Numerical investigation of solitary waves stability for quantum dissipative systems.

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Abstract

We consider a simple model describing the interaction of a quantum particle with a vibrational environment which eventually acts as a friction on the particle. This equation admits soliton-like solutions and we numerically investigate their stability when subjected to a small initial impulsion. Our findings illustrate the analogies with the behavior of classical particles and the relevance of asymptotic models.

Keywords. Open quantum systems. Particles interacting with a vibrational field. Schrödinger-Wave equation. Ground states. Orbital stability.

Math. Subject Classification. 35Q40 35Q51 35Q55

1 Introduction

In this paper we investigate on numerical grounds the dynamics of the following system, hereafter referred to as the *Schrödinger-Wave equation*

$$\left(i\partial_t u + \frac{1}{2}\Delta_x u\right)(t,x) = \left(\iint_{\mathbb{R}^d\times\mathbb{R}^n} \sigma_1(x-y)\sigma_2(z)\psi(t,y,z)\,\mathrm{d}y\,\mathrm{d}z\right) u(t,x), \qquad t\in\mathbb{R},\ x\in\mathbb{R}^d \quad (1a)$$

$$(\partial_{tt}^2\psi - c^2\Delta_z\psi)(t,x,z) = -c^2\sigma_2(z)\left(\int_{\mathbb{R}^d}\sigma_1(x-y)|u(t,y)|^2\,\mathrm{d}y\right), \qquad t\in\mathbb{R},\ x\in\mathbb{R}^d,\ z\in\mathbb{R}^n \quad (1b)$$

endowed with the initial data

$$u(0,x) = u_0(x), \qquad (\psi(0,x,z),\partial_t\psi(0,x,z)) = (\psi_0(x,z),\psi_1(x,z)). \quad (2)$$

This model has been introduced in [13] and it is intended to describe the behavior of a quantum particle interacting with its environment: u stands for the wave function of the quantum particle,

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which interacts with the vibrational field ψ, representing the environment. Here $c > 0$ is a fixed parameter, and σ_1, σ_2 are some God-given form functions which are supposed non-negative, infinitely smooth, radially symmetric and compactly supported. A key feature of the model is the fact that the particle motion holds in the space $\mathbb{R}^d$, but the vibrations hold in a *transverse direction* $\mathbb{R}^n$.

Several quantities are conserved by the dynamics: the mass of the wave function u

$$\mathscr{M}(t) = \int |u(t)|^2 \,\mathrm{d}x,$$

and, denoting $\chi = \partial_t \psi$, the total energy of the system

$$E(u,\psi,\chi) = \frac{1}{2}\int |\nabla_x u(x)|^2 \,\mathrm{d}x + \frac{1}{2}\iint \Big(\frac{|\chi|^2}{c^2} + |\nabla_z \psi|^2\Big)(x,z)\,\mathrm{d}z\,\mathrm{d}x \\ + \iiint \sigma_1(x-y)\sigma_2(z)\psi(y,z)|u(x)|^2 \,\mathrm{d}z\,\mathrm{d}y\,\mathrm{d}x, \quad (3)$$

and the total momentum

$$P(u,\psi,\chi) = \mathrm{Im}\int \nabla_x u(x)\overline{u(x)}\,\mathrm{d}x - \frac{1}{c^2}\iint \chi(x,z)\nabla_x \psi(x,z)\,\mathrm{d}x\,\mathrm{d}z \quad (4)$$

are conserved too. These conservation laws define a natural functional framework, in which a well-posedness theory can be established [13].

We are particularly interested in the stability of some specific solutions of the system (1a)–(1b). To this end, it is relevant to consider the regime $c \to +\infty$, which reveals the attractive dynamics of the system. Indeed, passing to the limit $c \to +\infty$ in (1a)–(1b) leads (at least formally) to the following system

$$i\partial_t \tilde{u} + \frac{1}{2}\Delta_x \tilde{u} = \Big(\sigma_1 \star_x \int \sigma_2 \tilde{\psi}\,\mathrm{d}z\Big)\,\tilde{u}, \qquad t \in \mathbb{R},\ x \in \mathbb{R}^d, \quad (5a)$$

$$-\Delta_z \tilde{\psi} = -\sigma_2(z)\left(\sigma_1 \star_x |\tilde{u}|^2\right)(x), \qquad t \in \mathbb{R},\ x \in \mathbb{R}^d,\ z \in \mathbb{R}^n. \quad (5b)$$

Let us denote $z \mapsto \Gamma(z)$ the solution of the auxilliary equation

$$\Delta_z \Gamma = \sigma_2.$$

Then, the solution of (5b) reads $\tilde{\psi}(x,z) = \Gamma(z)(\sigma_1 \star |\tilde{u}|^2)(x)$. Accordingly, (5a)–(5b) can be cast in the usual form of an Hartree type equation

$$i\partial_t \tilde{u} + \frac{1}{2}\Delta_x \tilde{u} = -\kappa\left(\Sigma \star_x |\tilde{u}|^2\right)\tilde{u}, \qquad t \in \mathbb{R},\ x \in \mathbb{R}^d, \quad (6)$$

where $\kappa = \|\nabla_z \Gamma\|^2_{L^2_z}$ and $\Sigma = \sigma_1 \star \sigma_1$. Since $\kappa > 0$ and σ_1 is non negative, this Hartree type equation looks like the Newton-Hartree equation, where the self-consistent potential is focusing. This observation motivates the study of solitary waves, particular solutions of the form $(u(t,x),\psi(x,z)) = (Q(x)e^{i\omega t}, \Psi(x,z))$. For such solutions, the natural dispersion of the linear Schrödinger equation is compensated by the non linear term. As a matter of fact, we check that $(u(t,x),\psi(x,z)) = (Q(x)e^{i\omega t}, \Psi(x,z))$ is a solution of (1a)–(1b) if and only if $\Psi(x,z) = \Gamma(z)\sigma_1 \star Q^2(x)$ and Q is a solution of the following Choquard equation

$$-\frac{1}{2}\Delta_x Q + \omega Q - \kappa(\Sigma \star Q^2)Q = 0. \quad (7)$$

The Choquard equation (7) has been intensively studied: see for example [14, 15], and the references therein. In particular, with the assumptions made on σ_1, we know that equation (7) has infinitely many non trivial solutions, and thus the Schrödinger-Wave system admits many solitary waves. It is worth pointing out that neither Ψ, nor the Choquard equation (7), depend on the wave speed c. This means that if $(u(t,x),\psi(x,z)) = (Q(x)e^{i\omega t},\Psi(x,z))$ is a solitary wave of the Schrödinger-Wave system for some $c_0 > 0$, then (u,ψ) is a solitary wave of the Schrödinger-Wave equation for every wave speed $c > 0$. This property equally applies for the asymptotic system (5a)–(5b). To be more specific, if $(u(t,x),\psi(x,z)) = (Q(x)e^{i\omega t},\Psi(x,z))$ is a solution of the Schrödinger-Wave system, then (u,ψ) (resp. u) is also a solution of (5a)–(5b) (resp. (6)).

The analysis of the Hartree system (5a)–(5b) provides some useful hints to understand the dynamics for finite c's. However the complex interactions between the particle and the environment are certainly poorly described by the asymptotic system — where the wave function is the only unknown, see (6) — and it is important to understand how the dynamics do differ. A crucial difference is that (6) is Galilean invariant while the Schrödinger-Wave system (1a)–(1b) is not. Hence, let Q be a solution of (7) with $M = \|Q\|^2_{L^2_x}$; we shall work with initial data

$$\tilde{u}_0(x) = Q(x)e^{i\frac{p_0}{M}\cdot x}.$$

Owing to Galilean invariance for (6), we find

$$\tilde{u}(t,x) = Q\Big(x - t\frac{p_0}{M}\Big)\cdot \exp\left(i\frac{p_0}{M}\cdot\Big(x - t\frac{p_0}{M}\Big)\right)\cdot\exp\left(i\omega t + i\frac{|p_0|^2}{2M^2}t\right). \tag{8}$$

In other words, if an impulsion p_0 is given to a solitary wave of mass M, then the solitary wave for (6) moves on a straight line with a uniform momentum p_0/M. We are going to compare this solution to the solution of (1a)–(1b), starting from the same initial data: we wish to investigate how the lack of Galilean invariance for the Schrödinger-Wave system modifies the *movement* of a solitary wave when this solitary wave is initially submitted to an impulsion p_0.

As we shall discuss in details below, this question has to be made more precise because, due to the lack of Galilean invariance, the solitary wave perturbed by an impulsion p_0 can be *deformed* during the time evolution of (1a)–(1b). That the discussion makes sense relies on a stability property of the system which asserts that the solution remains close to the original solitary wave. Such a stability property holds for the ground states of (1a)–(1b), the solitary waves which minimize the energy (3) under a mass constraint. The orbital stability results established in [13] precisely insure that for a small enough impulsion p_0, the solution remains, up to a translation and a change of phase, close to the original solitary wave, uniformly in time. The present study is based on the following statement [13].

Theorem 1.1 (i) Existence of ground states. *There exists $M_0 > 0$ such that for every $M \in (M_0,+\infty)$*

$$J_M = \inf\Big\{E(u,\psi,\chi)\ \textit{s.t.}\ (u,\psi,\chi)\in H^1_x\times L^2_x\dot{H}^1_z\times L^2_xL^2_z\ \textit{and}\ \|u\|^2_{L^2_x} = M\Big\}$$

is strictly negative and achieved at $(u,\psi,\chi) = (Q,\Psi,0)$ where $\Psi(x,z) = \Gamma(z)\sigma_1 \star Q^2(x)$ and Q is a solution of the Choquard equation (7) for some $\omega > 0$. Moreover, Q is a positive, radially symmetric, function which belongs to the Schwartz class, and its radial profile is decreasing. Such

minimizer (Q,Ψ) *of* J_M *is called a ground state.*
(ii) Orbital stability. *For every* $(u_0,\psi_0,\chi_0)\in H^1_x\times L^2_x\dot H^1_z\times L^2_xL^2_z$ *let us denote by* $(u,\psi,\chi=\partial_t\psi)$ *the unique solution of* (1a)–(1b) *associated to the initial data* (u_0,ψ_0,χ_0). *Let* $M>M_0$, $(Q,\Psi,0)$ *be a ground state of* J_M *and let us assume that* $\|u_0\|_{L^2_x}=\|Q\|_{L^2_x}$. *For every* $\varepsilon>0$ *sufficiently small, there exists* $\eta(\varepsilon)>0$ *and* $\delta(\varepsilon)>0$ *such that the following condition on the initial data*

$$\|u_0-Q\|^2_{H^1_x}+\|\psi_0-\Psi\|^2_{L^2_x\dot H^1_z}+\frac{1}{c^2}\|\chi_0\|^2_{L^2_xL^2_z}\le\eta(\varepsilon)^2\quad\textit{and}\quad W(u_0,\psi_0,\chi_0)-W(Q,\Psi,0)\le\delta(\varepsilon),$$

implies the existence of two continuous functions $t\mapsto x(t)\in\mathbb{R}^d$ *and* $t\mapsto\gamma(t)\in\mathbb{R}$ *such that*

$$\sup_{t\ge0}\left\|u(t)-e^{i\gamma(t)}Q(\cdot-x(t))\right\|^2_{H^1_x}+\|\psi(t)-\Psi(\cdot-x(t))\|^2_{L^2_x\dot H^1_z}+\frac{1}{c^2}\|\chi(t)\|^2_{L^2_xL^2_z}\le\varepsilon^2. \tag{9}$$

Assuming $|p_0|\ll1$, we can apply Theorem 1.1-ii) with $u_0(x)=Q(x)e^{i\frac{p_0}{M}\cdot x}$ and $(\psi_0,\psi_1)(x,z)=(\Psi(x,z),0)$. The modulation parameter $x(t)$ seems to be a natural candidate for the *position* of the ground state and we can thus study its *movement*. Nevertheless, although the modulation parameters $x(t)$ and $\gamma(t)$ are uniquely determined (thanks to some orthogonality conditions, see [13, Theorem 2.9]), the continuity of the translation operator on H^1_x implies that the stability estimate (9) equally applies when $x(t)$ is replaced by a function $y(t)$ such that $\|y-x\|_{L^\infty_t}\ll1$. Thus the notion of *position* of a ground state along time is not absolute (the function $y(t)$ could also be a definition of the position) but only defined up to a small translation. This remark raises the issue of clarifying the quantities of interest to study numerically the *movement* of a ground state.

1.1 Motivation

In order to motivate our study and to have some insight on what could be the dynamic of the position of a ground state, let us briefly recall the physical motivation of the Schrödinger-Wave equation. This system belongs to the large class of open systems modeling dissipative effects. Indeed, as suggested by A. Caldeira and A. Legget in [6, 7] the dissipation arising on a physical system might come from a coupling with a complex environment. In this approach, dissipation is interpreted as the transfer of energy from the single degree of freedom characterizing the system to the more complex set of degrees of freedom describing the environment; the energy is evacuated into the environment and does not come back to the system. To be more specific, the Schrödinger-Wave system is the quantum version of the classical model introduced by L. Bruneau and S. De Bièvre in [5]:

$$\ddot q(t)=-\iint\nabla\sigma_1(q(t)-y)\sigma_2(z)\psi(t,y,z)\,\mathrm{d}z\,\mathrm{d}y,\qquad t\in\mathbb{R} \tag{10a}$$

$$(\partial^2_{tt}\psi-c^2\Delta_z\psi)(t,z)=-c^2\sigma_2(z)\,\sigma_1(x-q(t)),\qquad t\in\mathbb{R},\ x\in\mathbb{R}^d,\ z\in\mathbb{R}^n \tag{10b}$$

completed by the initial data

$$(q(0),\dot q(0))=(q_0,p_0),\qquad(\psi(0,x,z),\partial_t\psi(0,x,z))=(\psi_0(x,z),\psi_1(x,z)). \tag{11}$$

In this system, $q(t)$ denotes the position of the classical particle and $\psi(t,x,z)$ still describes the state of the vibrational environment. Roughly speaking the environment can be thought of as a

(continuum) set of membranes, activated by the passage of the particle. On each position $x \in \mathbb{R}^d$, the particle exchanges momentum and energy with the membranes. The evacuation of energy through the membranes eventually leads to a sort of friction effect. In (1a)–(1b), the position-velocity pair (q, p) of the classical modeling is replaced by the wave function u governed by the Schrödinger equation. A fully quantized model is discussed in [4, 8]. We point out that here the wave equation is scaled differently than in the seminal paper [5], with an extra c^2-factor on the right hand side of (10b). We refer the reader to [13] for the justification of this rescaling. The main finding in [5] is precisely to exhibit the friction effects in the dynamics of (10a)–(10b), as illustrated by the following statement (see [5, Theorems 2 & 4] for further details).

