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DECOHERENCE FOR A HEAVY PARTICLE INTERACTING WITH A LIGHT PARTICLE: NEW ANALYSIS AND NUMERICS*

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Abstract. We study the dynamics of a quantum heavy particle undergoing a repulsive interaction with a light particle. The main motivation is the detailed description of the loss of coherence induced on a quantum system (in our model, the heavy particle) by the interaction with the environment (the light particle).

The content of the paper is analytical and numerical.

Concerning the analytical contribution, we show that an approximate description of the dynamics of the heavy particle can be carried out in two steps: first comes the interaction, then the free evolution. In particular, all effects of the interaction can be embodied in the action of a collision operator that acts on the initial state of the heavy particle. With respect to previous analytical results on the same topics, we turn our focus from the Møller wave operator to the full scattering operator, whose analysis proves to be simpler.

Concerning the numerical contribution, we exploit the previous analysis to construct an efficient numerical scheme that turns the original, multi-scale, two-body problem into two one-body problems which can be solved separately. This leads to a considerable gain in simulation time. We present and interpret some simulations carried out on specific one-dimensional systems by using the new scheme.

According to simulations, decoherence is produced by an interference-free bump which arises from the initial state of the heavy particle immediately after the collision. We support such a picture by numerical evidence as well as by an approximation theorem.

Key words. Quantum mechanics, Schrödinger equation, heavy-light particle scattering, interference, decoherence, asymptotic analysis, numerical discretization.

AMS subject classifications. 35Q41, 65M06, 81S22.

1. Introduction

In the present paper we describe, both through a theoretical analysis and numerical simulations, the following idealized experiment: a quantum particle lies in a state given by the superposition of two localized wave functions ("bumps"), initially separated and moving towards each other. At a certain time, the particle interacts with another particle that is considerably lighter. As a consequence, the quantum interference arising when the two bumps corresponding to the heavy particle eventually meet is damped. The damping of the interference is called *decoherence*, and provides a description of the transition from the quantum to the classical world (see [8, 9, 11, 16–20, 26]). Despite the conceptual relevance of decoherence to the foundations of quantum mechanics as well as in applications (e.g. in quantum computation) and, more generally, in the understanding of the classical picture of the macroscopic world, a rigorous and exhaustive description of this phenomenon is still at its beginnings; nevertheless, in the last decade many important steps have been accomplished (see e.g. [1–3, 10, 12–14]).

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According to the principles of quantum mechanics, the time evolution of the wave function $\psi_\varepsilon(t,X,x)$ representing the two-body quantum system is given by the Schrödinger equation

$$\begin{cases} i\partial_t\psi_\varepsilon = -\dfrac{1}{2M}\Delta_X\psi_\varepsilon - \dfrac{1}{2\varepsilon M}\Delta_x\psi_\varepsilon + \dfrac{1+\varepsilon}{\varepsilon}V(x-X)\psi_\varepsilon, \\ \psi_\varepsilon(0,X,x) = \psi_\varepsilon^0(X,x), \end{cases} \tag{1.1}$$

where we used units in which $\hbar=1$, M is the mass, and X is the spatial coordinate of the heavy particle, while εM is the mass and x is the spatial coordinate of the light one. So ε is the ratio between the mass of the light particle and the mass of the heavy one, and we study the regime $\varepsilon \ll 1$, which we call the *small mass ratio* regime.

The interaction is described by the potential $\frac{1+\varepsilon}{\varepsilon}V$; the uncommon coupling constant is chosen to be of order ε^{-1} so that even a single collision leaves an observable mark on the heavy particle; furthermore, the factor $1+\varepsilon$ hardly affects the dynamics and simplifies some expressions. We shall always choose a *factorized* initial state, i.e. ψ_ε^0 will be the product of functions depending only on the variable X and the variable x, respectively (see (2.1)). Physically, this means that initially the two particles are uncorrelated. We shall always assume that ψ_ε^0, and consequently $\psi_\varepsilon(t)$, is normalized in $L^2(\mathbb{R}^{2d})$.

The aim of the present paper is threefold: first, we rigorously derive a *collisional dynamics* for the heavy particle as an approximation of the underlying quantum evolution (1.1) in the limit $\varepsilon \to 0$ (sections 3 and 4); second, we employ such a collisional dynamics in order to build up an efficient numerical scheme (sections 5.1 and 5.2); third, we observe the appearance of decoherence through numerical simulation (Section 5.3). Eventually, simulations show an unpredicted mechanism for the occurrence of decoherence, which we are able to derive rigorously (sections 5.4 and 6.3).

The emergence of a collisional dynamics, well-known since [19] and rigorously deduced already in [1–3, 10, 12–14], can be explained by the fact that the characteristic evolution time is of order one for the heavy particle and of order ε for the light one, so the light particle diffuses almost instantaneously, while, during the interaction, the heavy particle hardly moves. Thus, the main effect of the interaction on the heavy particle is the reduction of the quantum interference among the two bumps. This, roughly speaking, is the content of the celebrated Joos–Zeh's heuristic formula (see e.g. [19, formula (3.43)]), which establishes that the state of the heavy particle has hardly changed, while the state of the light particle is transformed by the action of a suitable scattering operator.

In order to give a mathematical description to this scenery, in Section 3 we introduce a *collision operator* $\mathcal{I}_\chi$, whose action consists in multiplying the kernel $\rho^M(X,X')$ of the density operator ρ^M of the heavy particle by the *collision function*

$$I_\chi(X,X') := \langle S^{X'}\chi | S^X\chi\rangle,$$

where, following the physicist's habit, the Hermitian product $\langle\cdot|\cdot\rangle$ is anti-linear in the first factor and linear in the second. Furthermore, S^X stays for the one-particle scattering operator constructed assuming that the interaction potential is $V(\cdot - X)$. Notice that $0 \le |I_\chi| \le 1$; we will show in Section 4 that decoherence arises precisely when I_χ is not identically equal to one.

Several novelties are present with respect to previous achievements on analogous problems (see [2,3,10,13]). First, we use a different initial state for the light particle in order to replace the Møller wave operator with the scattering operator (Theorem 3.2); this choice makes it possible to provide explicit formulas for the function I_χ (Section 3). Second, in the present work the convergence of the two-body dynamics to the two separated one-body dynamics is given in Theorem 3.2, but the convergence rate in ε is not explicitly specified (see formula (3.3)). However, given an interaction potential V, one can compute the related scattering operator S and then use formula (3.4) in order to find the convergence rate. Third, we generalize Theorem 3.2 to the case of density operators in Theorem 3.4. Fourth, we give explicit formulas for the momentum and energy transfers between the two particles. To this regard, we remark that, even though the incoming particle has a negligible mass, the transfer of energy and momentum is not trivial, since in the limit $\varepsilon \to 0$ the colliding light particle has finite momentum and infinite energy.

Concerning the numerical part of the paper, we recall that in [4] the authors exhibited some numerical simulations aimed at checking the Joos–Zeh's approximation formula from a quantitative point of view: indeed, the error in such formulas, as computed in [2,3,13], contains a multiplicative constant whose optimal size is unknown (see e.g. [3, estimate (2.2)]). The numerical simulations in [4] show that, in spite of this indeterminacy, the approximation in [2,3] can be successfully employed at least under some hypotheses on the interaction potential (for details see [4, Section 3.2]). Those numerical results were achieved by using standard discretization arguments and a splitting (Peaceman–Rachford) procedure. The main drawback of such a method was that, for fixed grids, the precision was sensitive to the value of ε, so that, in order to follow the fast evolution of the light particle, one had to employ tiny meshes both in time and space, and the computations became expensive in time and memory.

Conversely, in the present approach the role of the light particle is limited to the computation of the collision function I_χ. The focus of the analysis is the dynamics of the heavy particle that, in our approximation, becomes free after the collision. In this way, the computational problem drastically simplifies and the numerical cost is considerably diminished, both in memory and in time; moreover, it becomes possible to simulate an experiment with many colliding light particles, which is crucial for the sake of studying the continuous damping of the interference.

As already stressed, our simulations lead to a description of decoherence that, at least to our knowledge, was never put in evidence before. Indeed, simulations show that, if the light particle initially has a non-vanishing mean momentum, then after the collision a fraction of the wave function of the heavy particle organizes itself into a bump that moves independently of the rest (see the first image in Figure 5.5). Moreover, the newborn bump is uncorrelated with the other components of the state of the heavy particle, so it does not take part in the interference. Thus, the damping of the interference pattern can be explained by the fact that a fraction of the initial wave function decouples from the rest. We give a rigorous result which portrays this phenomenon, if some hypotheses on the involved spatial scales are satisfied (Theorem 5.1).

For simplicity, our numerical treatment is limited to the one-dimensional case, even though the general idea and the theoretical results apply to systems in arbitrarily high dimension.

This paper is more concerned with a precise estimate on the dynamics of the heavy particle, than on interpretation of decoherence in terms of the foundations of quantum mechanics; nevertheless, some words on the conceptual background are in order.

In [4] we introduced and discussed an interpretation of decoherence based on the analysis of the configuration space of the system. According to such an interpretation, the two bumps representing the state of the heavy particle can be plotted as two bumps that, in the absence of the light particle, move one towards the other: the simulation shows that when the centres of the two bumps coincide, the overlap between the two bumps is complete and then interference is maximal (see the last image of [4, Figure 9]).

On the other hand, if the light particle is present, then its position appears as an additional dimension in the configuration space of the two-particle system. Now, since both bumps of the heavy particle undergo a collision with the light one, they will be perturbed in two different ways, so that the eventual overlap will not be complete and thus the interference is only partial (to this regard, see the second image in the first row of [4, Figure 9]). For the details of this explanation of decoherence we refer to [4, Section 4] and to Remark 5.2: what we would like to stress here is the presence of a portion of the two-body wave function that, in the (full) configuration space, is prevented from overlapping and hence from producing interference.

Such a description has the advantage of being clear and simple, both from the physical point of view and for the mathematics involved: the only mathematical object that is needed is the wave function. On the other hand, in the present paper we aim at getting rid of the coordinates of the light particle, reducing then the number of variables to consider, which is often important for numerical computations. The price we have to pay is that we lose the enlightening picture in the coordinate space and we have to deal with more complicated mathematical objects, like density operators.
The description of the decoherence phenomenon that emerges from our analysis can be summarized as follows, according to formula (5.11): each bump of the heavy particle interacts with the light particle only through the portion of its wave function corresponding to the reflection coefficient of the interaction. Then, the density operator of the heavy particle after the interaction turns out to be a convex combination of three density operators: the one corresponding to the suitably damped initial state, that did not interact when the light particle was transmitted, the one corresponding to the left bump when the light particle was reflected from the left, and the one corresponding to the right bump when the light particle was reflected from the right. Only the first one has preserved the capability to produce interference, while the two others did not. The overall interference is then damped due to the fact that the portion of the heavy particle that underwent interaction cannot interfere any more. The correspondence with the non-overlapping components of the two-body wave function, as displayed in the analysis in the configuration space, is explained briefly in Remark 5.2. Actually, we plan to investigate that correspondence in more details in a future work.

The outline of the present paper is the following. In Section 2 we introduce the mathematical framework and fix some notation. Section 3 provides the general approximation theorems, enabling one to replace the two-body Schrödinger picture by a suitable collisional dynamics. Section 4 is devoted to the study of the collision function I_χ: we give general formula, study some properties and provide approximations for some particular choices of the interaction potential V. In Section 5, we describe the numerical method and present results obtained with that scheme. In particular, we carefully analyze the decoherence effect carried on the heavy particle by the interaction with the light one, showing the appearance, after the collision, of an uncorrelated bump and explaining it theoretically. Finally, the last sections are devoted to the rigorous mathematical proofs of the main theorems of sections 3 and 5.4.

2. Preliminaries

Let us recall some elementary notions of quantum mechanics and fix some notation. The state of a pair of quantum particles in space dimension d can be represented by a function ψ in $L^2(\mathbb{R}^{2d})$ called the "wave function", whose norm equals one, to be interpreted according to the well-known Born's rule: given $\Omega_1, \Omega_2 \subseteq \mathbb{R}^d$, the quantity $\int_{\Omega_1}\int_{\Omega_2} |\psi(X,x)|^2\,dx\,dX$ is the joint probability of finding the heavy particle in the domain Ω_1 and the light one in Ω_2 after a measurement of their positions. In order to detect and measure the decoherence, one has to study the probability density $\int_{\mathbb{R}^d} |\psi(X,x)|^2\,dx$ of finding the heavy particle at a point X, averaged on the position of the light one.

As already stated, we assume that the ratio of the masses of the two particles is small, and fix the mass of the heavy particle to $M=1$ for the analytical investigations, while the mass of the light particle will be denoted by $m=\varepsilon \ll 1$. In the numerical section (Section 5) however we will choose different values for M for scaling reasons.

We assume that the interaction between the two particles can be modelled by a regular, rapidly decaying and non-negative potential V, that depends on the distance between the two particles only. Due to the regime of small mass ratio, in order to obtain a non-trivial evolution for the heavy particle, we suppose that the strength of the interaction is of the order of the inverse of the mass ratio (ε^{-1}). More precisely, as this choice simplifies the analysis and does not affect the results, we define the coupling constant as $\varepsilon^{-1}(\varepsilon+1)$, which is the inverse of the reduced mass of the two-body system.

Under such assumptions, the time evolution of the two-body wave function $\psi_\varepsilon(t,X,x)$ is given by (1.1), associated with the initial condition

$$\psi_\varepsilon(0,X,x) \;=:\; \psi_\varepsilon^0(X,x) \;=\; \varphi(X)[U_0(-\varepsilon^{-\gamma})\chi](x), \tag{2.1}$$

where φ and χ are regular functions (see next section for the exact regularity required) and $\gamma \in (0,1)$. The presence of the free propagator $U_0(-\varepsilon^{-\gamma})$ in the definition of the initial state of the light particle is useful to describe a situation in which the light particle comes from infinity and reaches $x=0$ in a time of order $\varepsilon^{1-\gamma}$. Furthermore, it makes it possible to treat χ as an incoming state in the sense of the scattering theory (see e.g. [23]).

2.1. Notation.

- For $p \in [1,\infty]$, the norm in $L^p(\mathbb{R}^d)$ or in $L^p(\mathbb{R}^{2d})$ is denoted by $\|\cdot\|_p$: the context will always clarify the domain we refer to. For the norm in $H^s(\mathbb{R}^d)$ for $s \in \mathbb{R}$, we use the symbol $\|\cdot\|_{H^s}$.
- We denote the free Hamiltonian operator in $L^2(\mathbb{R}^d)$ by

$$H_0 := -\frac{1}{2}\Delta, \quad H_0 : H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d),$$

which is self-adjoint in $L^2(\mathbb{R}^d)$ and generates the free Schrödinger propagator, denoted in the following by $U_0(t)$. The family of such operators is a strongly continuous unitary group (for more details, see e.g. [22], Ch. 8). At fixed t, $U_0(t)$ acts as the convolution with the integral kernel

$$U_0(t,x) \;=\; \frac{1}{(2\pi i t)^{d/2}} e^{i\frac{|x|^2}{2t}}, \qquad x \in \mathbb{R}^d.$$

- Whenever a tensor product appears, the first factor refers to the heavy particle or to its state, while the second refers to the light particle or to its state. The convention applies to operators and wave functions. Given a wave function χ_X for the light particle, where the coordinate X of the heavy particle enters as a parameter, $\varphi \otimes \chi_X$ will denote the wave function defined by

$$[\varphi \otimes \chi_X](X,x) := \varphi(X)\chi_X(x).$$

Of course, this is an abuse of notation since χ_X depends on X, but it will be useful and unambiguous in the sequel.

