Higher order Schrödinger equations

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HIGHER ORDER SCHRÖDINGER EQUATIONS

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Abstract. The purpose of this paper is to provide higher order Schrödinger equations from a finite expansion approach. These equations converge toward the semi-relativistic equation for particles whose norm of their velocity vector is below $\frac{c}{\sqrt{2}}$ and are able to take into account some relativistic effects with a certain accuracy in a sense that we define. So, it is possible to take into account some relativistic effects by using Schrödinger form equations, even if they cannot be considered as relativistic wave equations.

1. Introduction

In quantum mechanics, the Schrödinger equation is a fundamental non-relativistic quantum equation that describes how the wave-function of a physical system evolves over time. It was published in 1926 by Erwin Schrödinger [25]. This equation has been widely studied [1]. Then, the Klein-Gordon equation, developed by Oskar Klein and Walter Gordon [16, 9], was the first relativistic quantum equation. Unfortunately, it cannot be straightforwardly interpreted as a Schrödinger type equation for a quantum state, because it is of second order in time. It is possible to transform the Klein-Gordon equation into a Schrödinger type equation of two coupled differential equations of first order in time [10], but it is not a couple of equations of the wave-function. It was the Dirac equation, formulated by Paul Dirac [6], that gave the fundamental relativistic equation of first order in time. It is a four dimensional matrix partial differential equation.

In this paper, we provide Schrödinger form equations of first order in time coming from the Einstein's mass-energy equivalence and from a finite expansion approach, giving rise to higher order Schrödinger equations. Contrary to the Dirac equation, the proposed equations have a domain of validity related with a certain accuracy in a sense that we define and cannot be used for all particles. They are valid for norms of the velocity vector up to $\frac{c}{\sqrt{2}}$ with some constraints on the accuracy. Each higher order Schrödinger equation is a Schrödinger form equation and a unique equation, contrary to the Dirac equation which is a four dimensional matrix equation, having a higher order Schrödinger operator [5, 14]. It is not a relativistic wave equation because it is not a Lorentz covariant equation and it cannot consider particles with velocity close to the speed of light. However, the higher order Schrödinger equations converge toward the semi-relativistic equation and are able to take into account some relativistic effects in their domain of validity and their accuracy can be tuned. They are interesting in some practical cases, when the solutions can be defined as for instance with an additive bounded or linear potential, due to the simplicity of the Schrödinger form equation. The proposed equations are an interpolation between Schrödinger and semi-relativistic equations, valid in the lower half of the scale between non-relativistic and ultra-relativistic extremes. The semi-relativistic equation is studied in [12, 13] by using optimized Schrödinger operator inequalities and concavity properties. Moreover, the second order Schrödinger equation is mentioned in [19] and used in [15] for solitons with an additive nonlinear term. In this paper, the problem of the square root of the semi-relativistic equation is approximated by using a finite expansion leading to higher order Schrödinger equations.

The paper is organized as follows. After some notations and definitions given in Section 2, higher order Schrödinger equations are given and studied in Section 3. Finally, a conclusion is addressed in Section 4.

2. Backgrounds

2.1. **The Schrödinger and Klein-Gordon equations.** The *Einstein's mass-energy equivalence* is the concept that the mass of a body is a measure of its energy content and is given by the formula [8]

$$E = \gamma m \cdot c^2 \tag{2.1}$$

where E is the total internal energy of the body,

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

is the Lorentz factor with $v^2 = \|\vec{v}\|^2$ the square norm of the velocity vector $\vec{v}$ of the body, m the rest mass of the body and c the speed of light in the vacuum.

Let us recall that the non-relativistic equation for the energy of a particle is given by

$$E = V(\vec{r}, t) + \frac{\mathbf{p}^2}{2m} \tag{2.2}$$

where $V(\vec{r}, t)$ is its potential energy and $\mathbf{p} = \gamma m \vec{v}$ its momentum. By using the correspondence principle [2]

$$E \leftrightarrow i\hbar \frac{\partial}{\partial t} \qquad \mathbf{p} \leftrightarrow -i\hbar \frac{\partial}{\partial \vec{x}} = -i\hbar \vec{\nabla} \tag{2.3}$$

we obtain the *Schrödinger equation* for a particle

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = V(\vec{r}, t)\psi(\vec{r}, t) - \frac{\hbar^2}{2m}\Delta\psi(\vec{r}, t) \tag{2.4}$$

moving in a potential $V(\vec{r}, t)$, where $\Delta := \nabla^2$ is the Laplace operator and $\hbar = \frac{h}{2\pi}$ the reduced Planck constant. The *wavefunction* $\psi : \mathbf{R}^3 \times \mathbf{R}_+ \to \mathbf{C}$ describes the evolution in space and time of the quantum state. In the following ψ stands for $\psi(\vec{r}, t)$. A *Schrödinger type equation* is an equation