Theorem 1.2 *Let $n = 3$. For any $\eta \in (0, 1)$ there exists a critical wave speed $c_0 = c_0(\eta) > 0$ and constants $\gamma, K > 0$ (which do not depend on η) such that for any $c \geq c_0$ there exists $q_\infty = q_\infty(c) \in \mathbb{R}^d$ such that*

$$|\dot{q}(t)| + |q(t) - q_\infty| \leq K e^{-\frac{\gamma(1-\eta)}{c}t}.$$

Remark 1.3 *As explained above, we have adopted a different scaling of the wave equation: this is the reason why the corresponding result in [5] appears with a factor c^{-3} in the convergence rate instead of c^{-1} here.*

This result makes it concrete the dissipation mechanism of the interaction with the environment. The conditions on the dimension n of the vibrational field and on the wave speed c are quite critical, as confirmed by the numerical experiments in [12]. Indeed, the dissipative effect comes from the capability of evacuating the kinetic energy of the particle through the vibrations in the transverse directions: the condition $n \geq 3$ can be seen as a condition insuring a strong enough dispersion effect in the membranes. It implies that the energy given by the particle to the environment does not entirely come back to the particle. Of course, the shape of the form function σ_2, and the fact it is compactly supported, are crucial in this mechanism. Moreover, requesting c large enough can be interpreted as a condition ensuring that the energy is quickly evacuated in the membrane, out of the support of σ_2. Since the dispersion rate of the wave equation depends on the dimension n, the friction effect of the environment on the particle depends on n. The specific case $n = 3$ makes a linear relation appear between the asymptotic velocity of the particle and the resulting friction force (and thus an exponential convergence rate), as pointed out in [5, Section 2], see also Remark 1.6 below.

The stability of the ground states can be seen as a natural analog of these properties for the quantum model (1a)–(1b): we still expect that the vibrational field ψ produces a friction effect on the wave function u. The orbital stability result in Theorem 1.1 insures that, up to an error term of size ε, the solution associated to a small initial perturbation of the ground state stays close to $(Q(x - x(t))e^{i\gamma(t)}, \Psi(x - x(t), z))$. Then, if the environment ψ acts on the wave function u as a friction force, one can expect that the wave function u remains at a bounded distance of the original ground state $(Q(x), \Psi(x, z))$, which means that $t \mapsto x(t)$ is bounded. These are the issues we wish to numerically investigate.

1.2 Conjectures and main results

From now on, we fix a mass $M > M_0$, a ground state (Q, Ψ) such that $\|Q\|^2_{L^2_x} = M$ and an initial impulsion p_0. We consider an initial data for (1a)–(1b) of the form

$$u_0(x) = Q(x)e^{i\frac{p_0}{M}\cdot x} \qquad (\psi_0, \psi_1) = (\Psi, 0).$$

We denote by (u, ψ) the unique solution of (1a)–(1b) associated to this initial data. We assume that p_0 is small enough so that Theorem 1.1 applies. Thus there exists four functions $(t, x) \mapsto u^\varepsilon(t, x)$, $(t, x, z) \mapsto \psi^\varepsilon(t, x, z)$, $t \mapsto x(t)$ and $t \mapsto \gamma(t)$ such that

$$u(t, x) = Q(x - x(t))e^{i\gamma(t)} + u^\varepsilon(t, x) \qquad \psi(t, x, z) = \Psi(x - x(t), z) + \psi^\varepsilon(t, x, z)$$

and

$$\sup_{t\geq 0} \left(\|u^\varepsilon(t)\|_{H^1_x} + \|\psi^\varepsilon(t)\|_{L^2_x \dot{H}^1_z} + \frac{1}{c^2}\|\partial_t \psi^\varepsilon(t)\|_{L^2_x L^2_z} \right) \leq \varepsilon^2.$$

We wish to challenge on numerical grounds this stability result, the intuition on the problem and the analogy with the model for a single classical particle. To this end, we shall produce numerical approximations of the solutions: hereafter, we denote with a subscript h the numerical solution, where $h > 0$ refers to the discretization parameters. The following conjecture would be the analog of Theorem 1.2 for the quantum model.

Conjecture 1.4 *Let $n = 3$ and $c > 0$. There exists constants $\lambda, C > 0$ such that for any p_0 sufficiently small we can find a function $t \mapsto y(t) \in \mathbb{R}^d$ and $y_\infty \in \mathbb{R}^d$ such that the conclusion* (9) *of Theorem 1.1 still applies when the modulation parameter $x(t)$ is replaced by $y(t)$ and*

$$|\dot{y}(t)| + |y(t) - y_\infty| \leq Ce^{-\frac{\lambda}{c}t}.$$

Remark 1.5 *The conjecture is stated only when the conclusion of Theorem 1.1 is valid, and how p_0 has to be small depends on the assumptions of this theorem. However, in the regime $c \gg 1$ we believe that the assumptions can be weakened. To be more specific, since for $c \to +\infty$ the asymptotic system is Galilean invariant, we believe that the smallness assumption on $u_0 - Q$ can be relaxed in the direction $\exp(ip_0 \cdot x/M)$ when $c \gg |p_0|$. We will investigate numerically how p_0 has to be small depending on the value of c.*

We warn the reader that this conjecture involves a function $t \mapsto y(t)$ which could differ from the modulation parameter $x(t)$. This is related to the fact, mentioned above, that the position of a ground state for (1a)–(1b) along time is not absolute due to the possible deformation of the ground state. From the function y one can easily construct another smooth function $\bar{y}$ such that $\|\bar{y} - y\|_{L^\infty_t} \ll 1$ (and then such that (9) applies with $\bar{y}(t)$ replacing $x(t)$) and such that $\bar{y}(t)$ is rapidly oscillating around y_∞ without converging to it as $t \to +\infty$. For this function there exists $C > 0$ such that for every $\bar{y}_\infty \in \mathbb{R}^d$

$$\limsup_{t\to+\infty} |\dot{\bar{y}}(t)| + |\bar{y}(t) - \bar{y}_\infty| > C$$

and then Conjecture 1.4 fails with $\bar{y}(t)$. In particular, there is no reason to believe *a priori* that the conjecture applies with $y = x$.

This discussion raises the issue of the definition and computation of the *position* of a ground state along time. The definition of x relies on orthogonality relations, see [13], which can indeed be used to compute the modulation parameter $x(t)$. However, we shall introduce another quantity, which is more physical and which will allow us to perform finer predictions: the center of mass of the solution, which is given by

$$q(t) = \frac{\displaystyle\int x|u(t, x)|^2 \, \mathrm{d}x}{\displaystyle\int |u(t, x)|^2 \, \mathrm{d}x} = \frac{1}{M} \int x|u(t, x)|^2 \, \mathrm{d}x.$$

In order to investigate the validity of the conjecture we have first to check that $q(t)$ stays close to $x(t)$, uniformly in time. The following computation shows that this is formally the case:

$$\begin{aligned} Mq(t) &= x(t)\int |u(t,x)|^2\,\mathrm{d}x + \int (x-x(t))|u(t,x)|^2\,\mathrm{d}x \\ &= Mx(t) + \int (x-x(t))|Q(x-x(t))|^2\,\mathrm{d}x \\ &\qquad +2\mathrm{Re}\int (x-x(t))Q(x-x(t))e^{-i\gamma(t)}u^\varepsilon(t,x)\,\mathrm{d}x + \int (x-x(t))|u^\varepsilon(t,x)|^2\,\mathrm{d}x \\ &= Mx(t) + 0 + 2\mathrm{Re}\int (x-x(t))Q(x-x(t))e^{-i\gamma(t)}u^\varepsilon(t,x)\,\mathrm{d}x + \int (x-x(t))|u^\varepsilon(t,x)|^2\,\mathrm{d}x, \end{aligned}$$

where the second term is equal to zero because Q is radially symmetric. We thus get

$$|q(t)-x(t)| \le \frac{2}{M}\|xQ\|_{L^2_x}\|u^\varepsilon(t)\|_{L^2_x} + \frac{1}{M}\int |x-x(t)|\,|u^\varepsilon(t,x)|^2\,\mathrm{d}x.$$

Theorem 1.1 insures that $\|u^\varepsilon(t)\|_{H^1_x}$ is dominated by ε, uniformly in time. Thus the first term of the estimate is of order $\mathscr{O}(\varepsilon)$. However, we have no information on the boundedness of $\int |x-x(t)|\,|u^\varepsilon(t)|^2\,\mathrm{d}x$ along time, and the second term is only formally of order $\mathscr{O}(\varepsilon^2)$. Nevertheless it will be easy to check whether or not this behavior is confirmed numerically. Indeed, once the numerical approximation u_h of the wave function is computed, we will be able to compute its center of mass q_h and then to compute in some discrete norm the difference

$$\epsilon^1_h = |u_h| - Q_h(x-q_h). \tag{12}$$

This is the purpose of our first numerical investigation and we obtain the following conclusion.

Observation 1 *The quantity ϵ^1_h remains small, uniformly on the simulation time, in discrete L^2_x, H^1_x and L^∞_x-norms.*

This fact confirms the formal computation. From now on we will assume that the following decomposition is valid

$$u(t,x) = Q(x-q(t))e^{i\gamma(t)} + \widetilde{u^\varepsilon}(t,x) \tag{13}$$

where $\widetilde{u^\varepsilon}$ is of order $\mathscr{O}(\varepsilon)$.

It would be tempting to investigate the validity of the conjecture with $y(t) = q(t)$. Indeed, this quantity has a physical meaning and it is easier to compute than the modulation parameter $x(t)$. However, the computation of the center of mass requires the computation of the wave function u itself. Furthermore, a priori we have no information on the damping of this quantity and we cannot exclude that $q(t)$ does not converge exponentially fast to some asymptotic position but instead oscillates around it. Such oscillations can come from the part $\widetilde{u^\varepsilon}$ of the wave function which is not damped. Another (more optimistic) possible scenario is that $\widetilde{u^\varepsilon}$ is damped but with a rate slower than exponential: the possible oscillations of $q(t)$ can be damped but not with the expected exponential rate. For this reason, we decide to work with another relevant function y which is robust with respect to the small perturbations of the wave function. To this end, let us observe that the evolution of the center of mass is governed by

$$M\dot{q}(t) = p(t) \qquad \text{with } p(t) = \mathrm{Im}\int \nabla_x u(t)\bar{u}(t)\,\mathrm{d}x, \tag{14a}$$

$$\dot{p}(t) = -\int \nabla_x \left(\sigma_1 \star \int \sigma_2\psi(t)\,\mathrm{d}z\right)|u(t)|^2\,\mathrm{d}x, \tag{14b}$$

$$\partial^2_{tt}\psi - c^2\Delta_z\psi = -c^2\sigma_2(z)\,\sigma_1 \star |u(t)|^2, \tag{14c}$$

endowed with the initial data

$$(q(0),p(0)) = \left(\frac{1}{M}\int x|u_0|^2\,\mathrm{d}x, \mathrm{Im}\int \nabla_x u_0 \bar{u}_0\,\mathrm{d}x\right), \qquad (\psi_0,\psi_1) = (\Psi,0).$$

With the specific choice of initial data u_0 we have $q(0)=0$ and $p(0)=p_0$. Neglecting the fluctuation term $\widetilde{u^\varepsilon}$ in (13), we obtain the following simplified system

$$M\frac{\mathrm{d}}{\mathrm{d}t}q^a(t) = p^a(t) \tag{15a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}p^a(t) = -\int \nabla_x\left(\sigma_1 \star \int \sigma_2\psi^a(t)\,\mathrm{d}z\right) Q^2(x-q^a(t))\,\mathrm{d}x, \tag{15b}$$

$$\partial_{tt}^2\psi^a - c^2\Delta_z\psi^a = -c^2\sigma_2(z)\,\sigma_1\star Q^2(\cdot - q^a(t)), \tag{15c}$$

endowed with the initial data

$$(q^a(0),p^a(0)) = (0,p_0), \qquad (\psi_0^a,\psi_1^a) = (\Psi,0).$$

This closed system is similar to the model for a classical particle (10a)–(10b). Indeed, using the fact that σ_1 and Q^2 are radially symmetric one can check that the right hand side of (15b) is exactly the right hand side of (10a) when σ_1 is replaced by $\sigma_1\star Q^2$:

$$-\int \nabla_x\left(\sigma_1\star\int\sigma_2\psi^a(t)\,\mathrm{d}z\right)Q^2(x-q^a(t))\,\mathrm{d}x = -\nabla_x\left(\left(\sigma_1\star Q^2\right)\star\int\sigma_2\psi^a(t)\,\mathrm{d}z\right)(q^a(t)).$$

Then (15a)–(15c) is exactly (10a)–(10b) with a particle of mass M instead of mass 1 and with the form function $\sigma_1\star Q^2$ instead of σ_1.

By construction q^a does not depend on the fluctuations of the wave function u as we would like it to be. Using the decomposition given by the orbital stability result of Theorem 1.1 shows that the force term acting on the center of mass $q(t)$ in (14b) is of order $\mathscr{O}(\varepsilon)$:

$$\begin{aligned}\int \nabla_x\left(\sigma_1\star\int\sigma_2\psi(t)\,\mathrm{d}z\right)|u(t)|^2\,\mathrm{d}x &= \int \nabla_x\left(\sigma_1\star\int\sigma_2\Psi(\cdot-x(t),z)\,\mathrm{d}z\right)|Q(x-x(t)|^2\,\mathrm{d}x\\ &+2\mathrm{Re}\int\nabla_x\left(\sigma_1\star\int\sigma_2\Psi(\cdot-x(t),z)\,\mathrm{d}z\right)Q(x-x(t))e^{-i\gamma(t)}u^\varepsilon(t,x)\,\mathrm{d}x\\ &+\int\nabla_x\left(\sigma_1\star\int\sigma_2\psi^\varepsilon(t)\,\mathrm{d}z\right)|Q(x-x(t))|^2\,\mathrm{d}x\\ &+\int\nabla_x\left(\sigma_1\star\int\sigma_2\Psi(\cdot-x(t),z)\,\mathrm{d}z\right)|u^\varepsilon(t,x)|^2\,\mathrm{d}x\\ &+2\mathrm{Re}\int\nabla_x\left(\sigma_1\star\int\sigma_2\psi^\varepsilon(t)\,\mathrm{d}z\right)Q(x-x(t))e^{-i\gamma(t)}u^\varepsilon(t,x)\,\mathrm{d}x\\ &+\int\nabla_x\left(\sigma_1\star\int\sigma_2\psi^\varepsilon(t)\,\mathrm{d}z\right)|u^\varepsilon(t,x)|^2\,\mathrm{d}x.\end{aligned}$$

Every element of this decomposition is at least of order $\mathscr{O}(\varepsilon)$ except the first one which at first sight is of order $\mathscr{O}(1)$. But actually this term vanishes since

$$\begin{aligned}&\int\nabla_x\left(\sigma_1\star\int\sigma_2\Psi(\cdot-x(t),z)\,\mathrm{d}z\right)|Q(x-x(t))|^2\,\mathrm{d}x\\ &\qquad = -\kappa\int\nabla_x\left(\sigma_1\star Q^2(\cdot-x(t))\right)Q^2(x-x(t))\,\mathrm{d}x = 0.\end{aligned}$$

Therefore, the force term in (14b) is of order $\mathscr{O}(\varepsilon)$. The terms neglected in (14a)–(14c) are of the same order $\mathscr{O}(\varepsilon)$ and their effects on the dynamics, with possible deformations of the wave function u due to the nonlinear terms, cannot be considered as negligible, even on short time intervals. In particular, we do not know whether or not $q^a(t)$ remains close to the center of mass $q(t)$. We address this question numerically and we obtain the following conclusion.