• The interaction between the light and the heavy particle is described by the potential $V : \mathbb{R}^d \longrightarrow \mathbb{R}$. In theorems 3.2 and 3.4 the potential V is required to fulfill some general hypotheses (see assumptions (H1)–(H3) and related comments). For the numerical analysis (see Section 4.2) three different kinds of V are considered, which share the features of being non negative and rapidly decreasing, but are different in terms of local regularity.

• We denote by H_V the Hamiltonian

$$H_V := -\frac{1}{2}\Delta + V,$$

where V is the multiplication by $V(x)$. In all cases we consider, H_V is self-adjoint, and $U_V(t)$ denotes the unitary group generated by H_V, i.e.

$$U_V(t) := e^{-iH_V t}.$$

• We denote by S the scattering operator between the self-adjoint operators H_0 and H_V, i.e.

$$S_V := s - \lim_{t,t' \to +\infty} S_V(t,t'), \quad \text{where} \quad S_V(t,t') := U_0(-t')U_V(t+t')U_0(-t), \tag{2.2}$$

and the limit holds in the strong operator topology. In all cases we consider, S_V is well-defined and unitary.

• Consider the self-adjoint Hamiltonian operator H_V, its unitary group U_V and the related scattering operator S_V. Then, the shifts by any $X \in \mathbb{R}^d$, denoted respectively by H_V^X, U_V^X, and S_V^X, are also well-defined and share the properties of the unshifted ones. More explicitly,

$$H_V^X := -\frac{1}{2}\Delta + V(\cdot - X), \qquad U_V^X(t) := e^{-iH_V^X t},$$
$$S_V^X := s - \lim_{t,t' \to +\infty} S_V^X(t,t'), \quad \text{where} \quad S_V^X(t,t') := U_0(-t')U_V^X(t+t')U_0(-t).$$

When no confusion is possible, we will forget the subscript V and use the shorthand notation H, S, U and H^X, U^X, S^X.

• The two-particle free Hamiltonian operator and the Hamiltonian operator containing the interaction among the two particles shall be denoted respectively by

$$H_\varepsilon^f := -\frac{1}{2}\Delta_X - \frac{1}{2\varepsilon}\Delta_x, \qquad H_\varepsilon := -\frac{1}{2}\Delta_X - \frac{1}{2\varepsilon}\Delta_x + \frac{1+\varepsilon}{\varepsilon}V(|X-x|).$$

Both are unbounded self-adjoint operators on $L^2(\mathbb{R}^{2d})$. The associated unitary groups will be represented respectively by $U_\varepsilon^f(t)$ and $U_\varepsilon(t)$.
The unitary group generated by H_ε^f factorizes as

$$U_\varepsilon^f(t) = U_0(t) \otimes U_0(t/\varepsilon).$$

- The Fourier transform of a function $\phi\in L^2(\mathbb{R}^d)$ is denoted by $\widehat{\phi}$ and is defined by

$$\widehat{\phi}(k) := (2\pi)^{-\frac{d}{2}}\int_{\mathbb{R}^d} e^{-ik\cdot x}\phi(x)\,dx, \tag{2.3}$$

where $k\cdot x$ is the Euclidean scalar product in $\mathbb{R}^d$ between the vectors k and x.

- Given a functional space $H^s(\mathbb{R}^d)$ (possibly with $s=0$), we define the *translation operator* θ_X by

$$\theta_X\phi(x) = \phi(x-X),$$

for any $\phi\in H^s(\mathbb{R}^d)$. It turns out that θ_X is a unitary operator.

- The space of self-adjoint trace-class operators (see [22]) on $L^2(\mathbb{R}^d)$ or in $L^2(\mathbb{R}^{2d})$ is denoted by $\mathcal{L}^1$ and the norm of a generic element ρ in that space is given by

$$\|\rho\|_{\mathcal{L}^1} := \mathrm{Tr}|\rho|, \quad \forall\rho\in\mathcal{L}^1,$$

where Tr denotes the trace functional (see [22], Ch. VI). The subspace of the positive elements of $\mathcal{L}^1$ is denoted by $\mathcal{L}^1_+$, without specifying whether the operator of interest acts on $L^2(\mathbb{R}^{2d})$ or on $L^2(\mathbb{R}^d)$. Anyway, the context will always be unambiguous: if ρ is the density operator of a single particle, then $\|\rho\|_{\mathcal{L}^1}$ denotes its trace class norm as an operator on $L^2(\mathbb{R}^d)$. Conversely, if ρ is the density operator of a two-particle system, then $\|\rho\|_{\mathcal{L}^1}$ denotes its trace class norm as an operator on $L^2(\mathbb{R}^{2d})$.

- We shall make occasional use of the so-called Dirac's bra-ket notation: for example, the state of the heavy particle will be denoted by $|\varphi\rangle$, while the state of the light particle by $|\chi\rangle$. A scalar product between two states of the light particle shall be denoted by $\langle\chi'|\chi\rangle$, while the orthogonal projector along the span of $|\chi\rangle$ will be represented by $|\chi\rangle\langle\chi|$.
- We will always assume that wave functions φ, χ, and density operators ρ are normalized, i.e.

$$\|\varphi\|_2=\|\chi\|_2=1, \quad \rho\in\mathcal{L}^1_+, \quad \text{and} \quad \|\rho\|_{\mathcal{L}^1}=1.$$

2.2. Assumptions. We introduce three hypotheses that we shall use in theorems 3.2 and 3.4.

(H1) The Hamiltonian H_V is self-adjoint on $L^2(\mathbb{R}^d)$, its point spectrum is empty and zero-energy resonances are absent.

(H2) Asymptotic completeness holds for the couple of self-adjoint operators H_0 and H_V, and the scattering operator S_V is well-defined and unitary in $L^2(\mathbb{R}^d)$.

(H3) There exist $s\in\mathbb{R}$ and a constant $C_s>0$ such that

$$\forall\chi\in L^2(\mathbb{R}^d), \quad \||x|S_V\chi\|_2\le\||x|\chi\|_2+C_s\|\chi\|_{H^s}.$$

Let us comment on these hypotheses. The first one, (H1), requires self-adjointness of the Hamiltonian operator, which provides well-posedness of the associated Schrödinger equation and unitarity of the propagator; bound states, as well as zero-energy resonances are to be avoided for the wave operators to be well-defined. The second hypothesis (H2) prescribes the unitarity of the scattering operator. The third one (H3) is less common, and is a regularity assumption on the scattering operator S_V. For $d=1$, (H3) can be replaced by the stronger assumption

(H3') There exists an $s \in \mathbb{R}$ and a constant $C_s > 0$ such that the reflection and transmission amplitudes r_k and t_k (see Section 4.1) satisfy

$$|\partial_k t_k| + |\partial_k r_k| \leq C_s (1 + |k|^2)^{\frac{s}{2}}. \tag{2.4}$$

The fact that (H3') implies (H3) is proven in Lemma 4.1.

Roughly speaking, hypotheses (H1)–(H3) are fulfilled by non negative, regular potentials that decay fast enough at infinity. In dimension one, (H1)–(H3') are satisfied, among others, by the repulsive Dirac's delta potential and potential barriers, for which the transmission and reflection amplitudes are explicitly known. See Section 4 for more details.

3. Analytical results

In this section we give the analytical results that provide an approximate solution to the problem (1.1), (2.1) in the regime $\varepsilon \ll 1$. In Theorem 3.2 the case of a pure state (i.e. a wave function) is considered, and we give an approximate solution in which the evolution of the heavy particle is decoupled from the evolution of the light one, provided that the initial state has been suitably modified. In Theorem 3.4 we generalize the result to the case of a mixed state (i.e. a density operator), in which the problem (1.1), (2.1) is replaced by the operator differential equation (3.8). Theorem 3.4 provides an approximate density operator for the heavy particle whose dynamics is governed by a free evolution problem with modified initial data. The modification of the initial data is given by the action of the collision operator $\mathcal{I}_\chi$.

For the convenience of the reader, proofs are postponed to Section 6.

Theorems 3.2 and 3.4 supply the theoretical basis of the numerical method that will be introduced in Section 5.

Definition 3.1. *Given $\varepsilon > 0$, the operator $\mathcal{S}_\varepsilon$, acting on $L^2(\mathbb{R}^{2d})$ is the unique unitary extension of*

$$\mathcal{S}_\varepsilon(\varphi \otimes \chi) := \varphi \otimes \left[U_0(-\varepsilon^{-\gamma}) S^X \chi \right], \quad \forall \varphi, \chi \in L^2(\mathbb{R}^d); \tag{3.1}$$

Furthermore, the operator $\widehat{\mathcal{S}}$, acting on $L^2(\mathbb{R}^{2d})$, is the unique unitary extension of

$$\widehat{\mathcal{S}}(\varphi \otimes \chi) \;=\; \varphi \otimes S^X \chi.$$

Notice that, with our notation, $\mathcal{S}_\varepsilon = \left[\mathbb{I} \otimes U_0(-\varepsilon^{-\gamma}) \right] \widehat{\mathcal{S}}$.

Theorem 3.2. *Assume that the potential V is such that hypotheses (H1)–(H3) are satisfied and denote by s a real number for which (H3) holds. Choose $\varphi \in H^1(\mathbb{R}^d)$ such that $|X|\varphi \in H^1(\mathbb{R}^d)$, and $\chi \in H^{s+1}(\mathbb{R}^d)$ such that $|x|\chi \in H^1(\mathbb{R}^d)$.*

Let $\psi_\varepsilon(t)$ denote the solution to (1.1) with $M = 1$ and the initial condition (2.1); moreover let $\psi^a_\varepsilon(t)$ denote the solution to the free two-body Schrödinger equation

$$\begin{cases} i\partial_t \psi^a_\varepsilon = -\frac{1}{2}\Delta_X \psi^a_\varepsilon - \frac{1}{2\varepsilon}\Delta_x \psi^a_\varepsilon = H^f_\varepsilon \psi^a_\varepsilon \\ \psi^a_\varepsilon(0) = \varphi \otimes U_0(-\varepsilon^{-\gamma}) S^X \chi = \mathcal{S}_\varepsilon(\varphi \otimes \chi). \end{cases} \tag{3.2}$$

Then, the following estimate holds

$$\|\psi_\varepsilon(t) - \psi^a_\varepsilon(t)\|_2 \leq C_1 \left(\frac{1+\varepsilon}{\varepsilon} t - \varepsilon^{-\gamma}, \varepsilon^{-\gamma} \right) + C_2 \varepsilon + C_3 \varepsilon^{1-\gamma}, \tag{3.3}$$

where the constants are given by

$$C_1(\tau,\tau') := \|\varphi[S(\tau,\tau') - S]\chi(\cdot - X)\|_2 \tag{3.4}$$

$$C_2 := 2\sqrt{2}\big(\|\nabla\varphi\|_2 \||x|\chi\|_2 + \||X|\varphi\|_2 \|\nabla\chi\|_2 + \|X\cdot\nabla\varphi\|_2 + \|x\cdot\nabla\chi\|_2\big) \\ + \sqrt{2}C_s\big(\|\nabla\varphi\|_2\|\chi\|_{H^s} + \|\chi\|_{H^{s+1}}\big) \tag{3.5}$$

$$C_3 := 2\sqrt{2}\big(\|\nabla\varphi\|_2\|\nabla\chi\|_2 + 2\|\Delta\chi\|_2\big), \tag{3.6}$$

with s and C_s defined by the hypothesis (H3).

For the proof see Section 6.

REMARK 3.1.

i) The first term in (3.3) is quite implicit, nevertheless hypotheses (H1)–(H2) guarantee

$$\lim_{\tau,\tau'\to+\infty} C_1(\tau,\tau') = 0.$$

Indeed, the existence of the strong limit that defines the scattering operator (see (2.2)) implies that, for fixed X and χ, $\|S^X(\tau,\tau')\chi - S^X\chi\|_2 \to 0$ as $\tau,\tau' \to +\infty$, and therefore, observing that

$$C_1(\tau,\tau')^2 \le |\varphi(X)|^2 \left\|S^X(\tau,\tau')\chi - S^X\chi\right\|_2^2 \le 4|\varphi(X)|^2,$$

by dominated convergence one has $C_1(\tau,\tau') \to 0$ as $\tau,\tau' \to \infty$.

Notice that in order to explicitly estimate $C_1(\tau,\tau')$, one needs to study the one-body scattering of the light particle by the potential V. See Proposition A.2 for an example.

ii) The constant C_2 in Theorem 3.2 depends on the regularity properties of the scattering operator through the assumption (H3). If this hypothesis is not satisfied, then one can prove that the constant C_2 may be replaced by

$$C_2' := \Big\| |x| \left[\nabla\varphi \otimes S^X\chi + \varphi\otimes S^X\nabla\chi\right]\Big\|_2 + 5\big\| |x - X||\nabla\psi^0| \big\|_2.$$

REMARK 3.2. Matching Theorem 3.2 with Proposition A.2, one has that for the one-dimensional system with $V = \alpha\delta_0$, $\alpha > 0$, the solution ψ_ε to (1.1) is well-approximated by the solution ψ_ε^a to (3.2). More precisely, for any initial condition of the type treated in Theorem 3.2, there exists a constant C depending on φ and ψ such that

$$\forall t \ge 2\varepsilon^{1-\gamma}, \quad \|\psi_\varepsilon(t) - \psi_\varepsilon^a(t)\|_2 \le C\left[\left(\frac{\varepsilon}{t}\right)^{\frac14} + \varepsilon^{1-\gamma}\right].$$

REMARK 3.3. There are some differences with respect to the previously known results [2, 3]. First, we modified the initial state for the light particle by inserting the operator $U(-\varepsilon^{-\gamma})$. Physically, this means that in our idealized experiment the light particle enters the system at time $t = -\infty$ and immediately becomes entangled with the heavy one. On the other hand, in the physical situation depicted in [2, 3, 10, 13] each light particle is injected in the system at time zero. The mathematical consequence of our choice is that the initial state of the light particle is (approximately) transformed via the action of the scattering operator instead of the Møller wave operator. This is consistent with the original Joos–Zeh's formula ([19]).

The main advantage of our choice is that, in general, the operator S is rather simple to write in Fourier variables as it involves the Fourier transform only, while the Møller operator involves a different (and usually implicit) eigenfunction expansion. As a consequence, the scattering operator is better suited for a direct analytical study and for numerical simulations too.