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = H\psi(\vec{r}, t) \tag{2.5}$$

where H is the Hamiltonian of the system. If $H = H(\Delta)$, then the equation (2.4) is said to be a *Schrödinger form equation.*

By using the equality

$$\gamma^2 = \frac{\gamma^2 v^2}{c^2} + 1 \tag{2.6}$$

and the Einstein's mass-energy equivalence (2.1), we obtain

$$E = \gamma mc^2 = mc^2 \sqrt{\frac{\gamma^2 v^2}{c^2} + 1}. \tag{2.7}$$

Then we have the following relation

$$E^2 = m^2c^4 + \mathbf{p}^2c^2. \tag{2.8}$$

With the correspondence principle (2.3), we obtain the *Klein-Gordon equation*

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = m^2c^4\ \psi - \hbar^2 c^2 \Delta\psi. \tag{2.9}$$

As noted by Dirac, equation (2.9) is of second order in time contrary to the Schrödinger equation (2.4). So, it cannot be interpreted as a Schrödinger type equation for a quantum state.

2.2. **Mathematical tools.** To solve the Schrödinger equation in the absence of an external potential, it is convenient to use the Fourier transform. It turns out that the same approach can be used to solve the higher order Schrödinger equations (3.9). For the content of this subsection, we refer for instance to [24].

Notation. For $x \in \mathbf{R}^d$ (with d an integer not necessarily equal to 3), and $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbf{N}^d$, we denote by

$$x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_d^{\alpha_d}, \qquad |x| = \sqrt{x_1^2 + x_2^2 + \cdots + x_d^2}.$$

For $\beta \in \mathbf{N}^d$ and $f \in C^\infty(\mathbf{R}^d; \mathbf{C})$, we denote by

$$\partial^\beta f = \frac{\partial^{\beta_1}}{\partial x_1^{\beta_1}} \frac{\partial^{\beta_2}}{\partial x_2^{\beta_2}} \cdots \frac{\partial^{\beta_d}}{\partial x_d^{\beta_d}} f.$$

Introduce the Schwartz space

$$\mathcal{S}(\mathbf{R}^d) = \left\{ f \in C^\infty(\mathbf{R}^d; \mathbf{C}) \mid \sup_{x \in \mathbf{R}^d} \left| x^\alpha \partial^\beta f(x) \right| < \infty, \quad \forall \alpha, \beta \in \mathbf{N}^d \right\}.$$

For $f \in \mathcal{S}(\mathbf{R}^d)$, the (semi-classical) Fourier transform of f, denoted by $\widehat{f}$ or $\mathcal{F}(f)$, is defined by

$$\widehat{f}(p) = \frac{1}{(2\pi\hbar)^{d/2}} \int_{x \in \mathbf{R}^d} e^{-ix\cdot p/\hbar} f(x) \mathrm{d}x$$

where p is the Fourier variable. Then the function $\mathbf{R}^d \ni p \mapsto \widehat{f}(p)$ belongs to $\mathcal{S}(\mathbf{R}^d)$. The main properties that we will use concerning the Fourier transform are listed in the following proposition. In particular, the normalizing factor $(2\pi)^{-d/2}$ is chosen so that the Fourier Inversion Formula and the Plancherel formula below are simple.

Proposition 2.1. *Let $f \in \mathcal{S}(\mathbf{R}^d)$.*

- *For any $j \in \{1, \dots, d\}$,*

$$\mathcal{F}\left(\frac{\partial f}{\partial x_j}\right)(p) = i\frac{p_j}{\hbar}\widehat{f}(p). \tag{2.10}$$

- *For any $j \in \{1, \dots, d\}$,*

$$\frac{\partial \widehat{f}}{\partial p_j}(p) = -\frac{i}{\hbar}\mathcal{F}(x_j f)(p). \tag{2.11}$$

Fourier Inversion Formula: *We have*

$$f(x) = \frac{1}{(2\pi\hbar)^{d/2}} \int_{p\in\mathbf{R}^d} e^{+ix\cdot p/\hbar} \widehat{f}(p)\mathrm{d}p. \tag{2.12}$$