Observation 2 *We observe numerically that $\epsilon_h^2 = |q_h^a - q_h| + |p_h^a - p_h|$ remains small along time.*

The numerical simulations indicate that, for the considered initial data, $q^a(t)$ can be used to define the *position* of the ground state. This quantity does not depend on the small perturbations of the wave function around the moving ground state, and we have investigated the conjecture with $y(t) = q^a(t)$.

Observation 3 *We observe numerically that the momentum of the moving ground state converges exponentially fast to zero and its position converges to an asymptotic point with the same exponential rate. Moreover the exponential rate is proportional to c^{-1} and depends on the considering ground state Q. To be more precise there exists an asymptotic position q^∞ such that*

$$|p_h^a(t^n)| + |q_h^a(t^n) - q^\infty| \leq e^{-\frac{\lambda}{c}t^n}$$

where $\lambda = \lambda(Q)$ depends on Q.

Remark 1.6 *Let us discuss further the analogy between the classical and the quantum models. According to [5, Section 2], the force exerted by the environment when the particle has a uniform rectilinear motion can be explicitly computed, as a function of the particle's speed v. We get*

$$f(v) = -\iint_{\mathbb{R}^d\times\mathbb{R}^n} |\hat{\sigma}_2(\zeta)|^2 \left(\int_0^{+\infty} \frac{\sin(c|\zeta|\tau)}{c|\zeta|}\sigma_1(x+\tau v)\,\mathrm{d}\tau\right) \nabla_x\sigma_1(x)\,\mathrm{d}x\,\mathrm{d}\zeta.$$

It can be recast as

$$f(v) = f_r(|v|)\frac{v}{|v|}, \quad f_r(|v|) < 0$$

which makes the fact that the environment acts against the particle motion appear. Moreover, f_r vanishes when $v = 0$, and, more precisely it has the following behavior as $v \to 0$

$$f_r(|v|) = -\gamma\left(\frac{|v|}{c}\right)^{n-2} + o\left(\frac{|v|}{c}\right)^{n-2},$$

(this formula takes into account the rescaling of the current paper) where $\gamma > 0$ depends on the form functions σ_1 and σ_2:

$$\gamma = |\hat{\sigma}_2(0)|^2 \iint_{\mathbb{R}^d\times\mathbb{R}^n} \left(\int_0^{+\infty} \frac{\sin(\tau|\zeta|)}{|\zeta|}\sigma_1(x_1+\tau, x_\perp)\,\mathrm{d}\tau\right) \partial_{x_1}\sigma_1(x)\,\mathrm{d}x\,\mathrm{d}\zeta.$$

This formula shows the critical role of the dimension $n = 3$: when $n = 3$ it corresponds to a linear friction, with coefficient γ/c, when $n \geq 4$ the friction law becomes non linear with exponent $n-2$ (when $n = 1, 2$ the previous computations are meaningless; for instance the formula which defines γ is well defined only when $n \geq 3$).

Going back to the quantum model, this discussion can be adapted to make how λ depends on Q explicit. We assume that the soliton Q has a rectilinear uniform motion, at speed v, without deformation. We have already seen that in this case, replacing σ_1 by $\sigma_1 \star Q^2$, the systems (15a)–(15c) *and* (10a)–(10b) *are similar. Therefore $\lambda(Q)$ can be computed like γ, up to changing σ_1 into $\sigma_1 \star Q^2$; it leads to*

$$\lambda(Q) = |\hat{\sigma}_2(0)|^2 \iint_{\mathbb{R}^d \times \mathbb{R}^n} \left(\int_0^{+\infty} \frac{\sin(\tau|\zeta|)}{|\zeta|} \, \sigma_1 \star Q^2(x_1 + \tau, x_\perp) \, \mathrm{d}\tau \right) \partial_{x_1} (\sigma_1 \star Q^2)(x) \, \mathrm{d}x \, \mathrm{d}\zeta.$$

Up to now, we have focused the discussion on the translation of the ground state and neglected the change of phase. Let us go back to this issue now. To this end, we consider the asymptotic system (6) for which the Galilean invariance gives the explicit formula (8) and thus an exact knowledge of the phase of the solution. This formula can be rewritten by means of the center of mass of the solution: if we denote by $\tilde{q}(t)$ the center of mass of $\tilde{u}(t)$:

$$\tilde{q}(t) = \frac{1}{M} \int x |\tilde{u}(t,x)|^2 \, \mathrm{d}x,$$

then

$$M \frac{\mathrm{d}}{\mathrm{d}t} \tilde{q}(t) = \tilde{p}(t) \quad \text{with } \tilde{p}(t) = \mathrm{Im} \int \nabla_x \tilde{u}(t) \overline{\tilde{u}(t)} \, \mathrm{d}x, \tag{16a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \tilde{p}(t) = 0, \tag{16b}$$

and we eventually obtain

$$\tilde{u}(t,x) = Q(x - \tilde{q}(t)) \cdot \exp\left(i \frac{\tilde{p}(t)}{M} \cdot (x - \tilde{q}(t)) \right) \cdot \exp\left(i\omega t + \frac{i}{2M^2} \int_0^t |\tilde{p}(s)|^2 \, \mathrm{d}s \right).$$

We already know that $|u(t)| - Q(x - q^a(t))$ remains small along time, and (15a)–(15c) is asymptotic to (16a)–(16b). By analogy with the previous formula we expect that

$$\left\| u(t,x) - Q(x - q^a(t)) \cdot \exp\left(i \frac{p^a(t)}{M} \cdot (x - q^a(t)) \right) \cdot \exp\left(i\omega t + \frac{i}{2M} \int_0^t |p^a(s)|^2 \, \mathrm{d}s \right) \right\|$$

is uniformly small for all time. This conjecture is the purpose of our fourth numerical investigation.

Observation 4 *We observe numerically that the discrete quantity*

$$\epsilon_h^3 = u_h(t^n) - Q_h(x - q_h^a(t^n)) \cdot \exp\left(i \frac{p_h^a(t^n)}{M} \cdot (x - q_h^a(t^n)) \right) \cdot \exp\left(i\omega_h t^n + i\gamma_h^a(t^n) \right) \tag{17}$$

where γ_h^a stands for the discrete equivalent of

$$\gamma^a(t) = \frac{1}{2M^2} \int_0^t |p^a(s)|^2 \, \mathrm{d}s,$$

remains small for every t^n in discrete L_x^2, H_x^1 and L_x^∞-norms.

The paper is organized as follows. Section 2 we detail the numerical results and discuss on numerical grounds Observations 1-4 stated before. Section 3 describes the construction of the numerical method: we need a scheme for the Schrödinger-Wave system (1a)–(1b) and another one for solving the Choquard equation (7) in order to compute an approximation of a ground state. In Section 4 we investigate the energetic properties of the scheme discretizing (1a)–(1b).

2 Numerical results

For all the simulations discussed below we work with the form functions

$$\sigma_1(x) = K_1 \exp\Big(- \frac{1}{R_1^2 - x^2}\Big) \mathbf{1}_{|x| \leq R_1}$$

and

$$\sigma_2(z) = \tilde{\sigma}_2(|z|), \qquad \tilde{\sigma}_2(r) = K_2 \exp\Big(- \frac{1}{R_2^2 - x^2}\Big) \mathbf{1}_{r \leq R_2}.$$

The parameters used for the computational domain and the form functions are collected in Table 1. We refer the reader to the next Section for details on the numerical scheme. The wave equation is solved with the $\mathbb{P}_2$ Lagrange elements and we perform the simulations with a solitary wave of mass $M = 2$ (we did not take a mass $M = 1$ in order to test the validity of the mass dependence in (17)).

K_1	R_1	K_2	R_2	L	R_{max}	N_x	N_r	Δx	Δr	Δt
3	1	3	1	8π	$2R_2$	1024	512	$8\pi/1024$	$2/1024$	$1/256$

Table 1: General data for the numerical simulations.

The solitary wave Q_h and Υ_h are represented in Figure 1. The solitary wave is computed by

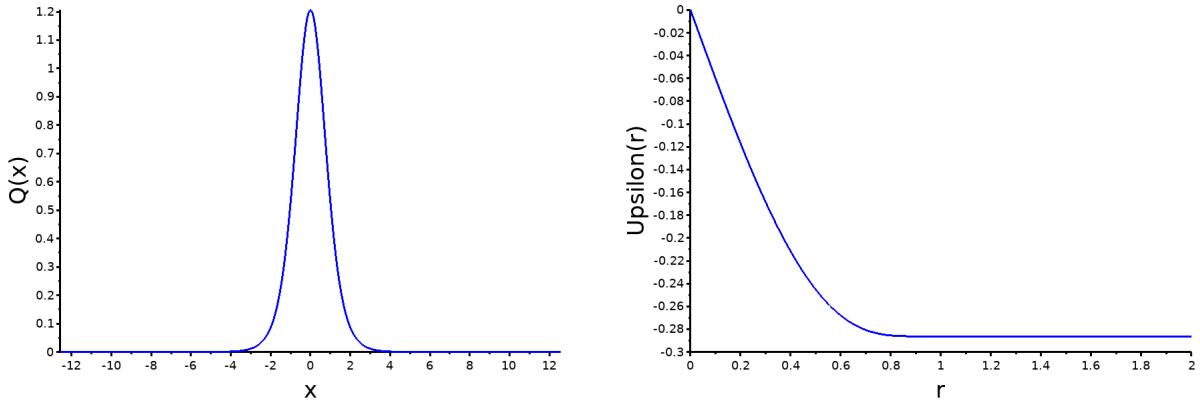

Figure 1: The solitary wave Q_h of mass $M = 2$ (left) and the solution Υ_h of $\partial^2_{rr}\Upsilon = \tilde{\sigma}_2$ (right). From these approximations we get $\omega_h \simeq 2.006$ and $\kappa_h \simeq 1.664$.

using the imaginary time method described in Section 3.2.2. We proceed in two steps. We first apply the imaginary time method with the initial data

$$v_0(x) = \frac{e^{-x^2}}{\| x \mapsto e^{-x^2} \|_{L^2_x}}.$$

It provides a solitary wave of mass $M = 1$. Then, we re-normalize this solitary wave in order to have a function of mass $M = 2$ and we apply again the imaginary time method with this new

initial data. In Figure 2, we have represented the evolution of the energy (25) when the imaginary time method is applied. In particular we observe, as at the continuous level, that this quantity is decreasing.

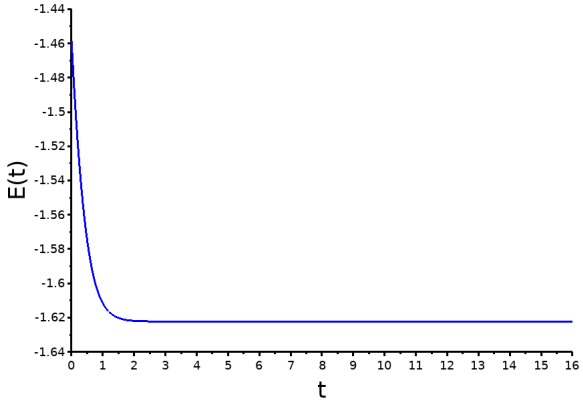

Figure 2: Evolution of energy (25) when the imaginary time method is applied.

Having the solitary wave at hand, we perform simulations with several values for p_0 and c, see Table 2, in order to see how the errors ϵ_h^1, ϵ_h^2 and ϵ_h^3, introduced in Observations 1, 2 and 4, are influenced by these parameters. Test 3 is the most challenging since it combines a large value of the initial impulsion p_0 and a moderate value of the wave speed c. The results are depicted in Figure 3–5.

	Test 1	Test 2	Test 3	Test 4
p_0	0.05	0.05	1.6	1.6
c	5	20	5	20
T	16	32	32	16

Table 2: Data for the study of the error terms ϵ_h^1, ϵ_h^2 and ϵ_h^3.

In particular, we see that these errors stay small along time. We also see that the smaller p_0, the smaller the errors and the larger c, the larger p_0 can be taken. Concerning Observation 4, note that the results are very sensitive to the accuracy of the evaluation of the Lagrange multiplier ω of the soliton: the errors on ω naturally produce an error on the phase, which grows linearly with time, as it can be observed in Figure 5. We also illustrate the dynamic of these solutions in Figure 6–7. In order to see on the figures the differences between $u_h(t^n, x)$ and

$$u_h^a(t^n, x) = Q_h(x - q_h^a(t^n)) \cdot \exp\left(i\frac{p_h^a(t^n)}{M} \cdot (x - q_h^a(t^n))\right) \cdot \exp\left(i\omega_h t^n + i\gamma_h^a(t^n)\right)$$

we make this illustration in the case of Test 3 where the error is the largest.