REMARK 3.4. Theorem 3.2 can be formally restated as follows:

$$U_\varepsilon(t)(\mathbb{I}\otimes U_0(-\varepsilon^{-\gamma})) \approx U_\varepsilon^f(t)\mathcal{S}_\varepsilon = U_\varepsilon^f(t)(\mathbb{I}\otimes U_0(-\varepsilon^{-\gamma}))\widehat{\mathcal{S}} \tag{3.7}$$

for times of order one. Pictorially, (3.7) states that for small ε the light particle is instantaneously scattered away by the heavy one, which may be considered as fixed during the interaction.

Let us generalize Theorem 3.2 to the formalism of density operators. Such a step is necessary in order to describe the dynamics of the heavy particle when interacting with several light particles: indeed, as we can see from (3.2), the initial condition for the limit model is not factorized, so after one collision the heavy particle lies in a mixed state that has to be described by the appropriate density operator.

Assume that the initial state of the heavy particle is given by the density operator $\rho^M(0)\in\mathcal{L}^1_+$, while, as before, the light particle at time zero lies in the state represented by the wave function $U_0(-\varepsilon^{-\gamma})\chi$. Then, the density operator $\rho_\varepsilon(t)$ that represents the state of the two-body system at time t solves the operator differential equation

$$\begin{cases} i\partial_t\rho_\varepsilon(t) & =[H_\varepsilon,\rho_\varepsilon(t)] \\ \rho_\varepsilon(0) & :=\rho^M(0)\otimes|U_0(-\varepsilon^{-\gamma})\chi\rangle\langle U_0(-\varepsilon^{-\gamma})\chi|, \end{cases} \tag{3.8}$$

where the symbol $[A_1,A_2]$ denotes the commutator of the operators A_1 and A_2.

For the sake of studying the dynamics of the heavy particle, the interesting quantity is the density operator of the heavy particle, which is denoted by $\rho_\varepsilon^M(t)$ and defined as

$$\rho_\varepsilon^M(t) := \mathrm{Tr}_m\rho_\varepsilon(t)=\sum_j\langle\chi_j|\rho_\varepsilon(t)|\chi_j\rangle, \tag{3.9}$$

where $\{\chi_j\}_{j\in\mathbb{N}}$ is a complete orthonormal set for the space $L^2(\mathbb{R}^d)$, and Tr_m denotes the so-called *partial trace w.r.t. the light particle.*

Let us be more precise on how to compute such a partial trace. As $\rho_\varepsilon(t)$ is compact, it can be represented as an integral operator whose kernel can be denoted, with a slight abuse of notation, by $\rho_\varepsilon(t,X,X',x,x')$. The integral kernel of the reduced density matrix for the heavy particle then reads

$$\rho_\varepsilon^M(t,X,X'):=\int_{\mathbb{R}^d}\rho_\varepsilon(t,X,X',x,x)\,dx. \tag{3.10}$$

There does not exist a closed equation for the time evolution of ρ_ε^M, but, as we shall see, as ε goes to zero and for any $t\neq 0$, the operator $\rho_\varepsilon^M(t)$ converges to an operator $\rho^{M,a}(t)$ that satisfies a closed equation. In order to state this result properly, we need to introduce a further operator on $\mathcal{L}_1$ which we call the *collision operator.*

DEFINITION 3.3 (Collision operator). *Suppose that the hypotheses (H1)–(H2) are satisfied. Then, we define the* collision operator

$$\mathcal{I}_\chi:\mathcal{L}^1(\mathbb{R}^d)\to\mathcal{L}^1(\mathbb{R}^d),\quad \rho^M\mapsto\mathrm{Tr}_m\big(\rho^M\otimes|S^X\chi\rangle\langle S^{X'}\chi|\big). \tag{3.11}$$

REMARK 3.5. It can be verified that the operator $\mathcal{I}_\chi$ is well-defined and completely positive (in particular it preserves positivity). Moreover, it satisfies the estimate

$$\mathrm{Tr}|\mathcal{I}_\chi \rho^M| \le \mathrm{Tr}|\rho^M| \quad \text{with equality if } \rho^M \in \mathcal{L}^1_+. \tag{3.12}$$

REMARK 3.6. In terms of integral kernels, the action of the collision operator reads

$$[\mathcal{I}_\chi \rho](X,X') = \rho(X,X')\, I_\chi(X,X'), \tag{3.13}$$

where the *collision function* I_χ is defined by

$$I_\chi(X,X') := \langle S^{X'}\chi | S^X \chi\rangle, \qquad X,X' \in \mathbb{R}^d \tag{3.14}$$

Notice that the function I_χ reaches its maximum modulus at $X = X'$, where it equals one.

THEOREM 3.4. *Assume that the potential V is s.t. the hypotheses (H1)–(H3) are satisfied, choose $\rho^M(0) \in \mathcal{L}^1_+$ s.t. $\nabla \rho^M(0) \nabla$ and $|\cdot|\nabla\rho^M(0)\nabla|\cdot| \in \mathcal{L}^1_+$; choose $\chi \in H^s(\mathbb{R}^d)$ for some $s \ge 1$. Denote by $\rho_\varepsilon(t)$ the solution to equation (3.8) and by $\rho^{M,a}(t)$ the unique solution to the problem*

$$\begin{cases} i\partial_t \rho^{M,a}(t) & = [H_0, \rho^{M,a}(t)] \\ \rho^{M,a}(0) & := \mathcal{I}_\chi \rho^M(0). \end{cases} \tag{3.15}$$

Then, the following estimate holds

$$\|\rho^M_\varepsilon(t) - \rho^{M,a}(t)\|_{\mathcal{L}^1} \le \widetilde{C}_1\left(\frac{1+\varepsilon}{\varepsilon} t - \varepsilon^{-\gamma}, \varepsilon^{-\gamma}\right) + \widetilde{C}_2 \varepsilon + \widetilde{C}_3 \varepsilon^{1-\gamma}, \tag{3.16}$$

where the constants are given by

$$\begin{aligned} \widetilde{C}_1(\tau,\tau') &:= 2\big\|\rho^M(0)|[S(\tau,\tau') - S]\chi(\cdot - X')\rangle\langle[S(\tau,\tau') - S]\chi(\cdot - X)|\big\|^{\frac{1}{2}}_{\mathcal{L}^1} \\ \widetilde{C}_2 &:= 4\sqrt{2}\big(\|\nabla\rho^M(0)\nabla\|^{\frac{1}{2}}_{\mathcal{L}^1} \||x|\chi\|_2 + \||X|\rho^M(0)|X|\|^{\frac{1}{2}}_{\mathcal{L}^1} \|\nabla\chi\|_2 \\ &\qquad + \big\||X|\nabla\rho^M(0)\nabla|X|\big\|^{\frac{1}{2}}_{\mathcal{L}^1} + \||x|\nabla\chi\|_2\big) \\ &\qquad + 2\sqrt{2}C_s\big(\|\nabla\rho^M(0)\nabla\|^{\frac{1}{2}}_{\mathcal{L}^1} \|\chi\|_{H^s} + \|\chi\|_{H^{s+1}}\big) \\ \widetilde{C}_3 &:= 4\sqrt{2}\big(\|\nabla\rho^M(0)\nabla\|^{\frac{1}{2}}_{\mathcal{L}^1} \|\nabla\chi\|_2 + 2\|\Delta\chi\|_2\big). \end{aligned}$$

The proof is given in Section 6.

The last step in our theoretical framework consists in the possibility of extending the previous procedure to the case of many light particles to be injected in the system one after another. To this purpose, one should use an approximation result analogous to Theorem 3.4, but adapted to a multi-particle system with light particles arriving at different times. Instead of following this approach, which is fully rigorous but cumbersome and very difficult to handle (see for instance [3] for a result with many simultaneous "collisions"), we will repeatedly use the approximation given by Theorem 3.4. This means that we treat the heavy particle as if it were interacting with only one light particle at a time.

Under that approximation, the multiple use of the collision operator $\mathcal{I}_\chi$ is justified, provided that the constants $\widetilde{C}_1$, $\widetilde{C}_2$, and $\widetilde{C}_3$ appearing in Theorem 3.4 do not explode when computed for $\rho^{M,a}(t)$ instead of $\rho^M(0)$. The behavior of such constants can be shown to depend on the regularity properties of the collision function I_χ only. In particular, the calculation of the kinetic energy of $\rho^{M,a}(0)$ in terms of $\rho^M(0)$ and I_χ, done in Proposition 4.2, may guarantee the correct behavior of the constants $\widetilde{C}_1$, $\widetilde{C}_2$ and $\widetilde{C}_3$, but we will not go into such details.

4. One-dimensional systems. Computation of $\mathcal{I}_\chi$

In this section we restrict to one-dimensional problems and provide a general expression for the collision function I_χ (see (4.11), (4.12), (4.13)) whose form shows that I_χ depends on the reflection and transmission amplitudes associated to the potential V and on the wave function of the light particle. Using this expression we compute the energy and momentum transfer occurring in a two-body collision.

Furthermore, assuming that the state of the light particle is represented by a Gaussian wave packet with a narrow spectrum in momentum, we prove an approximation of Θ_χ (see (4.22)) to be used in Section 5.4.

4.1. Scattering operator, reflection and transmission amplitudes. Consider a particle moving on a line under the action of the potential V, and assume hypotheses (H1)–(H3). We define the *transmission amplitude* t_k and the *reflection amplitude* r_k as the two complex coefficients s.t. the action of the scattering operator S, defined in (2.2), reads

$$(S\chi)(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} [t_k \widehat{\chi}(k) + r_{-k} \widehat{\chi}(-k)]\, e^{ikx}\, dk, \quad \forall x \in \mathbb{R}, \tag{4.1}$$

for any $\chi \in L^2(\mathbb{R})$. We stress that definition (4.1) corresponds to the following formal action on plane waves

$$S(e^{ikx}) = r_k e^{-ikx} + t_k e^{ikx},$$

which, in turn, agrees with the definition of reflection and transmission amplitudes usually found in physics textbooks, namely, t_k and r_k are the two complex coefficients s.t. the generalized eigenfunction ψ_k of the operator H_V corresponding to the generalized eigenvalue $E = \frac{k^2}{2} \neq 0, k > 0$ fulfills the asymptotics

$$\begin{aligned} \psi_k(x) &\sim \frac{1}{\sqrt{2\pi}} \left(e^{ikx} + r_k e^{-ikx} \right), \qquad x \to -\infty, \\ \psi_k(x) &\sim \frac{1}{\sqrt{2\pi}} t_k e^{ikx}, \qquad x \to +\infty. \end{aligned} \tag{4.2}$$

It proves useful to represent the action of S through the 2×2 matrices

$$S(k) := \begin{pmatrix} t_k & r_{-k} \\ r_k & t_{-k} \end{pmatrix}, \qquad k > 0, \tag{4.3}$$

that act on the vectors $(\widehat{\chi}(k), \widehat{\chi}(-k))_{k>0}$ as follows

$$\forall k > 0, \quad \begin{pmatrix} \widehat{S\chi}(k) \\ \widehat{S\chi}(-k) \end{pmatrix} = S(k) \begin{pmatrix} \widehat{\chi}(k) \\ \widehat{\chi}(-k) \end{pmatrix}. \tag{4.4}$$

Moreover, the unitarity of S implies, for $k \neq 0$,

$$|t_k|^2 + |r_k|^2 = 1, \quad r_k \overline{t_{-k}} + t_k \overline{r_{-k}} = 0, \quad |r_k| = |r_{-k}|. \tag{4.5}$$

The fact that S commutes with the Laplacian, together with its unitarity, gives

$$\|S\chi\|_{H^s} = \|\chi\|_{H^s}, \qquad \forall s \in \mathbb{R},\ \forall \chi \in H^s(\mathbb{R}).$$

We are ready to prove that, as stated in Section 2, the condition $(H3')$ in dimension one implies condition (H3).

LEMMA 4.1. *Suppose that for some $s \in \mathbb{R}$ and $C_s > 0$ the transmission and reflection coefficients satisfy*

$$|\partial_k t_k| + |\partial_k r_k| \leq C_s (1 + |k|^2)^{\frac{s}{2}} =: C_s \langle k \rangle^s. \tag{4.6}$$

Then, for all $\chi \in H^s(\mathbb{R})$

$$\|xS\chi\|_2 = \|\partial_k[\widehat{S\chi}]\|_2 \leq \|x\chi\|_2 + 2C_s \|\chi\|_{H^s}.$$

Proof. Since

$$\partial_k \begin{pmatrix} \widehat{S\chi}(k) \\ \widehat{S\chi}(-k) \end{pmatrix} = [\partial_k S(k)] \begin{pmatrix} \widehat{\chi}(k) \\ \widehat{\chi}(-k) \end{pmatrix} + S(k) \begin{pmatrix} \partial_k \widehat{\chi}(k) \\ \partial_k \widehat{\chi}(-k) \end{pmatrix},$$

one gets

$$\left\|\partial_k \widehat{S\chi}\right\|_2 \leq \left(\int_0^{+\infty} \left| [\partial_k S(k)] \begin{pmatrix} \widehat{\chi}(k) \\ \widehat{\chi}(-k) \end{pmatrix} \right|^2 dk \right)^{\frac{1}{2}} + \left(\int_0^{+\infty} \left| S(k) \begin{pmatrix} \partial_k \widehat{\chi}(k) \\ \partial_k \widehat{\chi}(-k) \end{pmatrix} \right|^2 dk \right)^{\frac{1}{2}}.$$

By unitarity of $S(k)$, the second term in the r.h.s. equals $\|\partial_k \widehat{\chi}\|_2 = \|x\chi\|_2$. Furthermore, by (4.6),

$$\begin{aligned} \int_0^{+\infty} \left| [\partial_k S(k)] \begin{pmatrix} \widehat{\chi}(k) \\ \widehat{\chi}(-k) \end{pmatrix} \right|^2 dk &\leq 4C_s^2 \int_0^{+\infty} \langle k \rangle^{2s} \left(|\widehat{\chi}(k)|^2 + |\widehat{\chi}(-k)|^2 \right) dk \\ &\leq 4C_s^2 \|\chi\|_{H^s}^2. \end{aligned}$$

This implies the claimed result. ∎

The effect of translation. If the potential V is translated by a quantity X, then the reflected wave is delayed by a phase equal to $2kX$ and the transmitted one remains unchanged. As a consequence, one has the following

LEMMA 4.2. *Let V be s.t. the Hamiltonian operator $H_V = -\frac{1}{2}\partial_x^2 + V$ satisfies assumptions (H1)–(H3). Then, the translated Hamiltonian operator $H_V^X = -\frac{1}{2}\partial_x^2 + V(\cdot - X)$ satisfies (H1)–(H3) and, denoting the corresponding reflection and transmission amplitudes by r_k^X and t_k^X, one has*

$$r_k^X = e^{2ikX} r_k, \qquad t_k^X = t_k, \quad \forall k \in \mathbb{R} \setminus \{0\}. \tag{4.7}$$

Proof. According to the notation of Section 2, we denote by θ_X the translation operator s.t. $\theta_X \chi = \chi(\cdot - X)$. Then, one easily gets

$$U_V^X(t) = \theta_X U_V(t) \theta_{-X}, \tag{4.8}$$

so that $U_V^X(t)$ and $U_V(t)$ are unitarily equivalent and assumptions (H1)–(H3) are preserved by translation. Furthermore, (4.8) implies

$$S_V^X = \theta_X S_V \theta_{-X}. \tag{4.9}$$

By direct computation $\widehat{\theta_{-X}\chi}(k) = e^{ikX}\widehat{\chi}(k)$, so one finally gets

$$\widehat{S_V^X \chi}(k) = e^{-2ikX} r_{-k} \widehat{\chi}(-k) + t_k \widehat{\chi}(k)$$

and the proof is complete. □

Corollary 4.1. *The matrix S_V^X reads*

$$S_V^X(k) = \begin{pmatrix} t_k & e^{-2ikX} r_{-k} \\ e^{2ikX} r_k & t_{-k} \end{pmatrix}. \tag{4.10}$$

Lemma 4.2 (and Corollary 4.1) allow us to get a rather simple expression for the collision function I_χ.