The Fourier transform is uniquely continuously extended to the space of tempered distributions, its dual space $\mathcal{S}'(\mathbf{R}^d)$*. The properties* (2.10) *and* (2.11) *remain valid in the sense of distributions, in* $\mathcal{S}'(\mathbf{R}^d)$*.*
Plancherel formula: *The Fourier transform is unitary on* $L^2(\mathbf{R}^d)$*,*

$$\|u\|_{L^2(\mathbf{R}^d)} = \|\widehat{u}\|_{L^2(\mathbf{R}^d)}, \quad \forall u \in L^2(\mathbf{R}^d). \tag{2.13}$$

Recall that $L^2(\mathbf{R}^d)$ is the space of square integrable functions, that is of measurable functions u such that

$$\int_{x\in\mathbf{R}^d} |u(x)|^2 \mathrm{d}x < \infty.$$

For $s \in \mathbf{R}$, we define the Sobolev space $H^s(\mathbf{R}^d)$ by

$$H^s(\mathbf{R}^d) = \left\{ f \in L^2(\mathbf{R}^d) \mid \|f\|^2_{H^s} := \int_{p\in R^d} \left(1+|p|^2\right)^s \left|\widehat{f}(p)\right|^2 \mathrm{d}p < \infty \right\}. \tag{2.14}$$

If moreover s is a non-negative integer, then the Sobolev space $H^s(\mathbf{R}^d)$ can be characterized as follows:

$$H^s(\mathbf{R}^d) = \left\{ f \in L^2(\mathbf{R}^d) \mid \partial^\alpha f \in L^2(\mathbf{R}^d), \quad |\alpha| \leqslant s \right\}.$$

3. The higher order Schrödinger equations

3.1. **The semi-relativistic equation.** In view of (2.8), we have

$$E = \sqrt{\mathbf{p}^2c^2 + m^2c^4}, \tag{3.1}$$

and then it leads to

$$E = mc^2 \sqrt{\frac{\mathbf{p}^2}{m^2c^2} + 1}. \tag{3.2}$$

Equation (3.1) leads, with the correspondence principle (2.3), to the following *semi-relativistic equation*

$$i\hbar\frac{\partial}{\partial t}\psi = \sqrt{-c^2\hbar^2\Delta + m^2c^4}\ \psi, \tag{3.3}$$

with the non local pseudo-differential operator $\sqrt{-c^2\hbar^2\Delta + m^2c^4}$ studied in [18, Chapter 7]; see also [4] for related studies. The semi-relativistic equation (3.3) with an arbitrary coordinate-dependent static interaction potential $V(\vec{r}) = V$ has been studied in [12, 13, 21]. This wave equation describes the bound states of spin-zero particles (scalar bosons) as well as the spin-averaged spectra of the bound states of fermions [23, 22]. With an additive nonlinear part $F(\psi)$, equation (3.3) is know as the *Hartree equation* [17].

If we use the Taylor series expansion of (3.2) given by

$$E = mc^2 \left(1 + \sum_{n=1}^{\infty} (-1)^{n+1}\alpha(n)\frac{\mathbf{p}^{2n}}{m^{2n}c^{2n}}\right), \tag{3.4}$$

and the correspondence principle (2.3), we obtain the following equation

$$i\hbar\frac{\partial\psi}{\partial t} = mc^2\ \psi - \sum_{n=1}^{\infty}\frac{\alpha(n)\hbar^{2n}}{m^{2n-1}c^{2n-2}}\Delta^n\psi, \tag{3.5}$$

where

$$\alpha(n) = \frac{(2n-2)!}{n!(n-1)!2^{2n-1}}. \tag{3.6}$$

This decomposition is given for instance in [11, 20].

Proposition 3.1. *Equations* (3.4) *and* (3.5) *hold for* $\frac{\mathbf{p}^2}{m^2c^2} < 1$*, which is equivalent to* $2v^2 < c^2$*.*

Proof. $\frac{\mathbf{p}^2}{m^2c^2} < 1$ is equivalent to $\frac{\gamma^2v^2}{c^2} < 1$. By using the definition of γ, it is also equivalent to $\frac{1}{1-\frac{v^2}{c^2}}\frac{v^2}{c^2} < 1$, which leads to the result. □

It means that equation (3.5) is equivalent to equation (3.3) for a norm $||\vec{v}||$ of the studied particle satisfying

$$||\vec{v}|| < \frac{c}{\sqrt{2}} \approx 211\ 985\ 280\, m.s^{-1}. \tag{3.7}$$

Equation (3.5) has an infinite number of terms. Thus, an infinite number of operators are required to specify the evolution of the wave-function ψ and it also leads to a highly non local theory [27]. Nevertheless, Equation (3.5) is a Schrödinger form equation with a restricted domain of validity.