Then we investigate how the environment acts on the solitary wave. For that purpose, for a given value of p_0 and depending on the value of c (see Table 3) we check that, as asserted in

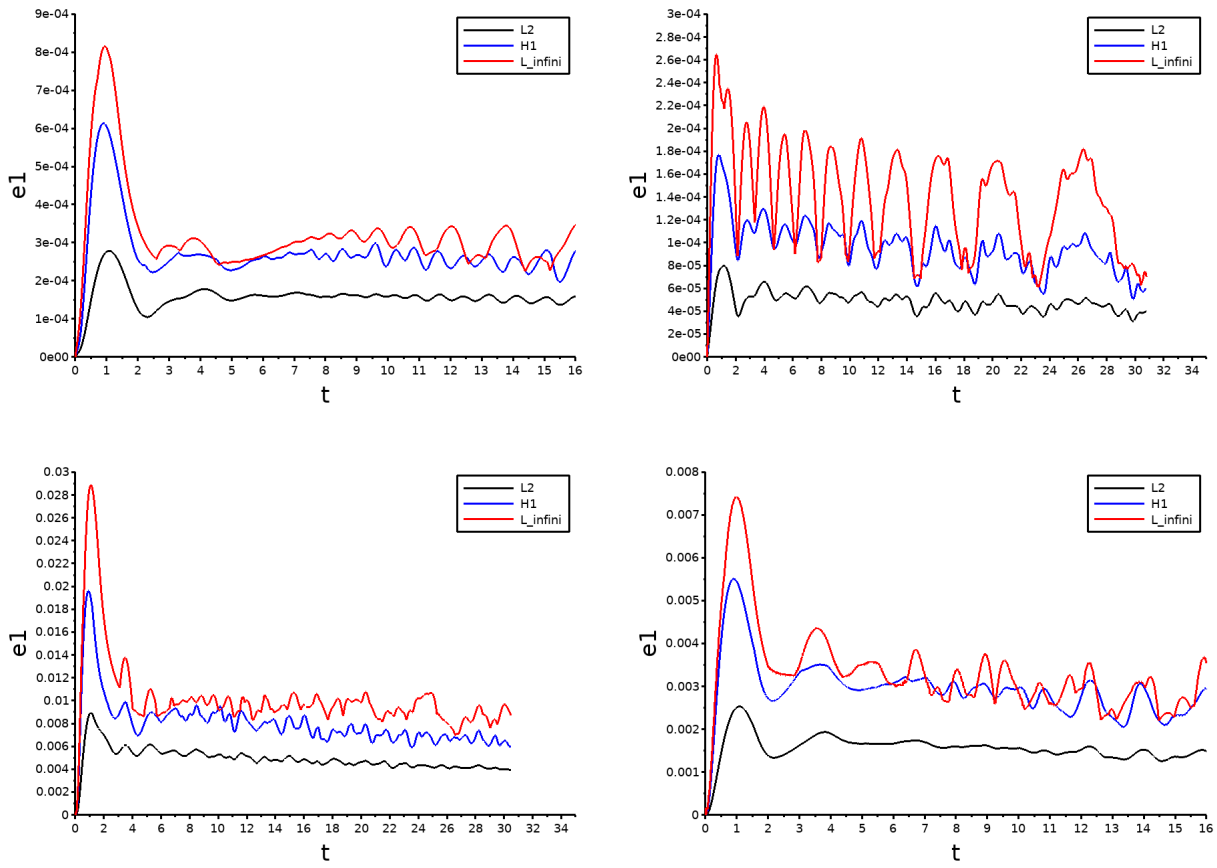

Figure 3: Evolution of the error term ϵ_h^1 along time (from left to right and top to bottom, Test 1 to 4, see Table 2)

	Test 1	Test 2	Test 3	Test 4
p_0	0.05	0.05	0.05	0.05
c	5	10	20	40
T	16	32	32	32

Table 3: Data for the study of the convergence rate to 0 of p_h^a (dependency on c).

Observation 3, p_h^a converges exponentially fast to zero and that the convergence rate is proportional to $1/c$: see Figure 8–9.

3 Numerical schemes

The numerical issues split into two parts: first, we explain how the Schrödinger-Wave system (1a)–(1b) is discretized and, second, we detail how we compute an approximation of a ground state (Q, Ψ). The latter step is crucial since this ground state is used to define the initial data for the

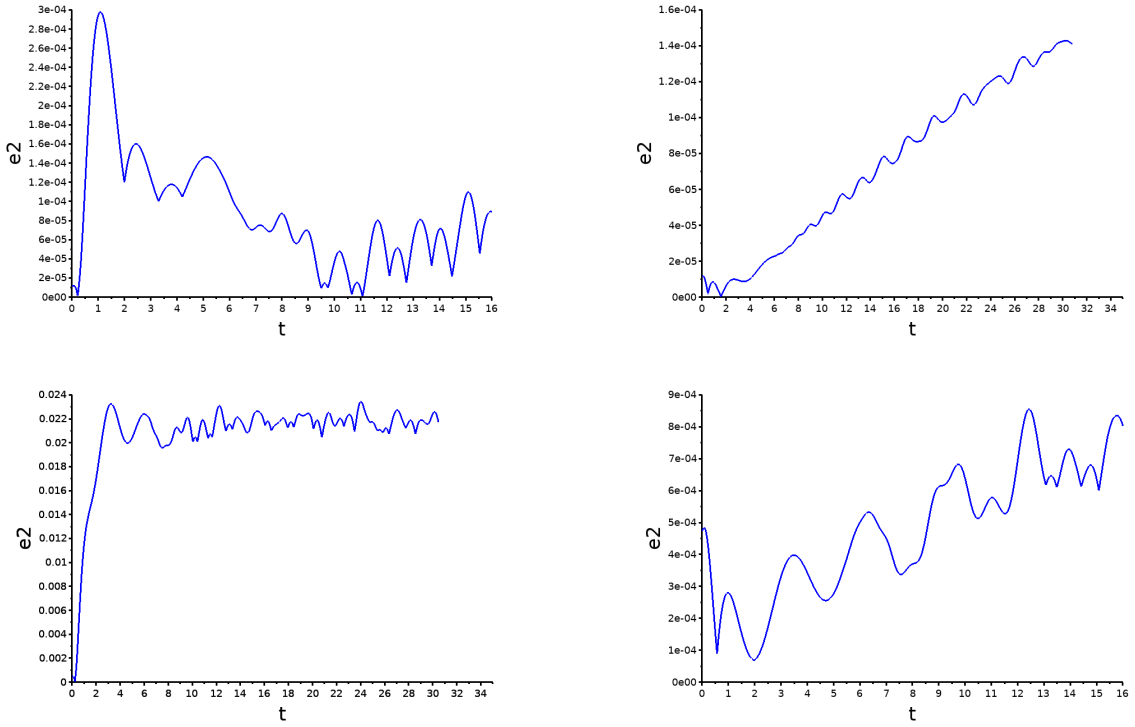

Figure 4: Evolution of the error term ϵ_h^2 along time (from left to right and top to bottom, Test 1 to 4, see Table 2)

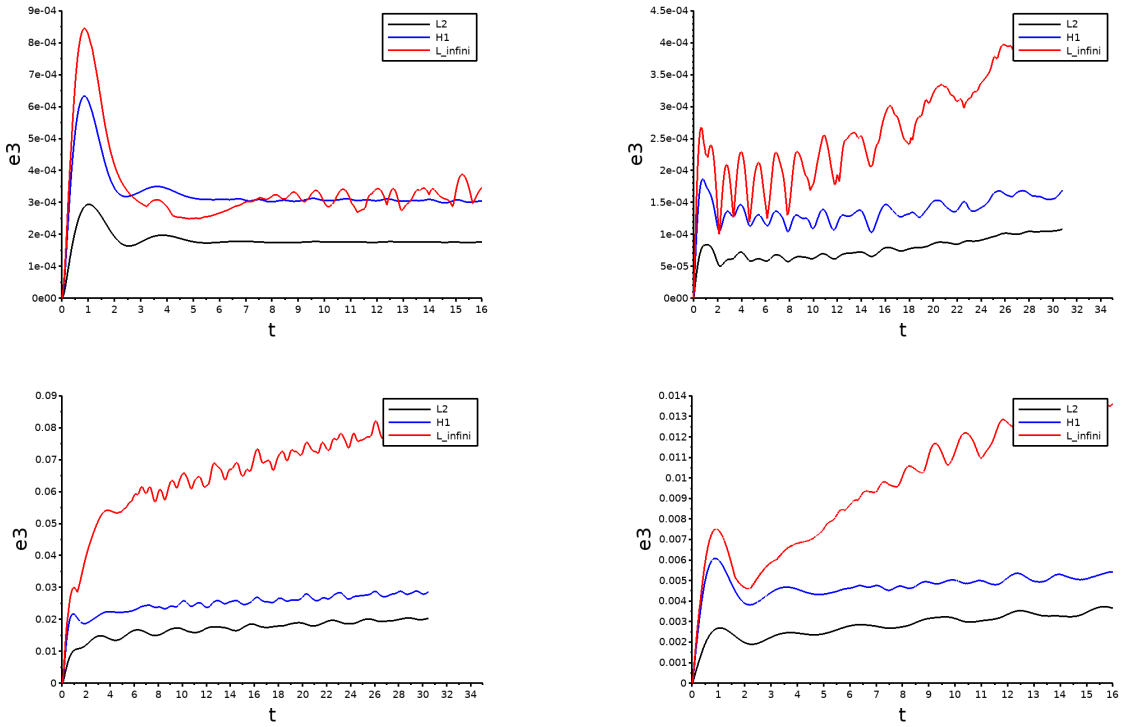

Figure 5: Evolution of the error term ϵ_h^3 along time (from left to right and top to bottom, Test 1 to 4, see Table 2)

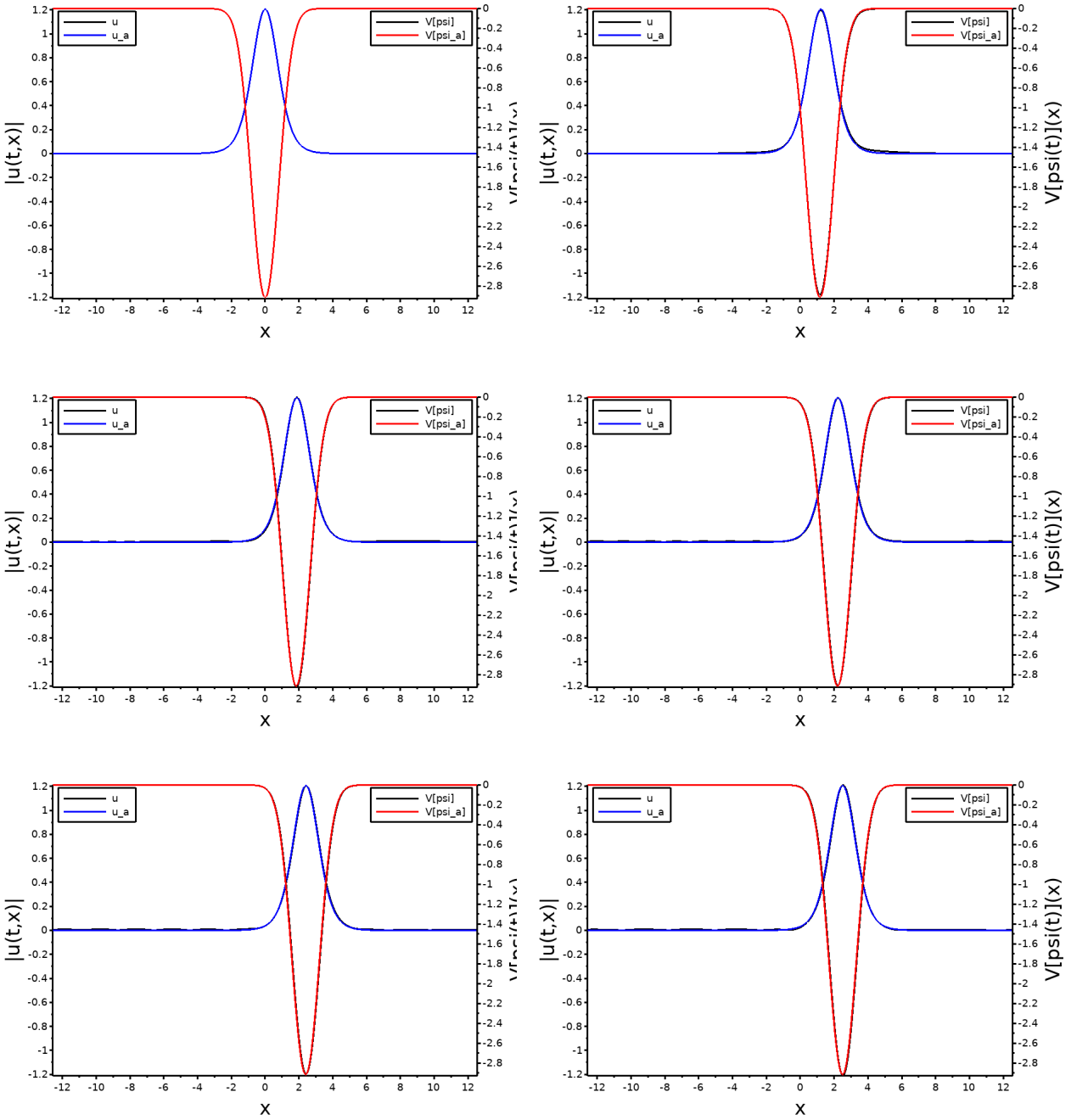

Figure 6: Evolution of the modulus of the wave function and of the potential created by the environment and acting on the wave function. From left to right and top to bottom $t^n = 0$, 2, 4, ..., 10.