Proposition 4.1. *For a one-dimensional two-particle system, endowed with an interaction potential V such that the hypotheses (H1)–(H3) are verified, the collision function I_χ defined in (3.14) can be expressed as*

$$I_\chi(X, X') = 1 - \Theta_\chi(X - X') + i\Gamma_\chi(X) - i\Gamma_\chi(X'), \tag{4.11}$$

with the definitions

$$\Theta_\chi(Y) := \int_{\mathbb{R}} \left(1 - e^{2ikY}\right) |r_k|^2 |\widehat{\chi}(k)|^2 \, dk, \tag{4.12}$$

$$\Gamma_\chi(X) := i \int_{\mathbb{R}} e^{2ikX} \, \overline{r_{-k}} \, t_k \, \overline{\widehat{\chi}(-k)} \, \widehat{\chi}(k) \, dk. \tag{4.13}$$

Proof. The proof is an elementary computation to be carried out using definition (3.14), the equation (4.1), the relations (4.5), and Lemma 4.2. □

Remark 4.1. By the change of variable $k \to -k$ in the integral defining I_χ and the relations (4.5), one immediately finds that $\Gamma_\chi(X)$ is real for any X.

Effect of the collision operator on kinetic energy and momentum of the heavy particle. In order to interpret the functions Θ_χ and Γ_χ we study the transfer of energy and momentum between the heavy and the light particle.

We recall that for a particle in the mixed state ρ lying in a d-dimensional space, the average momentum and kinetic energy are given by

$$P(\rho) = \mathrm{Tr}\left(\frac{1}{2}\left[(-i\nabla)\rho + \rho(-i\nabla)\right]\right) \qquad \text{or } P(\rho) = \frac{i}{2}\int_{\mathbb{R}^d} (\nabla_2 - \nabla_1)\rho(X, X) \, dX, \tag{4.14}$$

$$E_{kin}(\rho) = \frac{1}{2}\mathrm{Tr}(-i\nabla\cdot\rho[-i\nabla]) \qquad \text{or } E_{kin}(\rho) = \frac{1}{2}\int_{\mathbb{R}^d}\nabla_2\cdot\nabla_1\rho(X,X)\,dX. \quad (4.15)$$

The probability current $\overrightarrow{\mathrm{j}}$ is defined, in terms of the density operator, by

$$\overrightarrow{\mathrm{j}} := \frac{1}{2}\big[\rho(-i\nabla)+(-i\nabla)\rho\big] \qquad \text{or } \overrightarrow{\mathrm{j}}(X,X') := \frac{i}{2}(\nabla_2-\nabla_1)\rho(X,X'). \quad (4.16)$$

Remark that $P(\rho) = \mathrm{Tr}\,\overrightarrow{\mathrm{j}}$. For the sake of interpreting the forthcoming proposition, one can consider that, if ρ is the density operator representing the state of the heavy particle *before the collision*, then, in our approximation, $\mathcal{I}_\chi\rho$ is the density operator representing the state of the heavy particle *after the collision*.

PROPOSITION 4.2. *The momentum and the kinetic energy of a particle moving on a line, as it lies in the mixed state represented by the density operator $\mathcal{I}_\chi\rho$, are given by*

$$P\big(\mathcal{I}_\chi\rho\big) = P(\rho) + i\Theta'_\chi(0) + \frac{1}{2}\mathrm{Tr}\Big(\Gamma'_\chi\rho+\rho\Gamma'_\chi\Big), \quad (4.17)$$

$$E_{kin}(\mathcal{I}_\chi\rho) = E_{kin}(\rho) + i\Theta'_\chi(0)P(\rho) + \frac{1}{2}\Theta''_\chi(0) + \frac{1}{2}\mathrm{Tr}\big(\Gamma'_\chi j + j\Gamma'_\chi\big), \quad (4.18)$$

where Γ'_χ denotes the operator whose action is the multiplication by the derivative of Γ_χ and j is the only component of the current $\vec{j}$ that is present in the one-dimensional case.

Proof. From decomposition (4.11), one immediately gets

$$\partial_1 I_\chi(X,X') = -\Theta'_\chi(X-X') + i\Gamma'_\chi(X)$$
$$\partial_2 I_\chi(X,X') = \Theta'_\chi(X-X') - i\Gamma'_\chi(X'),$$

where ∂_j denotes the derivative w.r.t. the jth argument. By exploiting the second identity in (4.14), a straightforward computation yields

$$P\big(\mathcal{I}_\chi\rho\big) = P(\rho) + i\Theta'_\chi(0) + \int_{\mathbb{R}}\Gamma'_\chi(X)\rho(X,X)\,dX,$$

which may be rewritten as (4.17).
Concerning kinetic energy, by the second identity in (4.15) one gets

$$2E_{kin}(\mathcal{I}_\chi\rho) = 2E_{kin}(\rho) + \int_{\mathbb{R}}\big[(\partial_1 I_\chi)(X,X)(\partial_2\rho)(X,X) + (\partial_2 I_\chi)(X,X)(\partial_1\rho)(X,X)\big]\,dX$$
$$+\int_{\mathbb{R}}\big(\partial_2\partial_1 I_\chi\big)(X,X)\rho(X,X)\,dX.$$

Using decomposition (4.11), one finally has

$$E_{kin}(\mathcal{I}_\chi\rho) = E_{kin}(\rho) - \frac{1}{2}\Theta'_\chi(0)\int_{\mathbb{R}}\big[(\partial_2\rho)(X,X) - (\partial_1\rho)(X,X)\big]\,dX$$
$$+\frac{i}{2}\int_{\mathbb{R}}\Gamma'_\chi(X)\big[(\partial_2\rho)(X,X) - (\partial_1\rho)(X,X)\big]\,dX + \frac{1}{2}\Theta''_\chi(0).$$

This finally leads to (4.18). ∎

REMARK 4.2. First, by (4.12), one has $\Theta_\chi(0)=0$, $\mathrm{Re}(\Theta'_\chi(0))=0$, and $\mathrm{Im}(\Theta''_\chi(0))=0$, so that all quantities in Proposition 4.2 are real. In particular, notice that

$$i\Theta'_\chi(0)=2\int_{\mathbb{R}} k|r_k|^2|\widehat{\chi}(k)|^2\,dk, \tag{4.19}$$

which is in general different from zero, so that a transfer of momentum and energy is possible even though one could intuitively suspect that the light particle is in fact too light in order to exchange momentum or energy with the heavy one. In order to understand this fact, recall that the light particle has a momentum independent of ε and a kinetic energy of order ε^{-1}. Thus the collision occurs between two particles with momentum of the same order, for which exchanges of momentum and energy can take place.

Besides, the above formula (4.19) has a relatively simple interpretation. The plane wave e^{ikx} has a probability $|r_k|^2$ of being reflected, i.e. to gain a momentum $-2k$. Since the state of the incoming particle can be understood as a superposition of plane waves with weight $\widehat{\chi}(k)$, the average gain in momentum amounts to $-2\int_{\mathbb{R}} k|r_k|^2|\widehat{\chi}(k)|^2dk$ for the light particle. By conservation of momentum, the average gain in momentum for the heavy particle equals the r.h.s. of (4.19).

On the other hand, the last term in (4.17) does not have, at least to our concern, a clear interpretation. This is due to the fact that it takes into account the interference between the reflected and the transmitted waves, so that there is no classical counterpart to provide some understanding.

For the kinetic energy the situation is analogous: the sum of the second and the third term in the r.h.s. of (4.18)

$$\begin{aligned} i\Theta'_\chi(0)P(\rho)+\frac{1}{2}\Theta''_\chi(0) &= 2\int_{\mathbb{R}}(k+P(\rho))k|r_k|^2|\widehat{\chi}(k)|^2\,dk \\ &= \frac{1}{2}\int_{\mathbb{R}}\left[(2k+P(\rho))^2-P(\rho)^2\right]|r_k|^2|\widehat{\chi}(k)|^2\,dk \end{aligned}$$

can be understood similarly to the first term in the r.h.s. of (4.17), while the last term is due to a superposition effect between transmitted and reflected waves and its meaning is therefore less transparent.

The case of an initial Gaussian state for the light particle. Let us specialize to the case in which the initial state of the incoming light particle is represented by a Gaussian wave function, *i.e.*

$$\chi(x)=\frac{1}{(2\pi\sigma^2)^{1/4}}e^{-\frac{(x-x_l)^2}{4\sigma^2}+ipx}, \tag{4.20}$$

where $x_l\in\mathbb{R}$ is the centre of the wave packet, σ its spread, and p its mean momentum. Then,

$$\widehat{\chi}(k)=\left(\frac{2\sigma^2}{\pi}\right)^{1/4}e^{-\sigma^2(k-p)^2-i(k-p)x_l}.$$

We shall make this choice of state for the light particle in Section 5, when dealing with numerical simulations. For this reason, we give simplified expressions for Θ_χ and Γ_χ and we provide some related approximation formulas that prove easy to handle. In fact, for the Gaussian case definitions (4.12) and (4.13) yield

$$\begin{aligned}\Theta_{\sigma,p}(Y) &= \sigma\sqrt{\tfrac{2}{\pi}}\int_{\mathbb{R}}\left(1-e^{2ikY}\right)|r_k|^2 e^{-2\sigma^2(k-p)^2}\,dk,\\ \Gamma_{\sigma,p}(X) &= i\sigma\sqrt{\tfrac{2}{\pi}}e^{-2\sigma^2p^2}\int_{\mathbb{R}} t_k\overline{r_{-k}}\,e^{-2\sigma^2k^2+2ik(X-x_l)}\,dk.\end{aligned} \tag{4.21}$$

If the wave packet has a large spread in position, so that its support in momentum is small compared to the scale at which $|r_k|^2$ varies, then we can approximate $\Theta_{\sigma,p}$ by using $|r_p|^2$ instead of $|r_k|^2$ in the integral, and get the following approximation

$$\begin{aligned}\Theta^{app}_{\sigma,p}(Y) &:= |r_p|^2\left(1-\sigma\sqrt{\frac{2}{\pi}}\int_{\mathbb{R}} e^{2ikY-2\sigma^2(k-p)^2}\,dk\right)\\ &= |r_p|^2\left(1-e^{2ipY-\frac{Y^2}{2\sigma^2}}\right).\end{aligned} \tag{4.22}$$

Approximating Γ_χ turns out to be more difficult. However, as a first step, assuming that the light particle has a large momentum, we can approximate Γ_χ by 0 since the factor $e^{-2\sigma^2p^2}$ is negligible for σp large enough.

The approximations introduced here can be expressed in terms of density matrices. Indeed, one has the following proposition:

Proposition 4.3. *For any positive, self-adjoint operator ρ with $\mathrm{Tr}\rho = 1$, the following estimate holds*

$$\left\|\Theta_{\sigma,p}(X-X')\rho(X,X') - \Theta^{app}_{\sigma,p}(X-X')\rho(X,X')\right\|_{\mathcal{L}^1} \le \sqrt{\frac{2}{\pi\sigma^2}}\left\|\frac{d|r_k|^2}{dk}\right\|_\infty,$$
$$\left\|i[\Gamma_{\sigma,p}(X)-\Gamma_{\sigma,p}(X')]\rho(X,X')\right\|_{\mathcal{L}^1} \le 2e^{-2\sigma^2p^2},$$

where we denoted an operator by its integral kernel.

Proof. We will use the following simple estimates: for a wave packet χ with centre x_0, spread σ, and momentum p, we have

$$\begin{aligned}\int_{\mathbb{R}}\left||r_k|^2-|r_p|^2\right||\widehat{\chi}(k)|^2\,dk &\le \left\|\frac{d|r_k|^2}{dk}\right\|_\infty \int_{\mathbb{R}}|\widehat{\chi}(k)|^2|k-p|\,dk\\ &= \frac{2}{\sigma\sqrt{2\pi}}\left\|\frac{d|r_k|^2}{dk}\right\|_\infty\int_0^{+\infty} ke^{-k^2}\,dk\\ &= \frac{1}{\sigma\sqrt{2\pi}}\left\|\frac{d|r_k|^2}{dk}\right\|_\infty\end{aligned} \tag{4.23}$$

and

$$|\Gamma_{\sigma,p}(X)| \le \sigma\sqrt{\frac{2}{\pi}}e^{-2\sigma^2p^2}\int_{\mathbb{R}} e^{-2\sigma^2k^2}\,dk = e^{-2\sigma^2p^2}. \tag{4.24}$$

We shall only perform the proof in the case where ρ is a rank one projector: $\rho(X,X') = \varphi(X)\overline{\varphi(X')}$, where $\|\varphi\|_2 = 1$. The general case follows by diagonalisation of a general ρ and summation of the error given in the rank one case. Using (4.23), we get

$$
\begin{aligned}
&\left\|(\Theta^{app}_{\sigma,p}(X-X')-\Theta_{\sigma,p}(X-X'))\rho(X,X')\right\|_{\mathcal{L}_1}\\
&\quad\le \|\rho\|_{\mathcal{L}_1}\int_{\mathbb{R}}\left||r_k|^2-|r_p|^2\right||\widehat{\chi}(k)|^2\,dk+\left\|\int_{\mathbb{R}}(|r_k|^2-|r_p|^2)e^{2ik(X-X')}|\widehat{\chi}(k)|^2\rho(X,X')\,dk\right\|_{\mathcal{L}_1}\\
&\quad\le \frac{1}{\sigma\sqrt{2\pi}}\left\|\frac{d|r_k|^2}{dk}\right\|_\infty+\int_{\mathbb{R}}\left\|e^{2ikX}\varphi(X)e^{-2ikX'}\overline{\varphi(X')}\right\|_{\mathcal{L}_1}\left||r_k|^2-|r_p|^2\right||\widehat{\chi}(k)|^2\,dk\\
&\quad\le\sqrt{\frac{2}{\pi\sigma^2}}\left\|\frac{d|r_k|^2}{dk}\right\|_\infty.
\end{aligned}
$$

Before going to the estimate on $\Gamma_{\sigma,p}$, we recall that for any rank one operator ρ', i.e. operator with kernel of the form $\rho'(X,X')=\varphi_1(X)\overline{\varphi_2(X')}$, we have the equality $\|\rho'\|_{\mathcal{L}^1}=\|\varphi_1\|_2\|\varphi_2\|_2$. If we apply this to the rank one operators with kernel $\Gamma_{\sigma,p}(X)\varphi(X)\overline{\varphi(X')}$ and $\varphi(X)\overline{\Gamma_{\sigma,p}(X')\varphi(X')}$, we get

$$
\begin{aligned}
&\left\|i[\Gamma_{\sigma,p}(X)-\Gamma_{\sigma,p}(X')]\rho(X,X')\right\|_{\mathcal{L}^1}\\
&\le\left\|\Gamma_{\sigma,p}(X)\varphi(X)\overline{\varphi(X')}\right\|_{\mathcal{L}^1}+\left\|\Gamma_{\sigma,p}(X')\varphi(X)\overline{\varphi(X')}\right\|_{\mathcal{L}^1}\\
&\le 2\,\|\Gamma_{\sigma,p}\varphi\|_2\|\|\varphi\|_2\le 2\,\|\Gamma_{\sigma,p}\|_\infty\le 2\,e^{-2\sigma^2p^2}.
\end{aligned}
$$

This concludes the proof. ∎

4.2. Particular potentials of interest. Here, we briefly introduce three particular potentials that we shall use in the numerical simulations.