3.2. **The higher order Schrödinger equations as a finite expansion.** The main idea of what follows is to keep only the necessary terms of equation (3.5) for a certain accuracy in a sense that we define, by using a finite expansion.

Let us consider the following approximation

$$E_N = mc^2\left(1 + \sum_{n=1}^{N}(-1)^{n+1}\alpha(n)\frac{\mathbf{p}^{2n}}{m^{2n}c^{2n}}\right) \tag{3.8}$$

of the energy (3.4) with $N \geqslant 1$. By using the correspondence principle (2.3), we obtain the following *higher order Schrödinger equations*

$$i\hbar\frac{\partial\psi_N}{\partial t} = mc^2\ \psi_N - \sum_{n=1}^{N}\frac{\alpha(n)\hbar^{2n}}{m^{2n-1}c^{2n-2}}\Delta^n\psi_N. \tag{3.9}$$

Equation (3.9) has the advantages of a Schrödinger form equation without the drawbacks of equation (3.5).

3.3. **Convergence of the energy approximation.** The error $e_N = E - E_N$ between the full expression of the energy (3.4) and the approximation (3.8) is given by

$$e_N = mc^2\left(\sum_{n=N+1}^{\infty}(-1)^{n+1}\alpha(n)\frac{\mathbf{p}^{2n}}{m^{2n}c^{2n}}\right). \tag{3.10}$$

For $\mathbf{p}^2 < m^2c^2$, e_N corresponds to the remainder of an alternate series, hence

$$|e_N| \leqslant mc^2\alpha(N+1)\frac{\mathbf{p}^{2N+2}}{m^{2N+2}c^{2N+2}} = mc^2\alpha(N+1)\left(\frac{1}{\frac{c^2}{v^2}-1}\right)^{N+1}. \tag{3.11}$$

With the assumption that $2v^2 < c^2$, we have $0 < \frac{1}{\frac{c^2}{v^2}-1} < 1$. As $0 < mc^2 < 1$ for particles, we infer $|e_N| \leqslant \alpha(N+1)$, hence we have the following result:

Proposition 3.2. *We have*

$$\lim_{N\to\infty} |e_N| = 0 \tag{3.12}$$

and more precisely, Stirling formula yields

$$|e_N| = \mathcal{O}\left(\frac{1}{N^{3/2}}\right) \quad \text{as } N \to \infty.$$

Let

$$\varepsilon_N := mc^2\alpha(N+1)\frac{\mathbf{p}^{2N+2}}{m^{2N+2}c^{2N+2}} = mc^2\alpha(N+1)\left(\frac{1}{\frac{c^2}{v^2}-1}\right)^{N+1}. \tag{3.13}$$

In the following ε_N is called the *accuracy*. This accuracy concerns the energy of the studied particle and not the solutions ψ and ψ_N of equations (3.5) and (3.9). The convergence of the wave functions is studied in Subsection 3.6.

Example 3.3. Let us consider a free particle of mass m. First of all, keep the two first terms of equation (3.9) (i.e. $N = 1$). We obtain the following approximate equation

$$i\hbar\frac{\partial\psi_1}{\partial t} = mc^2\psi_1 - \frac{\hbar^2}{2m}\Delta\psi_1. \tag{3.14}$$

We recognize the Schrödinger equation (2.4) with an additive term $mc^2\psi_1$, where mc^2 is the rest energy of the studied particle. The relation between the semi-relativistic equation (3.3) and (3.14) had been noticed already in [26]. Suppose that the particle has a velocity satisfying $||\vec{v}|| = \frac{c}{100}$. The accuracy associated with equation (3.14) is

$$\varepsilon_1 \approx \frac{1}{8}\cdot m\cdot 9\times 10^{16}\cdot 10^{-8} \approx 1.125\times 10^8 m. \tag{3.15}$$

Then, by using the three first terms of equation (3.9) (i.e. $N = 2$), we obtain the following approximate equation

$$i\hbar\frac{\partial\psi_2}{\partial t} = \left(mc^2 + V\right)\psi_2 - \frac{\hbar^2}{2m}\Delta\psi_2 - \frac{\hbar^4}{8m^3c^2}\Delta^2\psi_2. \tag{3.16}$$