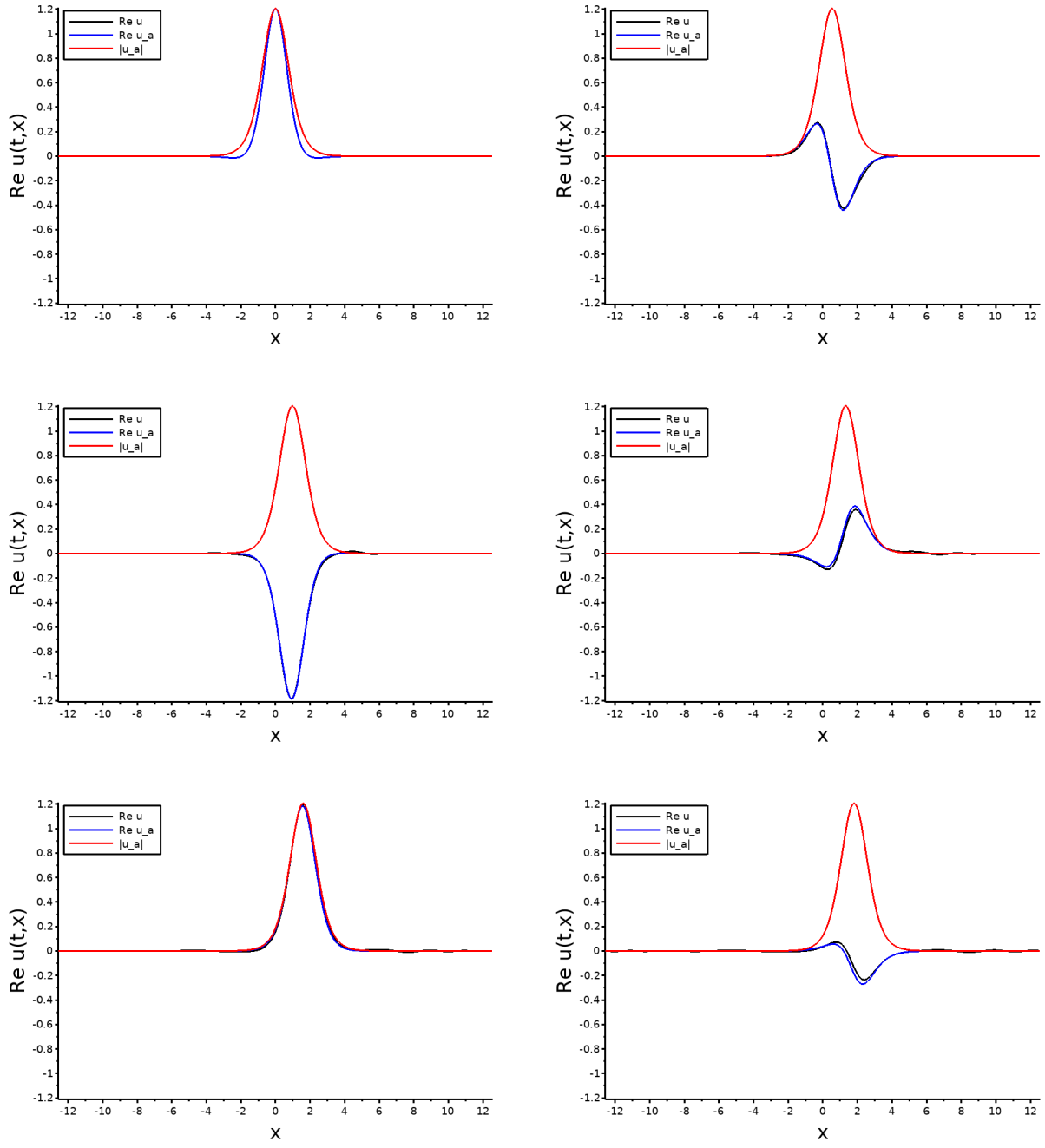

Figure 7: Evolution of the real part of the wave function. From left to right and top to bottom $t^n = 0,\ 0.75,\ 1.5,\ \ldots,\ 3.75$.

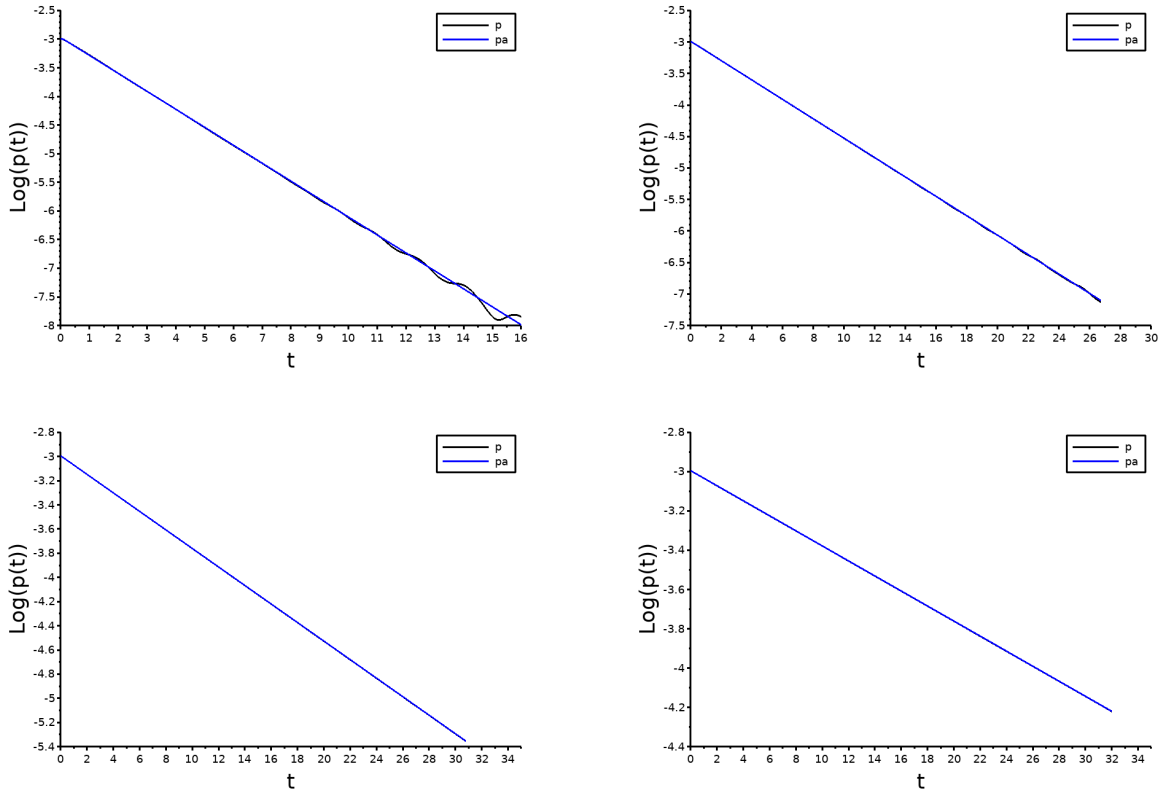

Figure 8: Exponential decay of $p_h^a(t)$ depending on c and comparison with the exponential decay of $p_h(t)$ (from left to right and top to bottom, Test 1 to 4, see Table 3). Top left we observe that when the ground state is almost stopped the exponential decay of the impulsion p_h oscillates while the exponential decreasing of p_h^a does not.

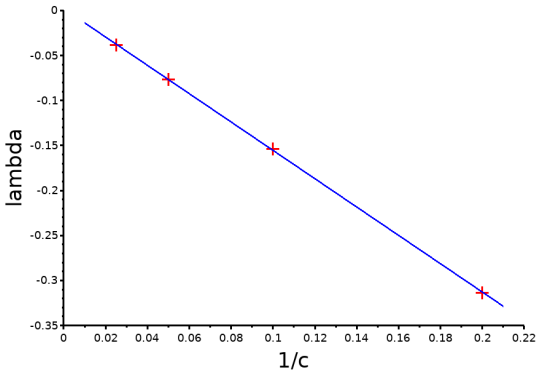

Figure 9: Investigation of the proportionality between the exponential decay to zero of p_h^a and $1/c$.

simulation of the Cauchy problem.

3.1 Discretization of the Schrödinger-Wave system

We restrict ourselves to the case where the wave function u evolves on the one-dimensional torus: $d = 1$ and $x \in \mathbb{T}_L := \mathbb{R}/(L\mathbb{Z})$. Of course, $L > 0$ is chosen at least larger than the diameter of the support of σ_1. The ground states Q decay exponentially fast, and we expect that by choosing $L > 0$ large enough the periodic boundary condition will induce a negligible effect on the computed solutions. This intuition is easily verifiable numerically by performing several numerical simulations with different values of L and comparing the solutions. Another approach could be to use some transparent boundary conditions [1]. For the Schrödinger equation, even in dimension $d = 1$, an exact formula for transparent boundary condition requires the computation of a non local operator; for the sake of simplicity we prefer to work on a sufficiently large computational domain with periodic boundary conditions.

As explained above, it is crucial to consider the wave equation in the three dimensional free space. Thus, we have to take $n = 3$ and we should pay attention to use transparent or absorbing conditions on the boundaries of the computational domain, in order to reproduce the necessary energy evacuation. In dimension $n = 1$, the transparent boundary conditions can be easily identified and computed, but in dimension $n \geq 2$ exact transparent boundary conditions are more involved and lead to some non local formula. The evaluation of the underlying non local operator is numerically costly [9]. Nevertheless in dimension $n = 3$, and for radially symmetric data, there exists a suitable transformation that allows us to reduce the problem to the classical wave equation in dimension $n = 1$ on the domain $[0, +\infty)$ with a Dirichlet boundary condition at $r = 0$, see e.g. [16]. This is the framework we adopt for the simulations. The form function $\sigma_2(z) = \tilde{\sigma}_2(|z|)$ is assumed radially symmetric, the initial data $(\psi_0, \psi_1) = (\Psi, 0)$ where $\Psi(x, z) = \Gamma(z)(\sigma_1 \star Q^2)(x)$ with $\Delta_z \Gamma = \sigma_2$ are radially symmetric too. In what follows, we denote $\Gamma(z) = \tilde{\Gamma}(|z|)$. Then, the solution ψ of (1b) is radially symmetric with respect to the z-variable: $\psi(t, x, z) = \tilde{\psi}(t, x, |z|)$. Setting $\chi(t, x, r) = r\tilde{\psi}(t, x, r)$ and using that $n = 3$ allow us to obtain that χ is a solution of the wave equation in dimension one

$$\partial_{tt}^2 \chi - c^2 \partial_{rr}^2 \chi = -c^2 r \tilde{\sigma}_2(r)(\sigma_1 \star |u(t)|^2)(x), \qquad t \geq 0,\ x \in [-L/2, L/2],\ r \in [0, +\infty), \tag{18a}$$

$$(\chi(0, x, r), \partial_t \chi(0, x, r)) = (r\tilde{\Gamma}(r)(\sigma_1 \star Q^2)(x), 0), \tag{18b}$$

$$\chi(t, x, 0) = 0. \tag{18c}$$

Note that the coupling potential in (1a) can be expressed only by means of the new unknown χ:

$$\phi(t, x) = \int_{-L/2}^{L/2} \sigma_1(x - y) \left(\int_{\mathbb{R}^3} \psi(t, y, z)\, \mathrm{d}z \right) \mathrm{d}y = 4\pi \int_{-L/2}^{L/2} \sigma_1(x - y) \left(\int_0^{+\infty} r\tilde{\sigma}_2(r)\chi(t, y, r) \right) \mathrm{d}y.$$

Moreover, the potential depends on χ only on the support of the function $\tilde{\sigma}_2$. Therefore, we have only to compute χ on a bounded domain $[0, R_{max}]$ with $\mathrm{supp}(\tilde{\sigma}_2) \subset [0, R_{max}]$ and to implement the exact transparent boundary condition on $r = R_{max}$

$$\partial_t \chi(t, x, R_{max}) + c\partial_r \chi(t, x, R_{max}) = 0.$$

We are thus led to discretize the following system:

$$i\partial_t u + \frac{1}{2}\Delta_x u = \left(\int_{-L/2}^{L/2}\int_0^{R_{max}} \sigma_1(x-y)\tilde{\sigma}_2(r)\chi(t,y,r)\,\mathrm{d}y\,\mathrm{d}r\right)u, \quad t\geq 0,\ x\in[-L/2,L/2], \tag{19a}$$

$$u(0,x) = Q(x)\cdot\exp(ip_0\cdot x/M), \qquad x\in[-L/2,L/2], \tag{19b}$$

$$u(t,-L/2) = u(t,L/2), \qquad t\geq 0, \tag{19c}$$

coupled with

$$\partial_{tt}^2\chi - c^2\partial_{rr}^2\chi = -c^2 r\tilde{\sigma}_2(r)(\sigma_1\star|u(t)|^2)(x), \qquad t\geq 0,\ x\in[-L/2,L/2],\ r\in[0,R_{max}], \tag{20a}$$

$$(\chi(0,x,r),\partial_t\chi(0,x,r)) = (r\tilde{\Gamma}(r)(\sigma_1\star Q^2)(x),0), \qquad x\in[-L/2,L/2],\ r\in[0,R_{max}] \tag{20b}$$

$$\chi(t,x,0) = 0, \qquad \partial_t\chi(t,x,R_{max}) + c\partial_r\chi(t,x,R_{max}) = 0, \qquad t\geq 0,\ x\in[-L/2,L/2]. \tag{20c}$$

Remark 3.1 (i) *In dimension $n=1$, the D'Alembert formula shows that a solution of the free wave equation is the sum of two profiles, one moving from right to left and another moving from left to right, both at velocity c. Thus, the part of the wave which goes out the domain $[-R_{max},R_{max}]$ satisfies the transport equation $\partial_t\chi \pm c\partial_r\chi$ at $r=\pm R_{max}$. For the equation set on $[0,+\infty)$ with Dirichlet boundary condition at $r=0$, the part of the wave moving from right to left is reflected at $r=0$ and move then from left to right; the part of the wave which travels from left to right goes out the domain at $r=R_{max}$ where it satisfies the transport equation $\partial_t\chi + c\partial_x\chi = 0$. This short argument can be used as an heuristic to justify the boundary condition* (20c).
(ii) *However this argument takes only into account the part of the wave which goes out the domain but not the part which goes from the outside to the inside. If the support of the moving profile from right to left is not included in the domain $[0,R_{max}]$, then after some time this part of the profile enters in the domain $[0,R_{max}]$ and modifies the solution. Such an effect cannot be taken into account in a simple way. Indeed the correct boundary condition at $r=R_{max}$ is $\partial_t\chi + c\partial_x\chi = f(t)$ where $f(t)$ is exactly the part of the wave coming from the outside of the domain and entering in it at time t. Such a boundary condition requires the knowledge of what happens outside of the computational domain, which is precisely disregarded at a numerical level.*
(iii) *This issue disappears when the support of the moving profile is bounded and the computational domain is larger than the support. One can apply the D'Alembert formula in order to prove this condition is fulfilled when the right hand side of the wave equation and the data $(\chi(0),\partial_t\chi(0))$ have a bounded support. In this case, if the support are included in $[0,R_{max}]$, then there is no incoming wave on $[0,R_{max}]$ and thus $f(t)=0$.*
(iv) *Therefore, we take R_{max} such that the support of $\tilde{\sigma}_2$ is included in $[0,R_{max}]$: the right hand side of* (20a) *is included in $[0,R_{max}]$ and does not generate incoming waves. This is also the case for $\partial_t\chi(0)\equiv 0$ but not for $\chi(0,x,r) = r\tilde{\Gamma}(r)(\sigma_1\star Q^2)(x)$. Indeed since Γ is defined as the solution of $\Delta_z\Gamma = \sigma_2$ where σ_2 is non negative, we know that the support of Γ spreads on the whole space $\mathbb{R}^3_z$ and the profile $\tilde{\Gamma}$ decays as $1/r$. Thus the coupling of* (19a)–(19c) *with* (20a)–(20c) *is not equivalent with the coupling of* (19a)–(19c) *with* (18a)–(18c).
(v) *This difficulty is handled as follows. The orbital stability result of Theorem 1.1 applies to any initial data close to $(Q,\Psi,0)$. Hence, we can consider an initial data with a small perturbation added to Ψ. We remark that $\Psi\in L^2_x\dot{H}^1_z$ implies*

$$\|\Psi\mathbf{1}_{|z|>R}\|_{L^2_x\dot{H}^1_z} \underset{R\to+\infty}{\longrightarrow} 0.$$

