_1$$
Result: $\boldsymbol{\psi}^N, \partial_t \boldsymbol{\psi}^N, \phi^N, \partial_t \phi^N, \vec{A}^N, \partial_t \vec{A}^N$

while $n = 0 \leqslant N$ **do**

Update the wavfeunction with Strang splitting

$$\boldsymbol{\psi}^{n+1} = U_1(\tfrac{\Delta t}{2})\; U_2(\tfrac{\Delta t}{2})\; U_3(\tfrac{\Delta t}{2})\; U_4(\Delta t)\; U_3(\tfrac{\Delta t}{2})\; U_2(\tfrac{\Delta t}{2})\; U_1(\tfrac{\Delta t}{2})\; \boldsymbol{\psi}^n$$

to obtain $\boldsymbol{\psi}^{n+1}$ using (OSS) with the fields ϕ^n and $\vec{A}^n$;

Calculate $\tilde{\rho}^n := \rho^n + 2|\psi^n|^2\phi^n$ and obtain $\tilde{\rho}^{n+1/2} := 2\tilde{\rho}^n - \tilde{\rho}^{n-1/2}$;

Obtain ϕ^{n+1} with CNS using ψ^n and
$F^{n+1} + F^n := 2\tilde{\rho}^{n+1/2} - 2|\psi^n|^2\phi^n - 2|\psi^{n+1}|^2\phi^{n+1}$;

Calculate J^{n+1} from ψ^{n+1} and $\vec{A}^n$;

Obtain $\vec{A}^{n+1}$ with CNS using $\vec{A}^n$ and $F^{n+1} + F^n := J^{n+1} + J^n$;

Numerical charge conservation - pseudo norm

- A fundamental difference of the Klein-Gordon equation is that its charge density ρ can be negative.
- In order to reflect this physical behavior properly we need a different tool to describe the conservation of charge

Definition (pseudo inner products)

Let $\mathcal{H}$ denote a Hilbert space of wavefunctions, where the inner product on $\mathcal{H}$ is denoted by $\langle \psi_1 | \psi_2 \rangle$ and let η be a hermitian operator such that we say η defines a pseudo inner product, according to

$$\langle \psi_1 | \psi_2 \rangle_\eta = \langle \psi_1 | \eta | \psi_2 \rangle = \int_{\mathbb{R}^n} \bar{\boldsymbol{\psi}}_1 \eta \boldsymbol{\psi}_2.$$

And the pseudo norm is defined as

$$\|\boldsymbol{\psi}\|_{L^2}^{\eta} = \langle \psi | \psi \rangle_\eta .$$

Numerical charge conservation - pseudo norm

- According to the definition of a pseudo inner product we define the pseudo adjoint of an operator Ω by the relation

$$\int_{\mathbb{R}^n} \bar{\psi_1}\, \eta\, \Omega\, \psi_2 = \int_{\mathbb{R}^n} \overline{\Omega^\dagger\, \psi_1} \eta\, \psi_2.$$

- We say that Ω is pseudo hermitian if

$$\eta^{-1}\, \Omega^\dagger\, \eta = \Omega.$$

- And we call U pseudo unitary if

$$\langle U\psi_1 | U\psi_2 \rangle_\eta = \langle \psi_1 | \psi_2 \rangle_\eta \quad \forall \psi_1, \psi_2 \in \mathcal{H}$$

and note that U satisfies the relation

$$\eta^{-1}\, U^\dagger\, \eta = U^{-1}.$$

Numerical charge conservation - pseudo norm

Lemma

Let H be a pseudo hermitian operator w.r.t. η then

$U = e^{-iH}$

is a pseudo unitary operator w.r.t. η.

- The idea of the proof is it to show that all H_i with $i \in \{1, 2, 3, 4\}$ are pseudo hermitian operators $\implies$ all U_i with $i \in \{1, 2, 3, 4\}$ are pseudo unitary operators $\implies$ they conserve the pseudo inner product $\implies$ they conserve the pseudo norm.
- Note that for $\eta = \tau_3$ we have

$$\|\psi\|_{L^2}^{\tau_3} := \int_{\mathbb{R}^n} \bar{\psi}\tau_3\psi = \int_{\mathbb{R}^n} \rho = Q.$$

Numerical charge conservation - pseudo norm

- The pseudo hermiticiy of the H_i with $i \in \{1, 2, 3, 4\}$ follows by straight forward calculation and finally implies that

Theorem ($\|\cdot\|_{L^2}^{\tau_3}$ Charge Conservation)

The operator splitting scheme conserves the total electric charge Q using Lie-Trotter and Strang splitting, i.e.

$$\|\psi^n\|_{L^2}^{\tau_3} = \left\|\psi^0\right\|_{L^2}^{\tau_3} = Q_0, \quad \forall n \in \mathbb{N},$$

where ψ^n is the vector valued wave function defined in (15) and Q_0 is the initial total charge determined by the initial wave function ψ^0.