The accuracy associated with equation (3.14) is given by

$$\varepsilon_2 \approx \frac{1}{16}\cdot m\cdot 9\times 10^{16}\cdot 10^{-12} \approx 5.625\times 10^3 m. \tag{3.17}$$

Thus, the result is that by taking into account a supplementary term in equation (3.9), we increase the accuracy (3.13) of five orders of magnitude for a particle having a velocity of $||\vec{v}|| = \frac{c}{100}$. When the norm of the velocity vector reaches $\frac{c}{\sqrt{2}}$, it is necessary to take into account higher-order terms of equation (3.9) to provide a sufficient accuracy. Thus, we can tune the accuracy by choosing an accurate number N of terms in equation (3.9). If the norm of the velocity vector becomes higher than $\frac{c}{\sqrt{2}}$, then equation (3.9) fails to describe correctly the evolution of the wave-function whatever the higher-order terms added to the equation. The Dirac equation must be used.

3.4. **Solving a generalized Schrödinger equation.** Let $G : \mathbf{R}_+ \to \mathbf{R}$ be a real-valued function, and consider the generalized Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} + G(-\hbar^2\Delta)\psi = 0; \quad \psi(x,0) = \psi_0(x). \tag{3.18}$$

The quantity $G(-\hbar^2\Delta)\psi$ is defined as a Fourier multiplier:

$$\mathcal{F}\left(G(-\hbar^2\Delta)\psi\right)(p) = G(|p|^2)\widehat{\psi}(p).$$

The most important aspect is that we want to encompass the following three cases:

- Schrödinger equation: $G(y) = -\frac{1}{2m}y$.
- Semi-relativistic equation (3.3): $G(y) = -\sqrt{c^2y + m^2c^4}$.
- Higher order Schrödinger equations (3.9):

$$G(y) = -mc^2 + \sum_{n=1}^{N} \frac{\alpha(n)}{m^{2n-1}c^{2n-2}}(-y)^n.$$

Applying the Fourier transform to (3.18) with respect to the space variable, we obtain formally a first order ordinary differential equation in time for $\widehat{\psi}$, in view of Proposition 2.1:

$$i\hbar \frac{\partial \widehat{\psi}}{\partial t} + G(|p|^2)\widehat{\psi} = 0; \quad \widehat{\psi}(0,p) = \widehat{\psi}_0(p).$$

It is solved explicitly:

$$\widehat{\psi}(p,t) = \widehat{\psi}_0(p)e^{-itG(|p|^2)}. \tag{3.19}$$

Since G is real-valued, $|\widehat{\psi}(p,t)| = |\widehat{\psi}_0(p)|$, and we obtain, from Proposition 2.1:

Proposition 3.4. *Let $s \in \mathbf{R}$ and $\psi_0 \in H^s(\mathbf{R}^d)$. Then the Cauchy problem* (3.18) *has a unique solution $\psi \in C(\mathbf{R}; H^s(\mathbf{R}^d))$, denoted by*

$$\psi(t) = e^{-itG(-\hbar^2\Delta)}\psi_0.$$

It is given by (3.19)*. Moreover, we have*

$$\|\psi(\cdot,t)\|_{H^s} = \|\psi_0\|_{H^s}, \quad \forall t \in \mathbf{R}.$$

In other words, the propagator $e^{-itG(-\hbar^2\Delta)}$ is unitary on every Sobolev space $H^s(\mathbf{R}^d)$.

3.5. **Higher order Schrödinger equations with an external potential.** Consider now (3.9) in the presence of an external potential. Dropping the index N to ease notations leads to

$$i\hbar \frac{\partial \psi}{\partial t} = V\psi - \sum_{n=0}^{N} \frac{\alpha(n)\hbar^{2n}}{m^{2n-1}c^{2n-2}}\Delta^n\psi; \quad \psi(x,0) = \psi_0(x), \tag{3.20}$$

where we use the convention $\alpha(0) = -1$. The potential V is real-valued. At least two cases can easily be concerned from the mathematical point of view: when V is bounded, and when V is linear with respect to the position x. These cases include for instance finite potential wells, neutrons in free fall in the gravity field and electrons accelerated by an electric field.

Bounded potential. By using perturbative arguments (based on Duhamel's formula), the following result can be proved by using Proposition 3.4.