Thus, for $R > 0$ sufficiently large, $\Psi(x,z)\mathbf{1}_{|z|\leq R}$ is a possible initial data. With this initial data the support of $\chi(0)$ is included in $[0,R]$, and there is no incoming wave on the domain $[0,R]$. Finally, we can consider the coupling of (19a)–(19c) *and* (20a)–(20c) *with $R_{max} \geq R$.*
(vi) *As a recap, at the numerical level we have to choose a sufficiently large computational domain for the wave equation in order to be sure that the incoming waves which are not computable have only a small influence on the solution.*

We discretize the system (19a)–(19c), (20a)–(20c) as follows. We use the classical Crank-Nicolson scheme to solve the Schrödinger equation. The wave equation is handled with a Finite Element Method (FEM) and the Newmark scheme in time (with parameter $(d,\theta) = (1/2, 1/4)$). We pay attention to the coupling in order to preserve at the discrete level the energy exchange dynamics. Let $\Delta t > 0$ be the time step. We set $t^n = n\Delta t$. We introduce a subdivision

$$0 = r_1 < r_2 < .... < r_K = R_{\max}$$

of $[0, R_{\max}]$ and a basis $(\varphi_1, ..., \varphi_{\mathcal{K}_K})$ (with $\mathcal{K}_K \geq K$) of polynomial functions associated to this partition and the choice of the family of finite elements. Next, we also define a subdivision of the physical domain

$$-\frac{L}{2} + \frac{\Delta x}{2} = x_1 < ... < x_i = -\frac{L}{2} + i\frac{\Delta x}{2} < ... < x_N = \frac{L}{2} - \frac{\Delta x}{2}$$

characterized by the (uniform) space step Δx. We denote $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ the cell centered at x_i. The numerical unknowns for the wave equation are denoted $\chi^n_{j,k}$; they define the following approximation χ^n of the wave at time t^n

$$\chi^n(x,r) = \sum_{j=1}^{N}\sum_{k=1}^{\mathcal{K}_k} \chi^n_{j,k}\mathbf{1}_{\left[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}\right]}(x)\varphi_k(r).$$

It is also convenient to introduce

$$\chi^n_k(x) = \sum_{j=1}^{N} \chi^n_{j,k}\mathbf{1}_{\left[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}\right]}(x),$$

so that

$$\chi^n_{j,k} = \frac{1}{\Delta x}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \chi^n_k(x)\,\mathrm{d}x.$$

We shall denote X^n_x and X^n_i the vector in $\mathbb{R}^{\mathcal{K}_K}$ with components $\chi^n_k(x)$ and $\chi^n_{i,k}$, respectively. Hence, the potential ϕ at time t^n can be approached by

$$\begin{aligned}\phi^n(x) &= 4\pi\int_{-L/2}^{L/2}\sigma_1(x-y)\left(\int_0^{R_{\max}} r\tilde{\sigma}_2(r)\chi^n(y,r)\,\mathrm{d}r\right)\mathrm{d}y \\ &= 4\pi\sum_{j=1}^{N}\sum_{k=1}^{\mathcal{K}_K}\chi^n_{j,k}\left(\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}}\sigma_1(x-y)\,\mathrm{d}y\right)\left(\int_0^{R_{\max}} r\tilde{\sigma}_2(r)\varphi_k(r)\,\mathrm{d}r\right),\end{aligned}$$

and we set

$$\phi_j^n = \frac{1}{\Delta x}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \phi^n(x)\,\mathrm{d}x.$$

Eventually we define the potential ϕ at time $t^{n+1/2}$ by

$$\phi^{n+\frac{1}{2}} = \frac{\phi^{n+1}+\phi^n}{2}.$$

The numerical unknowns for the Schrödinger equation are denoted u_j^n; they define the following approximation u^n of the wave function at time t^n

$$u^n(x) = \sum_{j=1}^{N} u_j^n \mathbf{1}_{\left[x_{j-\frac{1}{2}},x_{j+\frac{1}{2}}\right]}(x).$$

We set

$$(|u|^2)^n(x) = u^n(x)\overline{u^n}(x) = \sum_{j=1}^{N} u_j^n\overline{u_j^n}\mathbf{1}_{\left[x_{j-\frac{1}{2}},x_{j+\frac{1}{2}}\right]}(x),$$

and the approximation of the convolution $\sigma_1 \star |u|^2$ at time t^n becomes

$$\left(\sigma_1\star|u|^2\right)^n(x) = \sigma_1\star(|u|^2)^n(x) = \sum_{j=1}^{N} u_j^n\overline{u_j^n}\left(\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}}\sigma_1(x-y)\,\mathrm{d}y\right).$$

We eventually define the vectors $G^n(x) = (G_k^n(x))_k$ and $G_j^n = (G_{j,k}^n)_k \in \mathbb{R}^{\mathcal{K}_K}$ by

$$G_k^n(x) = -c^2\left(\sigma_1\star|u|^2\right)^n(x)\left(\int_0^{R_{\max}} r\tilde{\sigma}_2(r)\varphi_k(r)\,\mathrm{d}r\right) \quad \text{and} \quad G_j^n = \frac{1}{\Delta x}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} G^n(x)\,\mathrm{d}x.$$

We are now able to give the discretization of (19a)–(19c), (20a)–(20c). Assuming that the quantities $(\chi_{j,k}^{n-1})_{j,k}$, $(\chi_{j,k}^n)_{j,k}$ and $(u_j^n)_j$ are already known, we compute $(\chi_{j,k}^{n+1})_{j,k}$ and $(u_j^{n+1})_j$ as follows: for every $j \in \{1,\dots,N\}$

$$\mathcal{M}\frac{X_j^{n+1}-2X_j^n+X_j^{n-1}}{\Delta t^2} + \mathcal{C}\frac{X_j^{n+1}+X_j^{n-1}}{\Delta t} + \mathcal{R}\left(\frac{1}{4}X_j^{n+1}+\frac{1}{2}X_j^n+\frac{1}{4}X_j^{n-1}\right) = G_j^n, \tag{21a}$$

$$i\,\frac{u_j^{n+1}-u_j^n}{\Delta t} + \frac{1}{4}\,\frac{u_{j+1}^{n+1}-2u_j^{n+1}+u_{j-1}^{n+1}}{\Delta x^2} + \frac{1}{4}\,\frac{u_{j+1}^n-2u_j^n+u_{j-1}^n}{\Delta x^2} = \phi_j^{n+\frac{1}{2}}\,\frac{u_j^{n+1}+u_j^n}{2}, \tag{21b}$$

where $\mathcal{M}$, $\mathcal{C}$ and $\mathcal{R}$ are respectively the mass matrix, the diffusion matrix and the rigidity matrix associated to the chosen FEM. The Dirichlet boundary condition at $r=0$ is embodied in the mass matrix whereas the transparent boundary condition at $r = R_{max}$ is encoded in the diffusion matrix (the only non zero coefficients of $\mathcal{C}$ are indeed coming from this boundary condition). The scheme (21b) is completed by the periodic boundary condition $u_0^{n+1} = u_N^{n+1}$ and $u_{N+1}^{n+1} = u_1^{n+1}$.

3.2 Computation of a ground state (Q, Ψ)

Let $H : H^1_x \to \mathbb{R}$ be the functional defined by

$$H(u) = \frac{1}{2}\int |\nabla_x u|^2 \,\mathrm{d}x - \frac{\kappa}{2}\iint |u|^2(x)\Sigma(x-y)|u|^2(y)\,\mathrm{d}x\,\mathrm{d}y$$

where $\Sigma = \sigma_1 \star \sigma_1$ and $\kappa = \|\nabla_z \Gamma\|^2_{L^2_z}$ (with $\Delta_z \Gamma = \sigma_2$) and let K_M be the following minimization problem:

$$K_M = \inf\{H(u) \text{ s.t. } u \in H^1_x \text{ and } \|u\|^2_{L^2_x} = M\}.$$

One can prove that $E(u, \Gamma\, \sigma_1 \star |u|^2, 0) = H(u)$. Thanks to Theorem 1.1-i), if $J_M < 0$ we then get $K_M = J_M$ and if (Q, Ψ) is a minimizer of J_M, then $K_M = H(Q) = E(Q, \Psi, 0) = J_M$. Thus, instead of computing a minimizer of J_M we are going to compute a minimizer of K_M. To this end, we start by solving the Laplace equation $\Delta_z \Gamma = \sigma_2$ in order to have an approximation of the parameter κ. Next, we compute an approximation of a minimizer of K_M and eventually the formula $\Psi(x, z) = \Gamma(z)\sigma_1 \star Q^2(x)$ provides an approximation of Ψ.

3.2.1 Computation of κ

Reasoning as for the wave equation, with the radial symmetry, we set $\Upsilon(r) = r\tilde{\Gamma}(r)$. Then, instead of solving the $3d$-Laplace equation $\Delta_z \Gamma = \sigma_2$ it suffices to consider the following $1d$-Laplace equation on $[0, +\infty)$

$$\partial^2_{rr}\Upsilon(r) = r\tilde{\sigma}_2 r, \qquad \Upsilon(0) = 0, \qquad \Upsilon(r) \underset{r\to+\infty}{\longrightarrow} 0. \tag{22}$$

One possible strategy to solve numerically this equation is to mix a FEM on a bounded domain $[0, R_{max}]$ with an Infinite Element Method on the unbounded domain $[R_{max}, +\infty)$, see for example [10] and [11]. However, this equation has to be solved only once and instead we exploit the solver for the wave equation in dimension one endowed with the Dirichlet boundary condition at $r = 0$ and an exact transparent boundary condition at $r = R_{max}$. Namely, we solve the wave equation

$$\partial^2_{tt}\chi - c^2\partial^2_{rr}\chi = -c^2 r\tilde{\sigma}_2(r), \qquad t \geq 0,\ r \in [0, R_{max}], \tag{23a}$$

$$(\chi(0, r), \partial_t\chi(0, r)) = (0, 0), \qquad r \in [0, R_{max}] \tag{23b}$$

$$\chi(t, 0) = 0, \qquad \partial_t\chi(t, R_{max}) + c\partial_r\chi(t, R_{max}) = 0, \qquad t \geq 0. \tag{23c}$$

on a time interval $[0, T_f]$ sufficiently large so that the final solution $\chi(T_f, r)$ is a good approximation of $\Upsilon(r)$ for $r \in [0, R_{max}]$, since we know that $\chi(t) \to \Upsilon$ as $t \to +\infty$. We solve (23a)–(23c) with the classical Newmark scheme (21a). Here the unknown X^n does not depend on the index j since the considered wave equation does not depend on x and the right hand side is the constant vector $G = (G_k)_k \in \mathbb{R}^{\mathcal{K}_K}$ defined by

$$G_k = \int_0^{R_{max}} r\tilde{\sigma}_2(r)\varphi_k(r)\,\mathrm{d}r.$$

Let

$$\Upsilon_h(r) = \sum_{k=1}^{\mathcal{K}_K} \Upsilon_k \varphi_k(r)$$

be the computed approximation of $\Upsilon(r)$ on $[0, R_{max}]$ and V be the vector with component $(\Upsilon_k)_k$. Since $\kappa = 4\pi \int_0^{+\infty} |\partial_r \Upsilon(r)|^2 \, \mathrm{d}r$ we obtain the following approximation of κ:

$$\kappa_h = 4\pi \int_0^{R_{max}} |\partial_r \Upsilon_h(r)|^2 \, \mathrm{d}r = \frac{4\pi}{c^2} \langle \mathcal{R}V, V \rangle .$$

The accuracy of the approximation of κ is quite sensitive to the size of the computational domain: R_{max} should be chosen sufficiently large. In practice we compute κ_h for an increasing sequence of R^i_{max} and we consider the criterion $|\kappa_h^{i+1} - \kappa_h^i| \ll 1$ in order to detect when the size of the computational domain is sufficiently large.

3.2.2 Computation of Q

In order to compute a minimizer of K_M we appeal to the *imaginary time* method (see for example [2, 3] and the references therein). It consists in solving the following heat equation

$$\partial_t v - \frac{1}{2}\Delta_x v + \omega(v) v - \kappa(\Sigma \star |v|^2) v = 0, \qquad t \geq 0, \ x \in \mathbb{R}^d, \tag{24a}$$

$$\omega(v) = -\frac{1}{\|v\|^2_{L^2_x}} \left(\frac{1}{2} \int |\nabla_x v|^2 \, \mathrm{d}x - \kappa \iint |v|^2(x) \Sigma(x-y) |v|^2(y) \, \mathrm{d}x \, \mathrm{d}y \right), \tag{24b}$$

$$v(0,x) = v_0(x), \qquad \|v_0\|^2_{L^2_x} = M, \qquad x \in \mathbb{R}^d. \tag{24c}$$

A stationary solution of (24a) is a solution of the Choquard equation (7) and a direct computation shows that

$$\frac{\mathrm{d}}{\mathrm{d}t} \|v(t)\|^2_{L^2_x} = 0 \qquad \text{and} \qquad \frac{\mathrm{d}}{\mathrm{d}t} H(v(t)) = -2 \|\partial_t v(t)\|^2_{L^2_x} \leq 0.$$

Thus, when t goes to $+\infty$ the solution $v(t)$ converges to a (at least local) minimizer of K_M. We solve numerically (24a)–(24c) in dimension $d = 1$ and on a bounded domain $[-L/2, L/2]$ endowed with Dirichlet boundary conditions. Since a ground state Q of K_M decays exponentially fast, if L is chosen sufficiently large, this leads to small errors on the computed ground state Q_h. We solve the heat equation with a semi-Crank-Nicolson scheme: for every $j \in \{1, \dots, N\}$

$$\frac{\widetilde{v_j^{n+1}} - v_j^n}{\Delta t} - \frac{1}{4} \frac{\widetilde{v_{j+1}^{n+1}} - 2\widetilde{v_j^{n+1}} + \widetilde{v_{j-1}^{n+1}}}{\Delta x^2} - \frac{1}{4} \frac{v_{j+1}^n - 2v_j^n + v_{j-1}^n}{\Delta x^2} + \omega^n \frac{\widetilde{v_j^{n+1}} + v_j^n}{2} - \kappa \Phi_j^n \frac{\widetilde{v_j^{n+1}} + v_j^n}{2} = 0,$$

with the Dirichlet boundary condition $v_0^n = 0 = v_{N+1}^n$ and where

$$\Phi_j^n = \frac{1}{\Delta x} \sum_{j'=1}^{N} v_{j'}^n v_{j'}^n \left(\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \int_{x_{j'-\frac{1}{2}}}^{x_{j'+\frac{1}{2}}} \Sigma(x-y) \, \mathrm{d}x \, \mathrm{d}y \right).$$

Since this scheme does not preserve the discrete mass we renormalize

$$v_j^{n+1} = \frac{\sqrt{M}}{\sqrt{\Delta x \sum_{i=1}^{N} \widetilde{v_i^{n+1}} \widetilde{v_i^{n+1}}}} \widetilde{v_j^{n+1}},$$

and we eventually compute the new Lagrange multiplier ω^{n+1}:

$$\omega^{n+1} = -\frac{1}{M}\left(\frac{\Delta x}{2}\sum_{j=1}^{N}\frac{v_{j+1}^{n+1}-v_j^{n+1}}{\Delta x}\cdot\frac{v_{j+1}^{n+1}-v_j^{n+1}}{\Delta x} - \kappa\Delta x\sum_{j=1}^{N}\Phi_j^{n+1}v_j^{n+1}v_j^{n+1}\right).$$

As in the continuous case, we observe numerically (see Figure 2) that the discrete energy

$$H^n = \frac{\Delta x}{2}\sum_{j=1}^{N}\frac{v_{j+1}^{n+1}-v_j^{n+1}}{\Delta x}\cdot\frac{v_{j+1}^{n}-v_j^{n}}{\Delta x} - \kappa\frac{\Delta x}{2}\sum_{j=1}^{N}\Phi_j^{n}v_j^{n}v_j^{n} \tag{25}$$

decays along time.