Numerical conservation of the Lorentz gauge

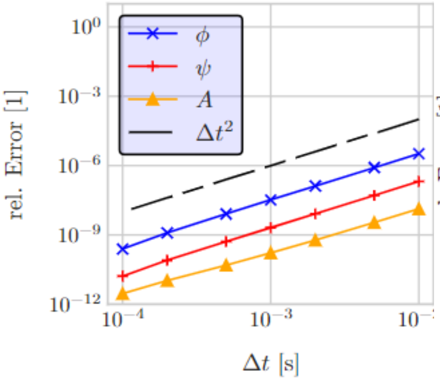
Lemma (Conservation of Lorentz gauge)

The Crank-Nicolson scheme (18) *preserves the Lorentz gauge condition in every time step, i.e.*

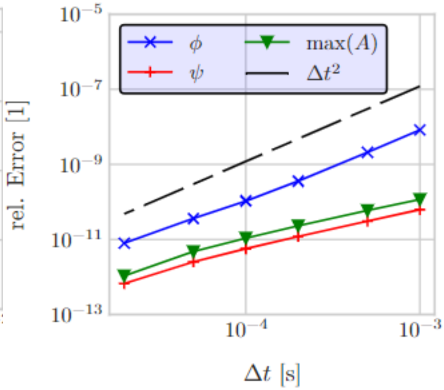
$$\partial_t \phi + \nabla \vec{A} = 0, \quad \forall n \in \mathbb{N}. \tag{19}$$

For more detail see (Huang et al. 2005)

Rate of convergence in Δt



(a) 1d



(b) 3d

Work in progress

- We are aiming to proof a convergence rate of order $p = 2$ in the L^2-norm.
- Our strategy is to use the Baker-Campbell-Hausdorff formula and to estimate all commutators occurring in there. The relevant decisions are
  - If we assume that $\vec{A}$ is smooth an will be updated between the splitting step we can shift all regularity towards it and we should be fine.
  - If we assume that $\vec{A}$ is dynamic we expect that the initial data for the magnetic potential $\vec{A_0} \in H^6$ and the wavefunction $\psi_0 \in H^3$ will do the job.

Relativistic dispersion

- We consider a free Gaussian wave packet in the rest frame its initial data is given by

$$\psi_0(\boldsymbol{x})_{\bar{\boldsymbol{p}}=0} = \tilde{\mathcal{N}} \int d^3p \quad \frac{1}{\sqrt{E}} \exp\left(-\frac{\boldsymbol{p}^2}{2\sigma^2} - i\boldsymbol{p}\boldsymbol{x}\right).$$

- In order to observe a non symmetric dispersion we boost this wave packet to the lab frame by choosing $\bar{\boldsymbol{p}} = 100$ in natural units, i.e.

$$\psi(\boldsymbol{x})_{\bar{\boldsymbol{p}}=0} \to \psi(\boldsymbol{x})_{\bar{\boldsymbol{p}}} = L(\bar{\mathrm{p}})\psi(\boldsymbol{x})_{\bar{\boldsymbol{p}}=0}\left(\Lambda^{-1}(\bar{\boldsymbol{p}})\boldsymbol{x}\right).$$

The Lorentz boost Λ (along the x-axis) is given by

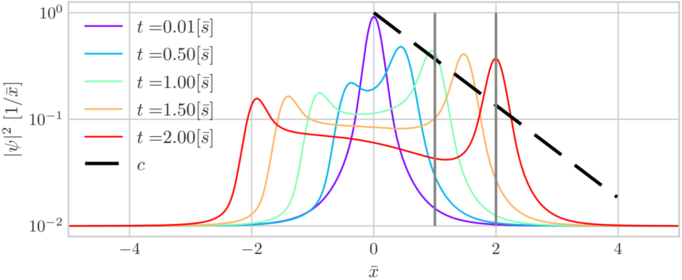
$$\Lambda = \begin{pmatrix} \gamma & \beta\gamma & 0 & 0 \\ \beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Relativistic dispersion

- The boosted initial data is obtained as

$$\psi_0(\boldsymbol{x})_{\bar{\boldsymbol{p}}} = \mathcal{N} \int \frac{d^3p'}{\sqrt{E'}} \sqrt{E' - c\beta \boldsymbol{p}'} \begin{pmatrix} 1 \pm E' \\ 1 \mp E' \end{pmatrix} \exp\left(-\frac{\boldsymbol{p}(\boldsymbol{p}')^2}{2\sigma^2} - i\boldsymbol{p}\boldsymbol{x} \right).$$

where the prime denotes the coordinates in the boosted system. By inspection the time evolution on spatial dimension we obtain



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