Proposition 3.5. *Suppose that $V \in L^\infty(\mathbf{R}^d)$. If $\psi_0 \in L^2(\mathbf{R}^d)$, then (3.20) has a unique solution $\psi \in C(\mathbf{R}; L^2(\mathbf{R}^d))$, and*

$$\|\psi(\cdot,t)\|_{L^2} = \|\psi_0\|_{L^2} \quad \forall t \in \mathbf{R}.$$

If in addition for some $s \in \mathbf{N}$, $\partial^\alpha V \in L^\infty(\mathbf{R}^d)$ for all $|\alpha| \leqslant s$, and $\psi_0 \in H^s(\mathbf{R}^d)$, then $\psi \in C(\mathbf{R}; H^s(\mathbf{R}^d))$.

Linear potential.

Proposition 3.6. *Suppose that V is of the form*

$$V(x,t) = E(t)\cdot x = E_1(t)x_1 + \cdots + E_d(t)x_d,$$

for $E \in L^\infty(\mathbf{R};\mathbf{R}^d)$. If $\psi_0 \in L^2(\mathbf{R}^d)$, then (3.20) has a unique solution $\psi \in C(\mathbf{R}; L^2(\mathbf{R}^d))$, and

$$\|\psi(\cdot,t)\|_{L^2} = \|\psi_0\|_{L^2} \quad \forall t \in \mathbf{R}.$$

It is given by its Fourier transform (in space)

(3.21)

$$\widehat{\psi}(p,t) = \widehat{\psi}_0\left(p+\pi(t)\right)\exp\left(\frac{i}{\hbar}\sum_{n=0}^N \frac{(-1)^n\alpha(n)}{m^{2n-1}c^{2n-2}}\int_0^t |p+\pi(t)-\pi(s)|^{2n}\,\mathrm{d}s\right),$$

where $\pi(t) = \int_0^t E(\tau)\mathrm{d}\tau$.

Sketch of the proof. Taking the Fourier transform in space in (3.20) yields

$$i\hbar\frac{\partial\widehat{\psi}}{\partial t} = E(t)\cdot\mathcal{F}\left(x\psi\right) - \sum_{n=0}^N \frac{\alpha(n)}{m^{2n-1}c^{2n-2}}(-|p|^2)^n\widehat{\psi};\quad \widehat{\psi}(p,0) = \widehat{\psi}_0(p).$$

Since $\mathcal{F}\left(x\psi\right) = i\hbar\nabla\widehat{\psi}$, we infer

$$i\hbar\left(\frac{\partial}{\partial t} - E(t)\cdot\nabla\right)\widehat{\psi} = -\sum_{n=0}^N \frac{\alpha(n)}{m^{2n-1}c^{2n-2}}(-|p|^2)^n\widehat{\psi};\quad \widehat{\psi}(p,0) = \widehat{\psi}_0(p).$$

This is an inhomogeneous transport equation, which can be solved by the method of characteristics: the above equation is treated like an ordinary differential equation thanks to the change of unknown $\widehat{\psi}(p,t) = w(p+\pi(t),t)$ (the equation for w is of the form $i\hbar\partial_t w = A(t,p)w$), and (3.21) follows. □

Remark 3.7. In the case of the Schrödinger equation, $N = 1$, and when E does not depend on time, the Fourier Inversion Formula (2.12) applied to (3.21) leads to the well-known Avron-Herbst formula (see e.g. [5, Chapter 7]). It was generalized in the case where E depends on time in [3]. On the other hand, such an explicit formula does not seem available as soon as $N \geqslant 2$, because (2.12) does not seem so helpful then: it is easy to compute the Fourier transform of $e^{i|p|^2}$ (it has the same form), while the Fourier transform of $e^{i|p|^4}$ is a special function.

Note the following property, which stems from Proposition 2.1: for $s \geqslant 0$,

$$\mathcal{F}\left(H^s(\mathbf{R}^d)\right) = \left\{ f \in L^2(\mathbf{R}^d) \mid \int_{x\in\mathbf{R}^d} |x|^{2s}|f(x)|^2\mathrm{d}x < \infty \right\}.$$

For $k \in \mathbf{N}$, set

$$\Sigma_N^k = H^{(2N-1)k}(\mathbf{R}^d) \cap \mathcal{F}\left(H^s(\mathbf{R}^d)\right).$$

Then we infer the following result from (3.21).