4 Discrete properties of the scheme

As stated in the introduction the Schrödinger-Wave system conserves the mass of the wave function, the total energy (3) and the total momentum of the system (4). It is then natural to ask that the scheme preserves the same discrete quantities. However the Schrödinger-Wave equation is a system where the wave function u exchanges energy with the environment ψ and it might be possible that at the discrete level a scheme preserves the discrete energy of the total system but such that the energy exchanges between the wave function and the environment are not consistent with the energy exchanges at the continuum level. Thus, first and foremost, a good scheme should be consistent with the energy exchanges. It can be difficult to construct a scheme which is consistent with both the energy and momentum exchanges. As we shall see below, the scheme we propose, primarily targeted on the energy balance, does not conserve the total momentum.

In order to specify what we mean by *consistency with the energy exchanges*, let us go back to the basic energetic properties of the Schrödinger-Wave system. If χ is the solution of a wave equation of the form

$$\partial_{tt}^2\chi - c^2\partial_{rr}^2\chi = c^2 f,$$

then the energy of χ defined by

$$E_{\text{wave}}(t) = 4\pi\iint\left(\frac{1}{2c^2}\left|\partial_t\chi(t,x,r)\right|^2 + \frac{1}{2}\left|\partial_r\chi(t,x,r)\right|^2\right)\mathrm{d}x\,\mathrm{d}r,$$

satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}E_{\text{wave}}(t) = 4\pi\iint\partial_t\chi(t,x,r)f(t,x,r)\,\mathrm{d}x\,\mathrm{d}r.$$

In particular the energy is conserved when $f = 0$. If u is a solution of a Schrödinger equation of the form

$$i\partial_t u + \frac{1}{2}\Delta_x u = \phi u,$$

(where ϕ is a real-valued potential) then the energy of u defined by

$$E_{\text{schro}}(t) = \frac{1}{2}\int\left|\nabla_x u(t,x)\right|^2\,\mathrm{d}x + \int\phi(t,x)\left|u(t,x)\right|^2\,\mathrm{d}x$$

satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}E_{\text{schro}}(t) = \int\partial_t\phi(t,x)\left|u(t,x)\right|^2\,\mathrm{d}x.$$

In particular the energy is conserved when ϕ is a stationary potential. Going back to the Schrödinger-Wave system, the total energy $E_{\text{tot}} = E_{\text{wave}} + E_{\text{schro}}$ is conserved because the source term f of the wave equation and the time-dependent potential ϕ fulfil the cancellation property

$$4\pi \iint \partial_t \chi(t,x,r) f(t,x,r)\,\mathrm{d}x\,\mathrm{d}r + \int \partial_t \phi(t,x)\,|u(t,x)|^2\,\mathrm{d}x = 0.$$

Therefore an energetically relevant scheme for the Schrödinger-Wave equation should satisfy the following basic requirements:

(i) the scheme for the wave equation conserves the analog of E_{wave} when the source term f vanishes,

(ii) the scheme for the Schrödinger equation conserves the discrete mass when the potential ϕ is real-valued and the discrete analog of E_{schro} when the potential ϕ does not depend on time,

(iii) the discrete coupling is such that the contributions from the analog of $4\pi \iint \partial_t \chi(t) f(t)\,\mathrm{d}x\,\mathrm{d}r$ and $\int \partial_t \phi(t) |u(t)|^2\,\mathrm{d}x$ cancel out.

We are going to check that the scheme (21a)–(21b) satisfies these three requirements. To this end, let us introduce a few notations. Let D be the discrete time derivative operator

$$(Da^n) = \frac{a^{n+1} - a^n}{\Delta t}$$

and let ∇^d be the discrete periodic gradient operator which associates to a real valued sequence $(b_j)_{1\le j\le N}$ the sequence defined by

$$\left(\nabla^d b\right)_{j+1/2} = \frac{b_{j+1} - b_j}{\Delta x}, \quad b_0 = b_N \quad \text{and} \quad b_{N+1} = b_1.$$

In the sequel we will repeatedly use the following discrete integration by part formula

$$\sum_{j=1}^{N} \left(\nabla^d a\right)_{j-1/2} b_j = -\sum_{j=1}^{N} a_j \left(\nabla^d b\right)_{j+1/2}. \tag{26}$$

The discrete mass of the wave function u at time t^n is given by

$$M^n = \int_{-L/2}^{L/2} |u^n(x)|^2\,\mathrm{d}x = \Delta x \sum_{j=1}^{N} u_j^n \overline{u_j^n}.$$

We define the following discrete energies at time t^n:

$$E^n_{\text{schro}} = \frac{\Delta x}{2} \sum_{j=1}^{N} (\nabla^d u^n)_{j+1/2} (\nabla^d \overline{u^n})_{j+1/2} + \Delta x \sum_{j=1}^{N} \phi_j^{n+\frac{1}{2}} u_j^n \overline{u_j^n}$$

and

$$\begin{aligned} E^n_{\text{wave}} &= \frac{4\pi}{2c^2} \int_{-L/2}^{L/2} \int_0^{R_{max}} |D\chi^n(x,r)|^2\,\mathrm{d}x\,\mathrm{d}r + \frac{4\pi}{2} \int_{-L/2}^{L/2} \int_0^{R_{max}} \left|\partial_r \chi^{n+\frac{1}{2}}(x,r)\right|^2 \mathrm{d}x\,\mathrm{d}r \\ &= \frac{2\pi\Delta x}{c^2} \sum_{j=1}^{N} \left\langle \mathcal{M} \frac{X_j^{n+1} - X_j^n}{\Delta t}, \frac{X_j^{n+1} - X_j^n}{\Delta t} \right\rangle + \frac{2\pi\Delta x}{c^2} \sum_{j=1}^{N} \left\langle \mathcal{R} \frac{X_j^{n+1} + X_j^n}{2}, \frac{X_j^{n+1} + X_j^n}{2} \right\rangle, \end{aligned}$$

where $\chi^{n+\frac{1}{2}} = (\chi^{n+1} + \chi^n)/2$.

Theorem 4.1 *Assume that for every $m \in \mathbb{N}$, $\mathcal{C}X_j^m = 0$. Then, the scheme* (21a)–(21b) *conserves the discrete mass M^n and the discrete total energy $E_{\rm tot}^n = E_{\rm schro}^n + E_{\rm wave}^n$. Moreover the scheme is consistent for the energy exchange, that means*

$$\int_{-L/2}^{L/2} D\phi^{n+\frac{1}{2}}(x)\,|u^{n+1}(x)|^2\,\mathrm{d}x + DE_{\rm wave}^n = 0.$$

Remark 4.2 *The assumption $\mathcal{C}X_j^m = 0$ means that the wave does not cross the boundary of the computational domain. We have to make this assumption since the part of the wave which goes out of the computational domain does not contribute anymore to the total energy (see the definition of $E_{\rm wave}^n$), and thus the discrete energy cannot be conserved. In practice this is not an issue since the energy that goes away the computational domain can be explicitly computed and incorporated in the energy balance.*

Before we detail the proof of this statement, let us say a few words on the discrete mass center and impulsion of the wave function u. The discrete mass of the wave function u is conserved and we denote by $M = M^n$ its value. Then the discrete center of mass of the wave function is defined by

$$q^n = \frac{1}{M}\int_{-L/2}^{L/2} x|u^n(x)|^2\,\mathrm{d}x = \frac{\Delta x}{M}\sum_{j=1}^{N} x_j u_j^n \overline{u_j^n}.$$

In order to define the discrete impulsion of the wave function we need to define its discrete gradient. To this end, we bear in mind that we have adopted a Finite Volume approach to discretize (1a), with a numerical unknown constant over the cells $C_j = [x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$. Hence, the discrete gradient is naturally thought of as the piecewise constant function on the staggered grid $C_{j+1/2} = [x_j, x_{j+1}]$:

$$(\partial_x u)^n(x) = \sum_{j=1}^{N} (\nabla^d u^n)_{j+1/2}\mathbf{1}_{[x_j,x_{j+1}]}(x), \qquad \nabla^d u_{j+1/2}^n = \frac{u_{j+1}^n - u_j^n}{\Delta x}.$$

This definition is consistent with the discrete Laplacian on C_j, with $(\Delta^d u)_j = \frac{1}{\Delta x}(\nabla^d u_{j+1/2} - \nabla^d u_{j-1/2})$, which can be seen as a combination of ∇^d's operators defined on the twin grids. Accordingly, the discrete impulsion of the wave function is defined by

$$p^n = \mathrm{Im}\int_{-L/2}^{L/2} (\partial_x u)^n(x)\overline{u^n(x)}\,\mathrm{d}x = \Delta x\,\mathrm{Im}\sum_{j=1}^{N} (\nabla^c u^n)_j \overline{u_j^n}$$

where $(\nabla^c b)_j = \frac{1}{2}[(\nabla^d b)_{j-1/2} + (\nabla^d b)_{j+1/2}]$ is the discrete periodic centered-gradient operator at x_j. Another justification for this definition is that at the continuous level the quantity $\int \nabla_x u\,\overline{u}\,\mathrm{d}x$ is purely imaginary. This property is conserved at the discrete level when the periodic centered-gradient operator is taken but it fails with the periodic right or left-gradient operators. It is also worth remarking that the energy $E_{\rm schro}^n$ can be rewritten as

$$E_{\rm schro}^n = \frac{1}{2}\int_{-L/2}^{L/2} |(\partial_x u)^n(x)|^2\,\mathrm{d}x + \int_{-L/2}^{L/2} \phi^{n+\frac{1}{2}}(x)\,|u^n(x)|^2\,\mathrm{d}x.$$

The discrete center of mass satisfies the following relation

$$M\,\frac{q^{n+1}-q^n}{\Delta t} = \Delta x\,\mathrm{Im}\sum_{j=1}^{N}\left(\nabla^d \frac{u^{n+1}+u^n}{2}\right)_{j+1/2} \frac{\overline{u_{j+1}^{n+1}} + \overline{u_{j+1}^n}}{2}.$$

The right hand side depends on both u^n and u^{n+1}, the latter being computed from u^n by (21b). We observe that

$$\begin{aligned}
&\mathrm{Im}\left\{\sum_{j=1}^{N}\left(\nabla^d\frac{u^{n+1}+u^n}{2}\right)_{j+1/2}\frac{\overline{u_{j+1}^{n+1}}+\overline{u_{j+1}^{n}}}{2}\right\}\\
&\quad=\frac{1}{4\Delta x}\mathrm{Im}\left\{\sum_{j=1}^{N}(u_{j+1}^{n+1}+u_{j+1}^{n}-u_j^{n+1}-u_j^n)(\overline{u_{j+1}^{n+1}}+\overline{u_{j+1}^{n}})\right\}\\
&\quad=-\frac{1}{4\Delta x}\mathrm{Im}\left\{\sum_{j=1}^{N}(u_j^{n+1}+u_j^n)(\overline{u_{j+1}^{n+1}}+\overline{u_{j+1}^{n}})\right\}=+\frac{1}{4\Delta x}\mathrm{Im}\left\{\sum_{j=1}^{N}(\overline{u_j^{n+1}}+\overline{u_j^{n}})(u_{j+1}^{n+1}+u_{j+1}^{n})\right\}\\
&\quad=+\frac{1}{4\Delta x}\mathrm{Im}\left\{\sum_{j=1}^{N}(\overline{u_j^{n+1}}+\overline{u_j^{n}})(u_{j+1}^{n+1}+u_{j+1}^{n}-u_j^{n+1}-u_j^n)\right\}\\
&\quad=\mathrm{Im}\sum_{j=1}^{N}\left(\nabla^d\frac{u^{n+1}+u^n}{2}\right)_{j+1/2}\frac{\overline{u_j^{n+1}}+\overline{u_j^{n}}}{2}=\mathrm{Im}\sum_{j=1}^{N}\left(\nabla^c\frac{u^{n+1}+u^n}{2}\right)_{j}\frac{\overline{u_j^{n+1}}+\overline{u_j^{n}}}{2}
\end{aligned}$$

and the evolution of the center of mass can be recast as follows:

$$M\,\frac{q^{n+1}-q^n}{\Delta t}=\mathrm{Im}\int_{L/2}^{L/2}\frac{(\partial_x u)^{n+1}(x)+(\partial_x u)^n(x)}{2}\,\frac{\overline{u^{n+1}(x)}+\overline{u^n(x)}}{2}\,\mathrm{d}x.$$

For the discrete impulsion, we have

$$\frac{p^{n+1}-p^n}{\Delta t}=-\Delta_x\mathrm{Re}\sum_{j=1}^{N}(\nabla^d\phi^{n+\frac12})_{j+1/2}\frac{u_{j+1}^{n+1}+u_{j+1}^n}{2}\,\frac{\overline{u_j^{n+1}}+\overline{u_j^n}}{2}.$$