Dirac's delta potential. In the case $V=\alpha\delta_0$, with $\alpha>0$, the reflection and transmission amplitudes are given by (see Proposition A.2)

$$
r_k=-\frac{\alpha}{\alpha-i|k|},\qquad t_k=-\frac{i|k|}{\alpha-i|k|},\quad \forall k\in\mathbb{R}. \tag{4.25}
$$

In the next section, we will use (4.25) to compute the function I_χ numerically via (4.11), (4.12), (4.13). To avoid the numerical integration, one can use formula (4.22), which gives

$$
\Theta^{\delta,app}_{\sigma,p}(Y)=\frac{\alpha^2}{\alpha^2+p^2}\left(1-e^{2ipY-\frac{Y^2}{2\sigma^2}}\right). \tag{4.26}
$$

Potential barrier. A further potential for which the scattering matrix can be explicitly computed is the potential barrier, i.e.

$$
V(x):=V_0\mathbb{1}_{[-a,a]},\qquad V_0=\frac{\alpha}{2a}\quad a>0,
$$

where $\mathbb{1}$ denotes the characteristic function and $\alpha>0$ measures the strength of the interaction. Letting $E=\frac{k^2}{2}$ denote the energy of the incoming wave and defining $k_0:=\sqrt{2(E-V_0)}\in\mathbb{C}$, the transmission and reflection amplitudes have the forms

$$
t_k=\frac{4kk_0e^{-2ika}}{(k+k_0)^2e^{-2ik_0a}-(k-k_0)^2e^{2ik_0a}},\quad \forall k\in\mathbb{R}\setminus\{0\}, \tag{4.27}
$$

$$
r_k=\frac{(k^2-k_0^2)e^{-2ika}(e^{-2ik_0a}-e^{2ik_0a})}{(k+k_0)^2e^{-2ik_0a}-(k-k_0)^2e^{2ik_0a}},\quad \forall k\in\mathbb{R}\setminus\{0\}. \tag{4.28}
$$

Numerical approximation for more general potentials. In the case of more general potentials, there is no analytic expression for the amplitudes r_k and t_k, however, we can compute them numerically.

We assume that the potential V rapidly decreases at infinity, and choose a sufficiently large a such that we can approximate V by 0 on $\mathbb{R}\setminus[-a,a]$. Let us shortly summarize the classical procedure to calculate the reflection and transmission amplitudes.

We look for generalized eigenfunctions ψ_k of the Hamiltonian $-\frac{1}{2}\Delta+V$ associated to the eigenvalue $E=\frac{k^2}{2}$. Due to our approximation, these eigenfunctions are combinations of the free waves e^{ikx} and e^{-ikx} outside the interval $[-a,a]$. For $k>0$ we look for solutions satisfying

$$\psi_k(x):=\begin{cases} e^{ik(x+a)}+r_k e^{-ik(x+a)} & \text{for } x<-a, \\ t_k e^{ik(x-a)} & \text{for } x>a. \end{cases} \tag{4.29}$$

In order to find the values of t_k and r_k, one must solve the stationary Schrödinger equation associated with transparent boundary conditions in the interval $[-a,a]$

$$\begin{cases} -\frac{1}{2}\psi_k''(x)+V\psi_k=E\psi, \quad x\in[-a,a], \\ \psi_k'(-a)+ik\psi_k(-a)=2ik, \\ \psi_k'(a)-ik\psi_k(a)=0. \end{cases} \tag{4.30}$$

Transparent boundary conditions express the fact that the wave function as well as its derivative are continuous at $\pm a$. Using the continuity of the wave function and of its derivative at $x=\pm a$, it can be checked that the boundary conditions in (4.30) are indeed satisfied if and only if conditions (4.29) are satisfied for some r_k and t_k. The reflection and transmission amplitudes are then given by

$$t_k:=\psi_k(a), \quad r_k:=\psi_k(-a)-1, \quad \forall k>0. \tag{4.31}$$

For a wave coming from the right, i.e. $k<0$, the procedure is analogous.

5. Numerical asymptotic resolution of the two-body Schrödinger system

In this section we use the approximations introduced in sections 3 and 4 in order to efficiently resolve the two body Schrdinger equation (1.1), with initial condition given by (2.1), in the regime $\varepsilon\ll 1$. The final aim is to quantify and study numerically the decoherence effect induced on the heavy particle by the interaction with the light one.

5.1. Model and initial data. According to Theorem 3.4, for small values of ε we can replace the resolution of the two-body Schrödinger equations (1.1)-(2.1) or, equivalently, of equation (3.8) for density operators, by the resolution of system (3.15) for the reduced density operator of the heavy particle. Rephrasing the latter as an equation for the integral kernel $\rho^{M,a}(t,X,X')$ of the operator $\rho^{M,a}(t)$, one gets

$$\begin{cases} i\partial_t\rho^{M,a}(t,X,X')=-\dfrac{1}{2M}(\Delta_X-\Delta_{X'})\rho^{M,a}(t,X,X'), \quad \forall (X,X')\in\mathbb{R}^2,\ \forall t\in\mathbb{R}^+ \\ \rho^{M,a}(0,X,X')=\rho_0^M(X,X')I_\chi(X,X'), \end{cases} \tag{5.1}$$

where the collision function I_χ is given by formulas (4.11), (4.12), (4.13), and $\rho_0^M(X,X')$ is the integral kernel of the operator ρ_0^M, which represents the state of the heavy particle before the collision. We set

$$\rho_0^M(X,X') := \varphi(X)\overline{\varphi(X')}, \tag{5.2}$$

where

$$\varphi(X) := N(\varphi_-(X) + \varphi_+(X)) \tag{5.3}$$

with

$$\varphi_\pm(X) := \frac{1}{(2\pi)^{1/4}\sqrt{\sigma_H}} e^{-\frac{(X\mp X_0)^2}{4\sigma_H^2}} e^{\mp i p_H X} \tag{5.4}$$

$$N := \sqrt{2}\left(1 + e^{-\frac{X_0^2}{2\sigma_H^2}} e^{-2\sigma_H^2 p_H^2}\right)^{\frac{1}{2}}. \tag{5.5}$$

The parameters X_0, p_H, and σ_H are positive.

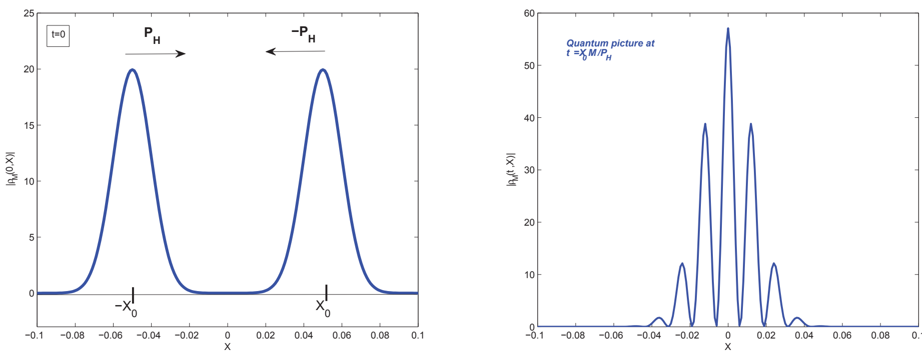

FIG. 5.1. *Left: Probability density associated to the initial state of the heavy particle. Right: Probability density associated to the state of the heavy particle in the case of no interaction, at the time of maximal overlap of the two bumps.*

Then, the integral kernel (5.2) can be rewritten as

$$\begin{aligned}\rho_0^M(0,X,X') &= N^2\left[\varphi_-(X)+\varphi_+(X)\right]\left[\overline{\varphi_-(X')}+\overline{\varphi_+(X')}\right]\\ &= N^2\left[\varphi_-(X)\overline{\varphi_-(X')}+\varphi_-(X)\overline{\varphi_+(X')}+\varphi_+(X)\overline{\varphi_-(X')}+\varphi_+(X)\overline{\varphi_+(X')}\right].\end{aligned} \tag{5.6}$$

The two terms $\varphi_\pm(X)\overline{\varphi_\pm(X')}$ are called *diagonal*, while the two terms $\varphi_\pm(X)\overline{\varphi_\mp(X')}$ are called *antidiagonal*. In fact, in view of definition (5.4) the products $\varphi_\pm(X)\overline{\varphi_\pm(X')}$ rapidly decay outside of a diagonal region $\{|X-X'|\simeq\sigma_H\}$, while the products $\varphi_\pm(X)\overline{\varphi_\mp(X')}$ are essentially supported in the region $\{|X+X'|\simeq\sigma_H\}$.

Physically, the density matrix "before the collision" ρ_0^M or, equivalently, the initial wave function (5.3), describes a state consisting of a quantum superposition of two localized bumps centred respectively at $\pm X_0$ and moving against each other with relative speed $2p_H/M$, as illustrated in the left plot of Figure 5.1. If no light particle or, more generally, no interaction is present, then one should use $\rho_0^M(X,X')$ as initial data in (5.1). Thus, at time MX_0/p_H the non-diagonal terms in (5.6) give rise to an interference pattern, shown in the right plot of Figure 5.1. The emergence of interference is due to the non-diagonal terms in (5.6). On the other hand, due to the collision, the initial data in (5.1) is is replaced by $\rho_0^{M,a}(X,X') = I_\chi(X,X')\rho_0^M(X,X')$. We will show in Section 5.3 that the presence of the factor I_χ dampens the interference.

5.2. Numerical domain and discretization. Here we give some brief explanation about the numerical resolution of equation (5.1).

First, we truncate the spatial domain $\mathbb{R}^2$ to a bounded simulation domain $\Omega_X^2 := (-H,H)\times(-H,H)$ and impose boundary conditions on $\partial\Omega_X$. To simplify computations, we choose homogeneous Neumann boundary conditions, which prescribe that the particle is reflected at the boundaries. However, if the domain is sufficiently large, the presence of the boundaries has negligible influence on the dynamics of the heavy particle.

Second, we discretize equation (5.1). For the discretization in time we employ the Peaceman–Rachford scheme which is unconditionally stable and second-order accurate. Let us explain in more detail the steps in the scheme. We start by discretizing the time interval $[0,T]$ and the simulation domain of the heavy particle $\Omega_X = (-H,H)$. Let us introduce the time and space steps

$$\Delta t = \frac{T}{L} > 0, \qquad h_X := \frac{2H}{J-1} > 0, \qquad \text{with } L, J \in \mathbb{N}$$

and define the homogeneous discretization $t_l := l\Delta t$, $X_j = -H + (j-1)h_X$, so that

$$0 = t_0 \le \cdots \le t_l \le \cdots \le t_L = T, \quad -H = X_1 \le \cdots \le X_j \le \cdots \le X_J = H.$$

Then, defining the operators $A, B : \mathcal{H} \subset L^2(\Omega_X) \to L^2(\Omega_X)$

$$A := -\frac{1}{2M}\Delta_X, \quad B := \frac{1}{2M}\Delta_{X'}, \quad \mathcal{H} := \{\phi \in H^2(\Omega_X) \,/\, \partial_n\phi = 0, \text{ on } \partial\Omega_X\},$$

where ∂_n denotes the outward normal to the boundary $\partial\Omega_X$, the Peaceman–Rachford scheme for the system (5.1) writes

$$\rho^{l+1} = \left(i\mathrm{Id} - \frac{\Delta t}{2}A\right)^{-1}\left(i\mathrm{Id} + \frac{\Delta t}{2}B\right)\left(i\mathrm{Id} - \frac{\Delta t}{2}B\right)^{-1}\left(i\mathrm{Id} + \frac{\Delta t}{2}A\right)\rho^l, \quad l = 0,\ldots,L-1, \tag{5.7}$$

where ρ^l (resp. ρ^l_{ij}) denotes the approximation of $\rho^{M,a}(t_l)$ (resp. $\rho^{M,a}(t_l, X_i, X_j)$). Notice that (5.7) is a sequence of Euler-explicit, Crank–Nicolson and Euler-implicit steps. Equivalently, one performs a sequential resolution of two 1D systems

$$\left(i\mathrm{Id} - \frac{\Delta t}{2}B\right)\rho^{l+1/2} = \left(i\mathrm{Id} + \frac{\Delta t}{2}A\right)\rho^l, \quad \left(i\mathrm{Id} - \frac{\Delta t}{2}A\right)\rho^{l+1} = \left(i\mathrm{Id} + \frac{\Delta t}{2}B\right)\rho^{l+1/2}.$$

Finally, we discretize the operators A and B in space via a standard second-order centred method.

The parameters employed in the simulations are summarized in Table 5.1.

Let us briefly explain the reasons why the present numerical method is faster than the one previously employed in [4].

First, thanks to Theorem 3.4 all information on the interaction is embodied in the collision operator $\mathcal{I}_\chi$ and is present in problem (5.1) through the initial condition only.

$2*H$	$2*10^{-1}$	J	201
T	$1.92*10^{-2}$	L	$120*20+1$
$\hbar$	1	p_H	$3.4*M$
M	100	p	$1.25; 2.5; 3.5*10^2$
σ_H, σ	$10^{-2}, 2*10^{-2}$	X_0, x_l	$5*10^{-2}, 2*10^{-1}$
α	$0,\dots,40*10^2$		

Table 5.1. *Parameters used in the numerical simulations.*

Therefore, one can get rid of any variable related to the light particle and thus of the fast time scale. The initial multi-scale problem then reduces to a one-scale problem, allowing a considerable gain in efficiency as compared to the method employed in [4]. Second, the scheme is an alternating-direction implicit (ADI) one, i.e. the actions of the two operators A and B, acting respectively on the variable X and X', are separated, so that, compared to a direct resolution of (5.1) via Crank–Nicolson method, the computational costs are drastically reduced.