Corollary 3.8. *Let $k, N \in \mathbf{N}$, and $\psi_0 \in \Sigma_N^k$. Suppose that V is of the same form as in Proposition 3.6. Then* (3.20) *has a unique solution $\psi \in C(\mathbf{R}; \Sigma_N^k)$.*

The case of the harmonic potential. Suppose that $V(x) = |x|^2$. Taking the Fourier transform in (3.20), we infer, from Proposition 2.1, that $\widehat{\psi}$ solves

$$i\hbar \frac{\partial \widehat{\psi}}{\partial t} = -\Delta \widehat{\psi} - \sum_{n=0}^{N} \frac{\alpha(n)}{m^{2n-1}c^{2n-2}} (-|p|^2)^n \widehat{\psi}; \quad \widehat{\psi}(p, 0) = \widehat{\psi}_0(p), \tag{3.22}$$

where now Δ stands for the Laplacian with respect to the variable p. The above equation is of the form $i\hbar \partial_t \widehat{\psi} = H \widehat{\psi}$, where

$$H = -\Delta - \sum_{n=0}^{N} \frac{\alpha(n)}{m^{2n-1}c^{2n-2}} (-|p|^2)^n.$$

In the case $N = 2$, it becomes, in view of (3.6),

$$H = -\Delta + mc^2 + \frac{|p|^2}{2m} - \frac{|p|^4}{8m^3c^2}.$$

It is well-known that H is not essentially self-adjoint on $C_0^\infty(\mathbf{R}^d)$ (see e.g. [7]). The reason is that classical trajectories may have an infinite speed of propagation, so there is a lack of uniqueness. Therefore, giving a rigorous meaning to the solution of (3.20) when V is an harmonic potential seems to be a very delicate issue, which we do not discuss further into details.

Remark 3.9 (Frequency localization). The issue described above could be avoided by using a frequency localization, which consists in replacing $\sqrt{\mathbf{p}^2c^2 + m^2c^4}$ in (3.1) with $\sqrt{\mathbf{p}^2c^2 \mathbf{1}_{\mathbf{p}^2<m^2c^2} + m^2c^4}$, where the function $\mathbf{1}_{\mathbf{p}^2<m^2c^2}$ is equal to 1 if $\mathbf{p}^2 < m^2c^2$, and 0 otherwise. In that case, the Taylor expansion (3.4) is always converging, thanks to the convergence of the entire series associated to $y \mapsto \sqrt{1+y}$. In the above example related to the harmonic potential, $|p|$ has to be replaced by $|p|\mathbf{1}_{|p|^2<m^2c^2}$, and the potential in H becomes bounded: there is no difficulty in solving the analogue of (3.22). On the other hand, introducing the indicating function makes the operator $\mathcal{F}^{-1}(|p|^2\mathbf{1}_{|p|^2<m^2c^2})$ non-local, and the benefit of the Taylor expansion is lost.

3.6. **Convergence of the wave function approximation.** We now study the convergence of ψ_N, solution to (3.9), to ψ solving (3.3), as N tends to infinity. We emphasize the fact that this study is performed in the absence of an external potential, $V = 0$: adapting it to either of the cases dealt with in Subsection 3.5 seems to be rather delicate.

Theorem 3.10. *Let $\psi_0 \in L^2(\mathbf{R}^d)$. Suppose that $\widehat{\psi}_0$ is smooth and compactly supported, $\widehat{\psi}_0 \in C_0^\infty(\mathbf{R}^d)$, with*

$$\widehat{\psi}_0(p) = 0 \quad \text{if } \left|\frac{p}{mc}\right| > 1.$$

Suppose that $\psi_{|t=0} = \psi_{N|t=0} = \psi_0$. *Then* $\psi_N \to \psi$ *as* $N \to \infty$, *in the following sense: for all* $T > 0$,

$$\sup_{t\in[0,T]} \|\psi(\cdot,t) - \psi_N(\cdot,t)\|_{L^2(\mathbf{R}^d)} \leqslant \frac{2T}{\hbar} mc^2 \alpha(N+1)\|\psi_0\|_{L^2} \underset{N\to\infty}{\longrightarrow} 0. \tag{3.23}$$

Remark 3.11. A more precise rate of convergence is available, in view of the estimate

$$\alpha(N) = \mathcal{O}\left(\frac{1}{N^{3/2}}\right) \text{ as } N \to \infty,$$

which stems from the expression (3.6) and Stirling formula.