Remark 4.3 *The shift index comes from the fact that at the discrete level the Leibniz formula for the derivative of a product is not satisfied. Moreover the time discretization of the wave equation seems not to be adapted to the conservation of the discrete total momentum of the system. This is not due to the choice of the space discretization, but to the choice of time discretization. The time discretization of both equations and the treatment of the coupling are constructed in order to ensure the conservation of the discrete total energy of the system, which is hardly compatible with the conservation of the discrete total momentum.*

Proof of Theorem 4.1. We begin with the mass conservation:

$$DM^n=\frac{M^{n+1}-M^n}{\Delta t}=\Delta x\sum_{j=1}^{N}\frac{u_j^{n+1}-u_j^n}{\Delta t}\,\overline{u_j^{n+1}}+\Delta x\sum_{j=1}^{N}u_j^n\,\frac{\overline{u_j^{n+1}}-\overline{u_j^n}}{\Delta t}.$$

Coming back to (21b) we have on the one hand

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}=\frac{i}{2}\left(\Delta^d u^{n+1}\right)_j+\frac{i}{2}\left(\Delta^d u^n\right)_j-i\,\phi_j^{n+\frac12}\,\frac{u_j^{n+1}+u_j^n}{2}$$

and on the other hand

$$\frac{\overline{u_j^{n+1}}-\overline{u_j^n}}{\Delta t}=-\frac{i}{2}\left(\Delta^d\overline{u^{n+1}}\right)_j-\frac{i}{2}\left(\Delta^d\overline{u^n}\right)_j+i\,\phi_j^{n+\frac12}\,\frac{\overline{u_j^{n+1}}+\overline{u_j^n}}{2}.$$

Then, thanks to the discrete integration by part property (26) we get

$$\begin{aligned}\Delta x \sum_{j=1}^{N} \frac{u_j^{n+1}-u_j^n}{\Delta t}\,\overline{u_j^{n+1}} \\ = -\frac{i\Delta x}{2}\sum_{j=1}^{N}\left[\left(\nabla^d u^{n+1}\right)_{j+1/2}\left(\nabla^d\overline{u^{n+1}}\right)_{j+1/2}+\left(\nabla^d u^{n}\right)_{j+1/2}\left(\nabla^d\overline{u^{n+1}}\right)_{j+1/2}\right] \\ -\frac{i\Delta x}{2}\sum_{j=1}^{N}\phi_j^{n+\frac12}\left(u_j^{n+1}\overline{u_j^{n+1}}+u_j^n\overline{u_j^{n+1}}\right)\end{aligned}$$

and

$$\begin{aligned}\Delta x \sum_{j=1}^{N} u_j^n\,\frac{\overline{u_j^{n+1}}-\overline{u_j^n}}{\Delta t} \\ = \frac{i\Delta x}{2}\sum_{j=1}^{N}\left[\left(\nabla^d u^{n}\right)_{j+1/2}\left(\nabla^d\overline{u^{n+1}}\right)_{j+1/2}+\left(\nabla^d u^{n}\right)_{j+1/2}\left(\nabla^d\overline{u^{n}}\right)_{j+1/2}\right] \\ +\frac{i\Delta x}{2}\sum_{j=1}^{N}\phi_j^{n+\frac12}\left(u_j^{n}\overline{u_j^{n+1}}+u_j^n\overline{u_j^{n}}\right)\end{aligned}$$

Eventually, gathering these two identities leads to

$$\begin{aligned}DM^n = -\frac{i\Delta x}{2}\sum_{j=1}^{N}\left[\left(\nabla^d u^{n+1}\right)_{j+1/2}\left(\nabla^d\overline{u^{n+1}}\right)_{j+1/2}-\left(\nabla^d u^{n}\right)_{j+1/2}\left(\nabla^d\overline{u^{n}}\right)_{j+1/2}\right] \\ -\frac{i\Delta x}{2}\sum_{j=1}^{N}\phi_j^{n+\frac12}\left(u_j^{n+1}\overline{u_j^{n+1}}-u_j^n\overline{u_j^{n}}\right).\end{aligned}$$

From here, since DM^n is a real number, we directly get the discrete mass conservation and we get for free that the discrete quantity

$$\begin{aligned}\int_{-L/2}^{L/2} D\left|\left(\partial_x u^n\right)(x)\right|^2+\phi^{n+\frac12}(x)\,D\left|u^n(x)\right|^2\,\mathrm{d}x \\ = \frac{\Delta x}{\Delta t}\sum_{j=1}^{N}\left[\left(\nabla^d u^{n+1}\right)_{j+1/2}\left(\nabla^d\overline{u^{n+1}}\right)_{j+1/2}+\phi_j^{n+\frac12}\,u_j^{n+1}\overline{u_j^{n+1}}\right] \\ -\frac{\Delta x}{\Delta t}\sum_{j=1}^{N}\left[\left(\nabla^d u^{n}\right)_{j+1/2}\left(\nabla^d\overline{u^{n}}\right)_{j+1/2}+\phi_j^{n+\frac12}\,u_j^{n}\overline{u_j^{n}}\right]=-\frac{2}{\Delta t}\mathrm{Im}\left(DM^n\right)=0\end{aligned}$$

is conserved by the scheme. This exactly means that the Crank-Nicolson scheme preserves the discrete mass and energy of any Schrödinger equation with a real and constant in time potential $\phi=\phi(x)$. Since

$$DE^n_{\mathrm{schro}}=\int_{-L/2}^{L/2}\left(D\left|\left(\partial_x u^n\right)(x)\right|^2+\phi^{n+\frac12}(x)\,D\left|u^n(x)\right|^2\right)\mathrm{d}x+\int_{-L/2}^{L/2}D\phi^{n+\frac12}(x)\left|u^{n+1}(x)\right|^2\mathrm{d}x,$$

the scheme preserves the discrete total energy E^n_{tot} if and only if it is consistent with the discrete

energy exchange, that means

$$\int_{-L/2}^{L/2} D\phi^{n+\frac{1}{2}}(x)\,|u^{n+1}(x)|^2\,\mathrm{d}x + D\,E^n_{\mathrm{wave}} = 0.$$

Let us compute the discrete time derivative of E^n_{wave}. For that purpose we rewrite (21a) as follows (the assumptions insure that the term of the form $\mathcal{C}X_j^m$ are equal to zero)

$$\mathcal{M}\frac{X_j^{n+1}-X_j^n}{\Delta t^2} = \mathcal{M}\frac{X_j^n-X_j^{n-1}}{\Delta t^2} - \mathcal{R}\left(\frac{1}{4}X_j^{n+1}+\frac{1}{2}X_j^n+\frac{1}{4}X_j^{n-1}\right)+G_j^n$$

and we take the scalar product of this quantity against the vector $X_j^{n+1}-X_j^n$

$$\begin{aligned}\left\langle \mathcal{M}\frac{X_j^{n+1}-X_j^n}{\Delta t}, \frac{X_j^{n+1}-X_j^n}{\Delta t}\right\rangle &= \left\langle \mathcal{M}\frac{X_j^{n}-X_j^{n-1}}{\Delta t}, \frac{X_j^{n+1}-X_j^n}{\Delta t}\right\rangle \\ &\quad - \left\langle \mathcal{R}\left(\frac{1}{4}X_j^{n+1}+\frac{1}{2}X_j^n+\frac{1}{4}X_j^{n-1}\right), X_j^{n+1}-X_j^n\right\rangle + \left\langle G_j^n, X_j^{n+1}-X_j^n\right\rangle.\end{aligned}$$

Besides, since the mass matrix $\mathcal{M}$ is symmetric

$$\left\langle \mathcal{M}\frac{X_j^{n}-X_j^{n-1}}{\Delta t}, \frac{X_j^{n+1}-X_j^n}{\Delta t}\right\rangle = \left\langle \mathcal{M}\frac{X_j^{n+1}-X_j^n}{\Delta t^2}, X_j^n-X_j^{n-1}\right\rangle,$$

we also get (by taking the scalar product against the vector $X_j^n-X_j^{n-1}$)

$$\begin{aligned}\left\langle \mathcal{M}\frac{X_j^{n}-X_j^{n-1}}{\Delta t}, \frac{X_j^{n+1}-X_j^n}{\Delta t}\right\rangle &= \left\langle \mathcal{M}\frac{X_j^{n}-X_j^{n-1}}{\Delta t}, \frac{X_j^{n}-X_j^{n-1}}{\Delta t}\right\rangle \\ &\quad - \left\langle \mathcal{R}\left(\frac{1}{4}X_j^{n+1}+\frac{1}{2}X_j^n+\frac{1}{4}X_j^{n-1}\right), X_j^{n}-X_j^{n-1}\right\rangle + \left\langle G_j^n, X_j^{n}-X_j^{n-1}\right\rangle.\end{aligned}$$

Gathering these two identities leads to

$$\begin{aligned}\left\langle \mathcal{M}\frac{X_j^{n+1}-X_j^n}{\Delta t}, \frac{X_j^{n+1}-X_j^n}{\Delta t}\right\rangle &= \left\langle \mathcal{M}\frac{X_j^{n}-X_j^{n-1}}{\Delta t}, \frac{X_j^{n}-X_j^{n-1}}{\Delta t}\right\rangle \\ &\quad - \left\langle \mathcal{R}\left(\frac{1}{4}X_j^{n+1}+\frac{1}{2}X_j^n+\frac{1}{4}X_j^{n-1}\right), X_j^{n+1}-X_j^{n-1}\right\rangle + \left\langle G_j^n, X_j^{n+1}-X_j^{n-1}\right\rangle.\end{aligned}$$

Since

$$\begin{aligned}&\left\langle \mathcal{R}\left(\frac{1}{4}X_j^{n+1}+\frac{1}{2}X_j^n+\frac{1}{4}X_j^{n-1}\right), X_j^{n+1}-X_j^{n-1}\right\rangle \\ &\qquad = \left\langle \mathcal{R}\left(\frac{X_j^{n+1}+X_j^n}{2}+\frac{X_j^{n}+X_j^{n-1}}{2}\right), \frac{X_j^{n+1}-X_j^n}{2}-\frac{X_j^{n}+X_j^{n-1}}{2}\right\rangle \\ &\qquad\qquad = \left\langle \mathcal{R}\frac{X_j^{n+1}+X_j^n}{2}, \frac{X_j^{n+1}+X_j^n}{2}\right\rangle - \left\langle \mathcal{R}\frac{X_j^{n}+X_j^{n-1}}{2}, \frac{X_j^{n}+X_j^{n-1}}{2}\right\rangle\end{aligned}$$

we eventually obtain the following relation

$$\left\langle \mathcal{M}\frac{X_j^{n+1}-X_j^n}{\Delta t},\frac{X_j^{n+1}-X_j^n}{\Delta t}\right\rangle + \left\langle \mathcal{R}\frac{X_j^{n+1}+X_j^n}{2},\frac{X_j^{n+1}+X_j^n}{2}\right\rangle$$
$$= \left\langle \mathcal{M}\frac{X_j^{n}-X_j^{n-1}}{\Delta t},\frac{X_j^{n}-X_j^{n-1}}{\Delta t}\right\rangle + \left\langle \mathcal{R}\frac{X_j^{n}+X_j^{n-1}}{2},\frac{X_j^{n}+X_j^{n-1}}{2}\right\rangle + \left\langle G_j^n, X_j^{n+1}-X_j^{n-1}\right\rangle$$

which implies that

$$DE_{\text{wave}}^n = \frac{2\pi\Delta x}{c^2\Delta t}\sum_{j=1}^{N}\left\langle G_j^{n+1}, X_j^{n+2}-X_j^n\right\rangle.$$

In particular this equality implies that the Newmark scheme conserves the energy of the free wave equation. We are left with the task to prove that

$$\Delta x\sum_{j=1}^{N}\frac{\phi_j^{n+1+\frac12}-\phi_j^{n+\frac12}}{\Delta t}u_j^{n+1}\overline{u_j^{n+1}} + \frac{2\pi\Delta x}{c^2\Delta t}\sum_{j=1}^{N}\left\langle G_j^{n+1}, X_j^{n+2}-X_j^n\right\rangle = 0.$$

On the one hand we get

$$\Delta x\sum_{j=1}^{N}\frac{\phi_j^{n+1+\frac12}-\phi_j^{n+\frac12}}{\Delta t}u_j^{n+1}\overline{u_j^{n+1}} = \frac{\Delta x}{2\Delta t}\sum_{j=1}^{N}(\phi_j^{n+2}-\phi_j^n)u_j^{n+1}\overline{u_j^{n+1}}$$
$$= \frac{2\pi}{\Delta t}\sum_{j,j'=1}^{N}\sum_{k=1}^{\mathcal{K}_K}(\chi_{j',k}^{n+2}-\chi_{j',k}^n)\left(\int_{x_{j-\frac12}}^{x_{j+\frac12}}\int_{x_{j'-\frac12}}^{x_{j'+\frac12}}\sigma_1(x-y)\,\mathrm{d}x\,\mathrm{d}y\right)\left(\int_0^{R_{max}} r\tilde{\sigma}_2(r)\varphi_k(r)\,\mathrm{d}r\right)u_j^{n+1}\overline{u_j^{n+1}}$$

while on the other hand we have

$$\frac{2\pi\Delta x}{c^2\Delta t}\sum_{j=1}^{N}\left\langle G_j^{n+1}, X_j^{n+2}-X_j^n\right\rangle = -\frac{2\pi}{\Delta t}\sum_{j,j'=1}^{N}\sum_{k=1}^{\mathcal{K}_K}u_{j'}^{n+1}\overline{u_{j'}^{n+1}}\left(\int_{x_{j-\frac12}}^{x_{j+\frac12}}\int_{x_{j'-\frac12}}^{x_{j'+\frac12}}\sigma_1(x-y)\,\mathrm{d}x\,\mathrm{d}y\right)$$
$$\times\left(\int_0^{R_{max}} r\tilde{\sigma}_2(r)\varphi_k(r)\,\mathrm{d}r\right)(\chi_{j,k}^{n+2}-\chi_{j,k}^n)$$

Since σ_1 is even, we have

$$\int_{x_{j-\frac12}}^{x_{j+\frac12}}\int_{x_{j'-\frac12}}^{x_{j'+\frac12}}\sigma_1(x-y)\,\mathrm{d}x\,\mathrm{d}y = \int_{x_{j'-\frac12}}^{x_{j'+\frac12}}\int_{x_{j-\frac12}}^{x_{j+\frac12}}\sigma_1(x-y)\,\mathrm{d}x\,\mathrm{d}y,$$

and we conclude that the scheme is consistent with the energy exchanges. Note that in practice the convolution with σ_1 in the definition of G_j^n and ϕ_j^n is computed with an numerical integration method. This numerical integration has to be consistent with the previous formula in order to insure that the scheme conserves the total energy of the system. ∎

Data Availability Statement

The data that supports the findings of this study are available within the article

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