5.3. Numerical results and interpretation. Here we present some numerical results obtained via the resolution method of the evolution equation (5.1) introduced in the previous section. We give a detailed analysis for the case of a Dirac's delta interaction potential, and then stress the main analogies with the cases of a potential barrier and of a Gaussian potential. Finally, we sketch the case with multiple light particles. For any choice of the interaction potential V, the reflection and transmission amplitudes are computed as detailed in Section 4 and the corresponding collision function I_χ is calculated numerically by formulas (4.11), (4.12), and (4.13).

5.3.1. Dirac's delta potential. Here we consider the case $V(x) = \alpha\delta_0(x)$, with $\alpha \in \mathbb{R}^+$.

The left plot in Figure 5.2 shows the quantity $|\rho_0^M(X,X')|$ (i.e. the state of the heavy particle before the collision with the light one). Notice that the non-trivial values of $\rho_0^M(X,X')$ are concentrated in four bumps. In accordance with the terminology introduced in Section 5.1, the two bumps located around the diagonal $X = X'$ are called *diagonal* while the two others, located around the set $X = -X'$, are called *antidiagonal*. The diagonal bumps give the probability density associated to the state of the heavy particle, while the antidiagonal bumps are responsible for the interference. Diagonal and antidiagonal bumps share the same shape and the same size.
The right plot in Figure 5.2 displays $|\rho^{M,a}(0,X,X')| = |I_\chi(X,X')\rho_0^M(X,X')|$ (i.e. the state of the heavy particle immediately after the collision) in the test case $\alpha = 10^3$. It is easily seen that, as an effect of the collision with the light particle, the antidiagonal bumps are damped, thus providing the expected attenuation of the interference.

Figure 5.3 is devoted to the collision function I_χ. In the left plot we show $|I_\chi(X,X')|$ corresponding to the right plot of Figure 5.2, while in the right plot of Figure 5.3 we give $|I_\chi(X,-X)|$ for different values of α. One can observe that, as the strength of the potential varies, the band width of $|I_\chi(X,-X)|$ remains unchanged; on the other hand, notice that the more the potential is intense, the more the quantity $|I_\chi(X,-X)|$ is reduced for large values of X. It is precisely this reduction which causes the damping of the antidiagonal bumps in Figure 5.2.

In order to examine how the decoherence effect varies with the momentum of the light particle, in Figure 5.4 we plot $|I_\chi(0.05,-0.05)|$ for several values of α and three

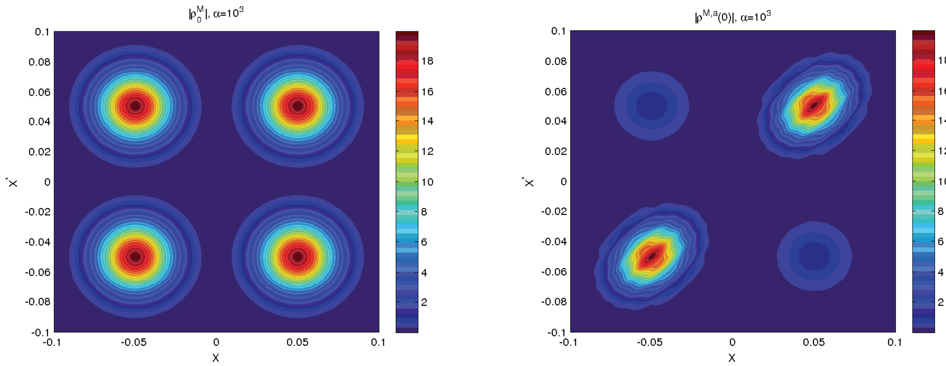

FIG. 5.2. *Test case: Dirac potential with* $\alpha = 10^3$. *Left: Plot of* $|\rho_0^M(X,X')|$ *before the collision; Right: Plot of* $|\rho^{M,a}(0,X,X')|$ *immediately after the collision.*

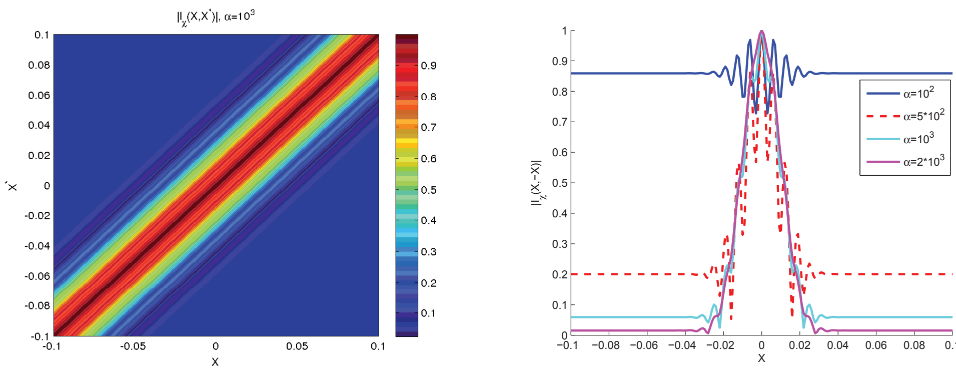

FIG. 5.3. *Left: Plot of* $|I_\chi(X,X')|$ *for* $\alpha = 10^3$. *Right: Plot of* $|I_\chi(X,-X)|$ *for several values of* α.

different momenta p of the light particle. We observe that the larger the momentum is, the smaller the decoherence effect on the heavy particle is. This can be explained by the fact that most of the light particle is transmitted when its momentum is large.

Finally, in Figure 5.5 we display the probability density $\rho^{M,a}(t_*,X,X)$ associated to the state of the heavy particle at the time $t_* = X_0 M/p_H$ of maximal overlap of the two diagonal bumps. The left plot in Figure 5.5 corresponds to a collision with a light particle arriving from the right with mean momentum $p = -2.5 * 10^2$, for several potential strengths α. One sees that the probability density associated to the state of the heavy particle splits into a component that exhibits complete interference and a bump that travels with mean momentum $p_H + p > p_H$ towards the right without experiencing interference. We refer to the component that displays interference as the *coherent part*, while the component in which interference is absent is referred to as the *decoherent part*. In the right plot, the light particle has momentum $p = 0$ and is located at the centre $x_l = 0$. The interference pattern exhibits a clear decoherence effect. In particular, notice that inside the pattern there are no points with zero probability. The corresponding plot is similar to the ones exhibited in [4] through a direct use of the Joos–Zeh formula. In fact, this plot too can be understood as the simultaneous presence of a coherent and of a decoherent part, except that here, since the momentum of the decoherent part is

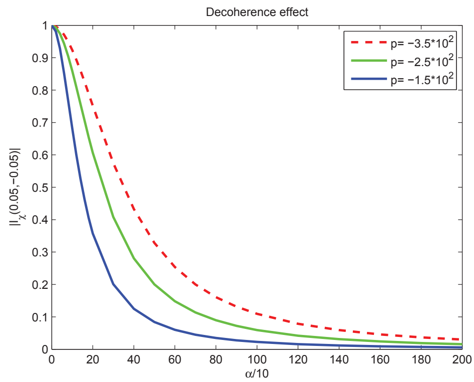

FIG. 5.4. *The quantity* $|I_{\chi}(0.05,-0.05)|$ *as a function of* α *for three different values of the momentum of the light particle.*

zero, the two components share the same support.

A theoretical explanation of the appearance of the decoherent bumps is given is Section 5.4.

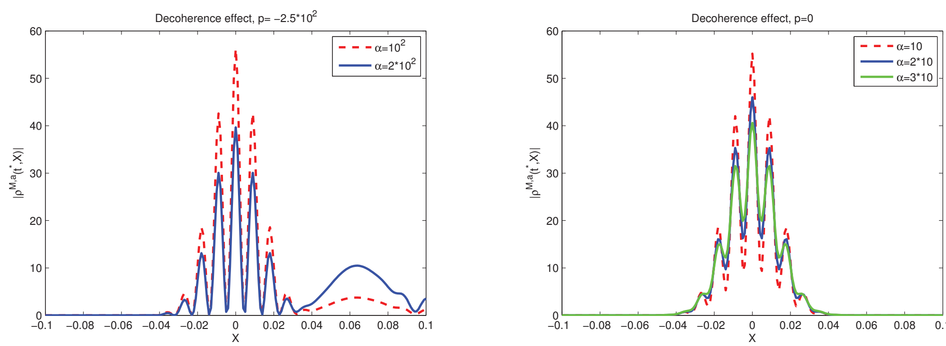

FIG. 5.5. *Attenuation of the interference pattern of the heavy particle, in the case that the light particle comes from the left with* $p = 2.5*10^2$ *(left) resp.* $p = 0$ *(right)*

5.3.2. Potential barrier and Gaussian potential. For the potential barrier

$$V(x) := V_0 \mathbb{1}_{[-a,a]}, \quad V_0 = \frac{\alpha}{2a}, \quad \alpha \in \mathbb{R}^+, \quad a \in [10^{-4}, 10^{-2}], \tag{5.8}$$

as well as for the Gaussian potential

$$V(r) := V_0 e^{-\frac{r^2}{2\sigma^2}}, \quad V_0 = \frac{\alpha}{\sqrt{2\pi}\sigma}, \quad \alpha \in \mathbb{R}^+, \quad \sigma \in [10^{-4}, 10^{-2}], \tag{5.9}$$

we carried out computations and simulations following the line of Section 5.3.1.

For the former case, reflection and transmission amplitudes are given by formulas (4.27),(4.28). For the latter case, we followed the computation of the reflection and transmission amplitudes as defined by the procedure detailed in (4.30),(4.31).

In both cases, the normalization constants V_0 have been chosen in order to guarantee that

$$\int_{\mathbb{R}} V(x)\,dx = \alpha,$$

so that the effects put in evidence in this section can be compared with the effects carried out by the Dirac's delta potential $\alpha\delta_0$.

As far as scattering is concerned, the only consequence of the interaction potential is the values of the reflection and transmission amplitudes. Thus, we just compare r_k, t_k and I_χ for the Dirac's delta, the potential barrier (5.8) and the Gaussian potential (5.9). The results are illustrated in figures 5.6 and 5.7 for fixed potential strength $\alpha = 5*10^2$, momentum $p = -2.5*10^2$ and several choices of a and σ. As expected, we found that the results obtained for the potential barrier as $a \to 0$, as well as those obtained for the Gaussian potential as $\sigma \to 0$, approach those obtained using the Dirac's delta potential.

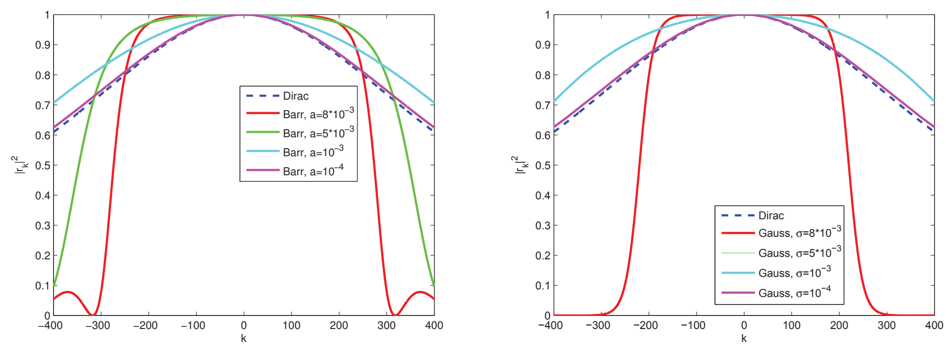

FIG. 5.6. *Comparison of the reflection amplitudes* $|r_k|^2$ *corresponding to three different interaction potentials, with fixed potential strength* $\alpha = 5*10^2$ *and various* a *and* σ *values. Left: Dirac's delta and potential barrier. Right: Dirac's delta and Gaussian potential.*

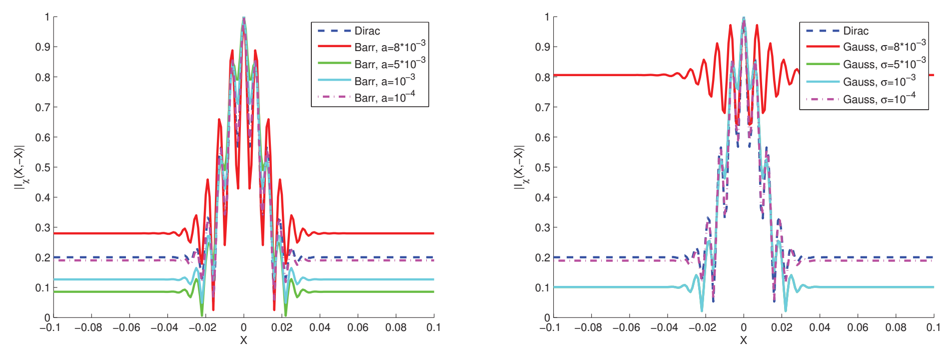

FIG. 5.7. *Comparison of the collision function* $I_\chi(X,-X)$ *corresponding to three different interaction potentials, with fixed potential strength* $\alpha = 5*10^2$ *and various* a *and* σ *values. Left: Dirac's delta and potential barrier. Right: Dirac's delta and Gaussian potential.*

5.3.3. Several light particles. We suppose that many light particles are injected one-by-one into the computation domain, in such a way that the heavy particle undergoes a finite sequence of collisions at times $t_k := 4k\Delta t$. At any collision, the state of the light particle is supposed to be the same, i.e., the kth colliding light particle lies in the state represented by the wave function $U_0(t_k - \varepsilon^{-\gamma})\chi$. Through any time interval (t_k, t_{k+1}) between two collisions, the heavy particle evolves freely. The state of the heavy particle after each collision $\rho(t_k^+)$ is then related to the state before collision $\rho(t_k^-)$ by

$$\rho(t_k^+) = \mathcal{I}_\chi[\rho(t_k^-)].$$

On the left plot of Figure 5.8 we show the probability density $\rho^{M,a}(t^*, X, X)$ associated to the state of the heavy particle at the time of maximal overlap. The plot refers to the case of a Dirac's delta potential with strength $\alpha = 10$, momentum of the light particle $p = 0$ and $N = 1,2,3$ collisions. As expected, multiple collisions enforce the destruction of the interference pattern.

If one is interested in the limit of infinite incoming light particles, then a significant re-scaling of the potential should be $\alpha/\sqrt{N}$ with fixed α: with this scaling, the decoherence effect should remain of order one (see the right plot in Figure 5.8). A detailed mathematical study of this effect in the case $N \to \infty$ will be treated in a subsequent paper.