Proof. The functions ψ and ψ_N solve

$$i\hbar\frac{\partial \psi}{\partial t} = -G(-\hbar^2\Delta)\psi, \qquad \text{with } G(y) = -\sqrt{c^2y + m^2c^4}.$$
$$i\hbar\frac{\partial \psi_N}{\partial t} = -G_N(-\hbar^2\Delta)\psi_N, \qquad \text{with } G_N(y) = \sum_{n=0}^{N} \frac{\alpha(n)}{m^{2n-1}c^{2n-2}}(-y)^n.$$

The difference $w_N = \psi - \psi_N$ solves $w_{N|t=0} = 0$ and

$$i\hbar\frac{\partial w_N}{\partial t} = -G(-\hbar^2\Delta)w_N + r_N, \quad \text{where } r_N = \left(G_N(-\hbar^2\Delta) - G(-\hbar^2\Delta)\right)\psi_N.$$

Multiply the above equation by $\overline{w_N}$, integrate in space, and take the imaginary part: the term involving $G(-\hbar^2\Delta)w_N$ disappears (because it is real), and we infer

$$\|w_N(t)\|_{L^2} \leqslant \frac{2}{\hbar}\int_0^t \|r_N(\tau)\|_{L^2}\mathrm{d}\tau. \tag{3.24}$$

In view of Plancherel formula (2.13), and since G and G_N are Fourier multipliers,

$$\|r_N(\tau)\|_{L^2} = \|\widehat{r}_N(\tau)\|_{L^2} = \left\|\left(G_N(|p|^2) - G(|p|^2)\right)\widehat{\psi}_N(\tau)\right\|_{L^2}.$$

We note that

$$G_N(|p|^2) - G(|p|^2) = mc^2 \sum_{n=N+1}^{\infty} (-1)^n \alpha(n) \left(\frac{|p|}{mc}\right)^{2n}.$$

Note that in view of the assumption on $\widehat{\psi}_0$, (3.19) implies that for all $\tau \geqslant 0$,

$$\widehat{\psi}_N(\tau,p) = 0 \quad \text{if } \left|\frac{p}{mc}\right| > 1. \tag{3.25}$$

Therefore, $\left(G_N(|p|^2) - G(|p|^2)\right)\widehat{\psi}_N(\tau)$ involves an alternate series, whose coefficients are decreasing, so

$$\begin{aligned}\left|\left(G_N(|p|^2) - G(|p|^2)\right)\widehat{\psi}_N(\tau,p)\right| &\leqslant mc^2\alpha(N+1)\left(\frac{|p|}{mc}\right)^{2N+2}\left|\widehat{\psi}_N(\tau,p)\right| \\ &\leqslant mc^2\alpha(N+1)\left|\widehat{\psi}_0(p)\right|,\end{aligned}$$

where we have used (3.25) and (3.19) to get the last inequality. The error estimate (3.23) then follows from (3.24) and the above estimate. □

It is worth noting that the assumption of Theorem 3.10 is the same condition as the one in Proposition 3.1, due to the relations between the momentum $\mathbf{p}$ and the Fourier variable p given by the correspondence principle (2.3) and the relation (2.10). It means that the higher order Schrödinger equations converge toward the semi-relativistic equation for the particles whose velocity vector satisfies (3.7).

Remark 3.12. Suppose that we have k particles of masses m_j evolving such that their velocities satisfy $\|\vec{v}_j\| < \frac{c}{\sqrt{2}}$ for $j = 1, \ldots, k$. The previous theory can be generalized as follows. The approximation of the energy of the system is given by

$$E_N = \sum_{j=1}^{k} m_j c^2 \left(1 + \sum_{n=1}^{N} (-1)^{n+1} \alpha(n) \frac{\mathbf{p}_j^{2n}}{m_j^{2n} c^{2n}} \right), \tag{3.26}$$

and higher order Schrödinger equations of the system are given by

$$i\hbar \frac{\partial \psi_N}{\partial t} = \sum_{j=1}^{k} \left(m_j c^2 \psi_N - \sum_{n=1}^{N} \frac{\alpha(n)\hbar^{2n}}{m_j^{2n-1} c^{2n-2}} \Delta_j^n \psi_N \right), \tag{3.27}$$

where $\psi_N = \psi_N(\vec{r}_1, \ldots, \vec{r}_k, t)$ with $\vec{r}_j$ the position vector associated with the particle j.

4. Conclusion

This paper provides higher order Schrödinger equations, coming from a finite expansion approach. The sequence of equations converges toward the semi-relativistic equation as the truncation index goes to infinity, and is then able to take into account some relativistic effects in a restricted relativistic domain of validity related to a desired accuracy. It is an interpolation between Schrödinger and semi-relativistic equations which takes into account higher-order terms.

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