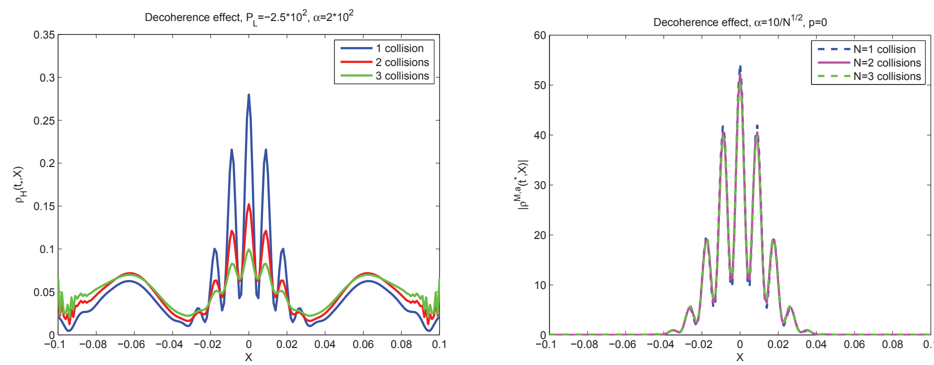

FIG. 5.8. *Attenuation of the interference pattern of the heavy particle in the case of several collisions. Test case: Dirac's delta potential, $p = 0$. Left: Fixed $\alpha = 10$ and several collisions $N = 1,2,3$. Right: $N = 1,2,3$ with $\alpha = 10/\sqrt{N}$.*

5.4. Theoretical explanation. Here we propose a theoretical explanation for the plots in Figure 5.5, described in Subsection 5.3.1 as the decomposition of the probability density associated to the heavy particle into a coherent and a decoherent part.

To this purpose, we first assume $\sigma p \gg 1$, which means that the light particle must travel fast enough; as proven in Proposition 4.3, this assumption makes the function Γ_χ, defined in (4.13), negligible. Besides, owing to this hypothesis, the normalization constant N defined in (5.5) can be approximated by one.

Second, we suppose $\left\| \frac{d|r_k|^2}{dk} \right\|_\infty \ll \sigma$, so that the variation of the reflection amplitude is slow, and r_k can be always considered as equal to r_p.

By these assumptions one easily gets

$$I_\chi(X,X') \approx 1 - \Theta^{app}_{\sigma,p}(X-X') = 1 - |r_p|^2 + |r_p|^2 e^{2ip(X-X') - \frac{(X-X')^2}{2\sigma^2}},$$

where $\Theta^{app}_{\sigma,p}$ was defined in (4.22).

Now, the main assumption states that the following ordering holds between the spatial scales involved in the collision:

$$\sigma_H \ll \sigma \ll X_0. \tag{5.10}$$

The physical meaning of (5.10) is transparent: if $\sigma \ll X_0$, then the incoming light particle can distinguish the two bumps of the heavy particle from each other; furthermore, if $\sigma_H \ll \sigma$, then any bump of the heavy particle approximately acts on the light particle as a pointwise scattering centre.

From Table 5.1 one has that this condition is satisfied if one replaces the symbol "$\ll$" by "$<$"; this fact suggests that the following explanation can hold also under more relaxed hypotheses.

Due to (5.10), referring to the initial density matrix as expressed in (5.6), the two diagonal terms $\varphi_\pm(X)\overline{\varphi_\pm(X')}$ are essentially supported in the region $|X-X'| \ll \sigma$, while the non-diagonal terms $\varphi_\pm(X)\overline{\varphi_\mp(X')}$ are essentially supported in the region $|X+X'| \ll \sigma$. Therefore, we can further approximate I_χ in the two regions $\{|X-X'| \ll \sigma\}$ and $\{|X-X'| \gg \sigma\}$ by

$$I_\chi(X,X') \approx \begin{cases} 1-|r_p|^2 & \text{if } |X-X'| \gg \sigma, \\ 1-|r_p|^2 + |r_p|^2 e^{2ip(X-X')} & \text{if } |X-X'| \ll \sigma. \end{cases}$$

so that, using also $N \approx 1$, one obtains $\rho^{M,a}(0,X,X') \approx \rho^{M,b}(0,X,X')$, where

$$\begin{aligned} \rho^{M,b}(0,X,X') := |t_p|^2 \rho^M_0(X,X') + \frac{|r_p|^2}{2} e^{2ipX} \varphi_-(X)\overline{e^{2ipX'}\varphi_-(X')} \\ + \frac{|r_p|^2}{2} e^{2ipX} \varphi_+(X)\overline{e^{2ipX'}\varphi_+(X')}. \end{aligned} \tag{5.11}$$

Thus, the approximated initial state $\rho^{M,b}(0)$ can be understood as the *statistical mixing* of three pure states:

- the initial pure state $\rho^M(0)$ with weight $|t_p|^2$;
- the pure state represented by the wave function $e^{2ip\cdot}\varphi_-$ with weight $\frac{1}{2}|r_p|^2$;
- the pure state represented by the wave function $e^{2ip\cdot}\varphi_+$ with weight $\frac{1}{2}|r_p|^2$.

We remark that the wave functions $e^{2ip\cdot}\varphi_\pm$ show the same spatial localization as $\varphi_\pm$, respectively, but their momentum has increased by $2p$. Therefore, the wave function $e^{2ip\cdot}\varphi_-$ ($e^{2ip\cdot}\varphi_+$) describes the heavy particle localized on the left (right) and accelerated by the reflection of the light one.

We are now ready to interpret Figure 5.5. Let us evolve $\rho^{M,b}$ according to the free dynamics (5.1). At the time t^* of maximal overlap of the two initial bumps, the first pure state on the r.h.s. of (5.11) shows the expected interference fringes as in Figure 5.1, but such fringes are damped by the factor $|t_p|^2$. This explains the fringes in the images on the left of Figure 5.5. We remark in particular that all the oscillations reach the zero value, as it occurs when the heavy particle lies in a pure state. At the same time, the pure states corresponding to the second and third terms in (5.11) are also overlapping, since they are both accelerated by the same quantity. But, since the r.h.s. of (5.11) is a statistical mixture, the two bumps will superpose classically, without giving rise to interference fringes. This explains the bump on the right side of the left diagram in Figure 5.5.

In the image on the right of Figure 5.5, this interpretation can still hold, but since in that case $p=0$, the interference fringes of the first state are also superposed with the two bumps created by the second and third states of the mixing, so the decomposition (5.11) is not so clearly readable.

The content of the present subsection can be made rigorous by proving that the approximation (5.11) holds in the trace-class norm. This is indeed the case since we have the following result:

Theorem 5.1. *Let the initial state φ of the heavy particle have the form stipulated in (5.3)–(5.5), and let the incoming state χ of the light particle be chosen as in (4.20). Define the density matrix $\rho^{M,a}(0)$ as in (3.15), and let $\rho^{M,b}(0)$ denote the density matrix with integral kernel having the form (5.11).*

Then, the following estimate holds:

$$\|\rho^{M,a}(0)-\rho^{M,b}(0)\|_{\mathcal{L}^1}\leq C\left(e^{-\sigma^2p^2}+\frac{1}{\sigma}\left\|\frac{d|r_k|^2}{dk}\right\|_\infty+\frac{\sigma_H}{\sigma}+e^{-\frac{2X_0^2}{\sigma^2}}+e^{-\frac{X_0^2}{2\sigma_H^2}}\right). \tag{5.12}$$

Remark 5.1. As an immediate consequence, if

$$\sigma_H\ll\sigma\ll X_0,\quad \left\|\frac{d|r_k|^2}{dk}\right\|_\infty\ll\sigma,\quad\text{and}\quad \frac{1}{\sigma}\ll p,$$

then the difference between $\rho^{M,a}$ and $\rho^{M,b}$ is small.

The proof of Theorem 5.1 is given in Section 6.3.

Remark 5.2 (Entanglement between the two particles). Under the same hypotheses of Theorem 5.1, one can work out a simpler expression for the initial two-particle wave function than the one given in Theorem 3.2. First, the assumption $\|\frac{dr_k}{dk}\|_\infty\ll\sigma$ gives

$$S\chi\approx S^{app}\chi_\varepsilon:=t_p\chi_\varepsilon+r_pR_0\chi_\varepsilon,$$

where $\chi_\varepsilon=U(-\varepsilon^{-\gamma})\chi$, and the reflection operator R_0 is defined by $R_0\chi_\varepsilon(x):=\chi_\varepsilon(-x)$ (its action is invariant under Fourier transformation). Second, by translational invariance

$$S^{X,app}\chi_\varepsilon:=t_p\chi_\varepsilon+r_p\theta_{2X}R_0\chi_\varepsilon, \tag{5.13}$$

where $\theta_{2X}u=u(\cdot-2X)$. Thus, after some computations (that can be performed more easily in the Fourier space), one can replace the initial condition of the limit equation (3.2) by

$$\varphi\otimes S^X\chi_\varepsilon\approx\varphi\otimes S^{X,app}\chi_\varepsilon\approx t_p\varphi\otimes\chi_\varepsilon+\frac{r_p}{\sqrt{2}}e^{2ipX}\varphi_-\otimes\left(e^{-2ipX_0}\theta_{-2X_0}R_0\chi_\varepsilon\right)$$
$$+\frac{r_p}{\sqrt{2}}e^{2ipX}\varphi_+\otimes\left(e^{2ipX_0}\theta_{2X_0}R_0\chi_\varepsilon\right). \tag{5.14}$$

The new phase factors come from the approximation of θ_{2X} by θ_{2X_0} or θ_{-2X_0}. Remark that the phase factor on the light particle is constant and thus not important; on the contrary, the phase factor on the heavy particle means that it is accelerated by $2p$. The two-body wave function in (5.14) represents an entangled state: the light particle is transmitted when the heavy particle remains in its initial state, it is reflected from $-X_0$ when the heavy particle is located at $-X_0$ (and accelerated) and so on. Since the three states of the light particle that appear in the previous approximation are almost orthogonal under the assumptions of Theorem 5.1, the associated density matrix for the heavy particle turns out to be well approximated by (5.11).

6. Proofs

The present section contains the proofs of the approximation theorems presented in Section 3. In particular, Section 6.1 deals with Theorem 3.2 and Section 6.2 with Theorem 3.4.

6.1. Proof of Theorem 3.2. We preliminarily warn the reader that part of this section is devoted to the proof of results that are analogous to those contained in [2, Theorem 1]. We include this section anyway, both for the sake of completeness and because the results we need are slightly different from the one in [2]. All proofs presented here are new.

The reduced variables and a useful lemma. Let us first introduce the centre of mass R and the relative position r of the two-body problem. We define

$$R := \frac{X+\varepsilon x}{1+\varepsilon}, \qquad r := x - X,$$

or, equivalently,

$$X := R - \frac{\varepsilon x}{1+\varepsilon}, \qquad x = R + \frac{r}{1+\varepsilon}.$$

The new variables naturally induce a unitary transformation on $L^2(\mathbb{R}^d)$, given by

$$(\mathcal{T}_\varepsilon \psi)(R,r) := \psi\left(R - \frac{\varepsilon x}{1+\varepsilon}, R + \frac{r}{1+\varepsilon}\right), \qquad (\mathcal{T}_\varepsilon^{-1}\phi)(X,x) := \phi\left(\frac{X+\varepsilon x}{1+\varepsilon}, x - X\right).$$

The previous definition can be extended to the case $\varepsilon = 0$. The following lemma compares $\mathcal{T}_\varepsilon\psi$ and $\mathcal{T}_0\psi$.

Lemma 6.1. *For any $\psi \in L^2(\mathbb{R}^{2d})$ s.t. $(x-X)\cdot(\nabla_X + \nabla_x)\psi \in L^2(\mathbb{R}^{2d})$, we have the following estimate*

$$\|\mathcal{T}_\varepsilon\psi - \mathcal{T}_0\psi\|_2 \le \varepsilon\|(x-X)\cdot(\nabla_X+\nabla_x)\psi\|_2 \ \le\ \varepsilon\|r\cdot\nabla_R\mathcal{T}_0\psi\|_2.$$

Proof. Denoting $\phi = \mathcal{T}_0\psi$ and

$$\hat{\phi}(k,r) \ = \ \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} e^{-ik\cdot R}\phi(R,r)\,dR$$

one has

$$\begin{aligned}
\|\mathcal{T}_\varepsilon\psi - \mathcal{T}_0\psi\|_2^2 &\le \|\mathcal{T}_\varepsilon\mathcal{T}_0^{-1}\phi - \phi\|_2^2 \\
&= \int_{\mathbb{R}^{2d}} \left|\phi\left(R - \frac{\varepsilon r}{1+\varepsilon}, r\right) - \phi(R,r)\right|^2 dR\,dr \\
&= \int_{\mathbb{R}^{2d}} \left|e^{-ik\cdot\frac{\varepsilon r}{1+\varepsilon}} - 1\right|^2 |\hat{\phi}(k,r)|^2\,dk\,dr \\
&\le \varepsilon^2\|r\cdot\nabla_R\phi\|_2^2,
\end{aligned}$$

and we get the claimed inequality using that $\nabla_R \phi(R,r) = (\nabla_X + \nabla_x)\psi(R, R+r)$. □

Moreover, $\mathcal{T}_0$ has the following property

$$\mathcal{T}_0 \widehat{\mathcal{S}} = [\mathbb{I} \otimes S]\mathcal{T}_0, \tag{6.1}$$

which is a consequence of the definition of $\widehat{\mathcal{S}}$ (see Definition 3.1). In that definition the action of $\widehat{\mathcal{S}}$ includes the scattering of the light particle by a potential centred at the location of the heavy particle, while in the reduced variables, the scattering takes place in the relative position variable. We will also use the following elementary identity, which may be proved directly.

LEMMA 6.2. *For all $j = 1, \ldots, d$, any $\tau \in \mathbb{R}$, and any $\chi \in L^2(\mathbb{R}^d)$ such that $|x|\chi \in L^2(\mathbb{R}^d)$*

$$x_j U_0(\tau)\chi \;=\; U_0(\tau)\big[i\tau\partial_j \chi + x_j \chi\big]. \tag{6.2}$$

This implies in particular that

$$\|\,|x| U_0(\tau)\chi\|_2 \;\le\; \sqrt{2}\big[\|\,|x|\chi\|_2 + \tau\|\nabla\chi\|_2\big]. \tag{6.3}$$

Step 1. Rewriting the problem in reduced variables. Let ψ_ε be the solution to (1.1), (2.1) with $M = 1$. Denoting

$$\widetilde{\psi}_\varepsilon := \mathcal{T}_\varepsilon \psi_\varepsilon, \qquad \widetilde{\psi}^a_\varepsilon := \mathcal{T}_\varepsilon \psi^a_\varepsilon, \tag{6.4}$$

one has that $\widetilde{\psi}_\varepsilon$ and $\widetilde{\psi}^a_\varepsilon$ are respectively solutions to

$$\begin{cases} i\partial_t \widetilde{\psi}_\varepsilon = -\frac{1}{2(1+\varepsilon)}\Delta_R \widetilde{\psi}_\varepsilon + \frac{1+\varepsilon}{\varepsilon}\Big(-\frac{1}{2}\Delta_r \widetilde{\psi}_\varepsilon + V(r)\widetilde{\psi}_\varepsilon\Big), \\ \widetilde{\psi}^\varepsilon(0) = \mathcal{T}_\varepsilon \psi^0_\varepsilon = \mathcal{T}_\varepsilon\big[\mathbb{I} \otimes U_0(-\varepsilon^{-\gamma})\big]\psi, \end{cases} \tag{6.5}$$

and

$$\begin{cases} i\partial_t \widetilde{\psi}^a_\varepsilon = -\frac{1}{2(1+\varepsilon)}\Delta_R \widetilde{\psi}_\varepsilon - \frac{1+\varepsilon}{2\varepsilon}\Delta_r \widetilde{\psi}_\varepsilon, \\ \widetilde{\psi}^a_\varepsilon(0) = \mathcal{T}_\varepsilon \mathcal{S}_\varepsilon \psi = \mathcal{T}_\varepsilon[\mathbb{I} \otimes U(-\varepsilon^{\gamma})]\widehat{\mathcal{S}}\psi, \end{cases} \tag{6.6}$$

where $\psi := \varphi \otimes \chi$. Notice that in problem (6.5) the variables R and r are decoupled, therefore we can express the solution in terms of semigroups acting separately on R and r, i.e.

$$\widetilde{\psi}_\varepsilon(t) = \Big[U_0\Big(\tfrac{t}{1+\varepsilon}\Big) \otimes U_V\Big(\tfrac{(1+\varepsilon)t}{\varepsilon}\Big)\Big]\mathcal{T}_\varepsilon\big[\mathbb{I} \otimes U_0(-\varepsilon^{-\gamma})\big]\psi, \tag{6.7}$$

$$\widetilde{\psi}^a_\varepsilon(t) = \Big[U_0\Big(\tfrac{t}{1+\varepsilon}\Big) \otimes U_0\Big(\tfrac{(1+\varepsilon)t}{\varepsilon}\Big)\Big]\mathcal{T}_\varepsilon\big[\mathbb{I} \otimes U_0(-\varepsilon^{-\gamma})\big]\widehat{\mathcal{S}}\psi. \tag{6.8}$$

In order to estimate the distance between $\psi_\varepsilon(t)$ and $\psi^a_\varepsilon(t)$ we introduce two intermediate terms $\psi^b_\varepsilon(t)$ and $\psi^c_\varepsilon(t)$, defined as follows

$$\widetilde{\psi}^b_\varepsilon(t) = \Big[U_0\Big(\tfrac{t}{1+\varepsilon}\Big) \otimes U_V\Big(\tfrac{(1+\varepsilon)t}{\varepsilon}\Big)\Big]\mathcal{T}_0\big[\mathbb{I} \otimes U_0(-\varepsilon^{-\gamma})\big]\psi \tag{6.9}$$

$$\widetilde{\psi}^c_\varepsilon(t) = \Big[U_0\Big(\tfrac{t}{1+\varepsilon}\Big) \otimes U_0\Big(\tfrac{(1+\varepsilon)t}{\varepsilon}\Big)\Big]\mathcal{T}_0\big[\mathbb{I} \otimes U_0(-\varepsilon^{-\gamma})\big]\widehat{\mathcal{S}}\psi. \tag{6.10}$$

Then,

$$\|\psi_\varepsilon(t)-\psi^a_\varepsilon(t)\|_2 \le \|\widetilde{\psi}_\varepsilon(t)-\widetilde{\psi}^b_\varepsilon(t)\|_2+\|\widetilde{\psi}^b_\varepsilon(t)-\widetilde{\psi}^c_\varepsilon(t)\|_2+\big\|\widetilde{\psi}^c_\varepsilon(t)-\widetilde{\psi}^a_\varepsilon(t)\big\|_2. \tag{6.11}$$

A control of $\widetilde{\psi}_\varepsilon(t)-\widetilde{\psi}^b_\varepsilon(t)$ may be obtained thanks to lemmas 6.1 and 6.2, and the same lemmas together with the hypothesis (H3) allows us to control $\widetilde{\psi}^c_\varepsilon(t)-\widetilde{\psi}^a_\varepsilon(t)$. This will be explained in Step 2. To control the term $\widetilde{\psi}^b_\varepsilon(t)-\widetilde{\psi}^c_\varepsilon(t)$, we will use the commutation properties of $\widehat{\mathcal{S}}$. We explain in Step 3 how it leads to the term involving C_1 in the estimate (3.3).

Step 2. The approximation of infinitely massive particle. In fact, the replacement of $\mathcal{T}_\varepsilon$ by $\mathcal{T}_0$ is equivalent to the approximation that the massive particle has an infinite mass, so that it does not move during the evolution of the light one. Using definition (6.9), the unitarity of U_0 and U_V, and Lemma 6.1 we get

$$\begin{aligned}
\|\widetilde{\psi}_\varepsilon(t)-\widetilde{\psi}^b_\varepsilon(t)\|_2 &= \|(\mathcal{T}_\varepsilon-\mathcal{T}_0)[\mathbb{I}\otimes U_0(-\varepsilon^\gamma)]\psi\|_2\\
&\le \varepsilon\,\|(x-X)\cdot(\nabla_X+\nabla_x)[\mathbb{I}\otimes U_0(-\varepsilon^\gamma)]\psi\|_2\\
&\le \varepsilon\|(x-X)\cdot(\nabla\varphi\otimes U_0(-\varepsilon^{-\gamma})\chi+\varphi\otimes U_0(-\varepsilon^{-\gamma})\nabla\chi)\|_2,\\
\varepsilon^{-1}\|\widetilde{\psi}_\varepsilon(t)-\widetilde{\psi}^b_\varepsilon(t)\|_2 &\le \|\nabla\varphi\|_2\||\cdot|U_0(-\varepsilon^{-\gamma})\chi\|_2+\|X\cdot\nabla\varphi\|_2\\
&\qquad +\|x\cdot U_0(-\varepsilon^{-\gamma})\nabla\chi\|_2+\|X\varphi\|_2\|\nabla\chi\|_2,
\end{aligned}$$

where we used the fact that U_0 commutes with derivatives and that $\|\varphi\|_2=\|\chi\|_2=1$. Using Lemma 6.2, one can get rid of the propagators $U_0(-\varepsilon^{-\gamma})$ in the previous estimate, namely

$$\begin{aligned}
\varepsilon^{-1}\|\widetilde{\psi}_\varepsilon(t)-\widetilde{\psi}^b_\varepsilon(t)\|_2 \le{}& \sqrt{2}\|\nabla\varphi\|_2\big(\||\cdot|\chi\|_2+\varepsilon^{-\gamma}\|\nabla\chi\|_2\big)+\|X\cdot\nabla\varphi\|_2\\
&+\sqrt{2}\big(\|x\cdot\nabla\chi\|_2+\varepsilon^{-\gamma}\|\Delta\chi\|_2\big)+\||\cdot|\varphi\|_2\|\nabla\chi\|_2,
\end{aligned}$$

so that eventually

$$\begin{aligned}
&\|\widetilde{\psi}_\varepsilon(t)-\widetilde{\psi}^b_\varepsilon(t)\|_2 \le K_1\varepsilon+K_2\varepsilon^{1-\gamma}, \qquad (6.12)\\
\text{with}\quad &K_1:=\sqrt{2}\big(\|\nabla\varphi\|_2\||x|\chi\|_2+\|x\cdot\nabla\chi\|_2\big)+\||X|\varphi\|_2\|\nabla\chi\|_2+\|X\cdot\nabla\varphi\|_2,\\
&K_2:=\sqrt{2}\big(\|\nabla\varphi\|_2\|\nabla\chi\|_2.+\|\Delta\chi\|_2\big).
\end{aligned}$$

Similarly, from definitions (6.8) and (6.10) one gets

$$\begin{aligned}
\|\widetilde{\psi}^c_\varepsilon(t)-\widetilde{\psi}^a_\varepsilon(t)\|_2 &= \|(\mathcal{T}_\varepsilon-\mathcal{T}_0)[\mathbb{I}\otimes U_0(-\varepsilon^\gamma)]\widehat{\mathcal{S}}\psi\|_2\\
&\le \varepsilon\,\|r\cdot[\mathbb{I}\otimes U_0(-\varepsilon^\gamma)][\mathbb{I}\otimes S]\nabla_R\mathcal{T}_0\psi\|_2,
\end{aligned}$$

where we have used that U_0 commutes with translation, the relation (6.1), and the fact that ∇_R commutes with $\mathbb{I}\otimes S$ and $\mathbb{I}\otimes U_0(\tau)$. Applying Lemma 6.2 (integrated on R) to the function $\bar{\phi}:=[\mathbb{I}\otimes U_0(-\varepsilon^\gamma)][\mathbb{I}\otimes S]\nabla_R\mathcal{T}_0\psi$, we get

$$2^{-1/2}\|\widetilde{\psi}^c_\varepsilon(t)-\widetilde{\psi}^a_\varepsilon(t)\|_2 \le \varepsilon\,\|r\cdot[\mathbb{I}\otimes S]\mathcal{T}_0(\nabla_X+\nabla_x)\psi\|_2+\varepsilon^{1-\gamma}\|\nabla_r[\mathbb{I}\otimes S]\mathcal{T}_0(\nabla_X+\nabla_x)\psi\|_2,$$

where in the last line we used that $\psi=\varphi\otimes\chi$. In order to bound the second term in the r.h.s. we can use the conservation of the kinetic energy under the action of S and get

$$\|\nabla_r[\mathbb{I}\otimes S]\mathcal{T}_0(\nabla_X+\nabla_x)\psi\|_2=\|\mathcal{T}_0\nabla_x(\nabla_X+\nabla_x)\psi\|_2$$

$$\leq \|\nabla\varphi\|_2\|\nabla\chi\|_2+\|\Delta\chi\|_2.$$

Using the regularity assumption (H3) on the scattering operator to bound the first term of the r.h.s. we get

$$\begin{aligned}
&\|r\cdot[\mathbb{I}\otimes S]\mathcal{T}_0(\nabla_X+\nabla_x)\psi\|_2\\
&\leq\||r|\mathcal{T}_0(\nabla_X+\nabla_x)\psi\|_2+C_s\|\mathcal{T}_0(\nabla_X+\nabla_x)\psi\|_{L^2_R(H^s_r)}\\
&\leq\||x-X|(\nabla_X+\nabla_x)\psi\|_2+C_s\big(\|\psi\|_{L^2_X(H^{s+1}_x)}+\|\nabla_X\psi\|_{L^2_X(H^s_x)}\big)\\
&\leq\|\nabla\varphi\|_2\||x|\chi\|_2+\||X|\nabla\varphi\|_2+\||x|\nabla\chi\|_2+\||X|\varphi\|_2\|\nabla\chi\|_2\\
&\qquad\qquad+C_s\big(\|\nabla\varphi\|_2\|\chi\|_{H^s}+\|\chi\|_{H^{s+1}}\big),
\end{aligned}$$

where we used the fact that $\psi_0=\varphi\otimes\chi$ is factorized. Putting all together, we get

$$\begin{aligned}
&\|\psi^c_\varepsilon(t)-\psi^a_\varepsilon(t)\|_2\leq K_3\varepsilon+K_4\varepsilon^{1-\gamma}, \qquad (6.13)\\
&\quad\text{with } 2^{-1/2}K_3:=\|\nabla\varphi\|_2\||x|\chi\|_2+\||X|\nabla\varphi\|_2+\||x|\nabla\chi\|_2+\||X|\varphi\|_2\|\nabla\chi\|_2\\
&\qquad\qquad\qquad+C_s\big(\|\nabla\varphi\|_2\|\chi\|_{H^s}+\|\chi\|_{H^{s+1}}\big),\\
&\qquad 2^{-1/2}K_4:=\|\nabla\varphi\|\|\nabla\chi\|+\|\Delta\chi\|.
\end{aligned}$$

Step 3. The approximation of a fast scattering. Now we estimate $\|\widetilde{\psi}^b_\varepsilon(t)-\widetilde{\psi}^c_\varepsilon(t)\|$. Starting from definitions (6.9) and (6.10), using the fact that $\mathcal{T}_0$ commutes with $\mathbb{I}\otimes U_0(t)$ and the relation (6.1), we obtain

$$\begin{aligned}
\widetilde{\psi}^b_\varepsilon(t)&=\left[U_0\left(\tfrac{t}{1+\varepsilon}\right)\otimes U_V\left(\tfrac{(1+\varepsilon)t}{\varepsilon}\right)\right]\left[\mathbb{I}\otimes U_0(-\varepsilon^{-\gamma})\right]\mathcal{T}_0\psi\\
&=\left[U_0\left(\tfrac{t}{1+\varepsilon}\right)\otimes U_0\left(\tfrac{(1+\varepsilon)t}{\varepsilon}-\varepsilon^{-\gamma}\right)\right]\left[\mathbb{I}\otimes S(\tau,\tau')\right]\mathcal{T}_0\psi\\
\text{and}\quad \widetilde{\psi}^c_\varepsilon(t)&=\left[U_0\left(\tfrac{t}{1+\varepsilon}\right)\otimes U_0\left(\tfrac{(1+\varepsilon)t}{\varepsilon}-\varepsilon^{-\gamma}\right)\right][\mathbb{I}\otimes S]\mathcal{T}_0\psi,
\end{aligned}$$

where we introduced $\tau=\varepsilon^{-\gamma}$ and $\tau'=\frac{(1+\varepsilon)t}{\varepsilon}-\varepsilon^{-\gamma}$. Using the unitarity of U_0, we get

$$\begin{aligned}
\|\widetilde{\psi}^b_\varepsilon(t)-\widetilde{\psi}^c_\varepsilon(t)\|_2&=\|\mathbb{I}\otimes[S(\tau,\tau')-S]\mathcal{T}_0\psi\|_2\\
&=\|\varphi[S(\tau,\tau')-S]\chi(\cdot-X)\|_2. \qquad (6.14)
\end{aligned}$$

Conclusion. Putting together (6.11), (6.12), (6.13), and (6.14) the proof is complete.

6.2. Proof of Theorem 3.4. We preliminarily recall that the initial density operator $\rho^M(0)$ of the heavy particle (see (3.8)) is a compact, positive, self-adjoint operator whose trace equals one. Thus by the spectral theorem there exists a sequence $0\leq\lambda_j\leq 1$, $\sum_j\lambda_j=1$, and a complete orthonormal set $|\varphi_j\rangle\in L^2(\mathbb{R}^d)$ such that

$$\rho^M(0)\;=\;\sum_j\lambda_j|\varphi_j\rangle\langle\varphi_j|. \qquad (6.15)$$

Estimate of the difference of the two-body density operators $\rho_\varepsilon(t)$ and $\rho^a_\varepsilon(t)$. We recall from Section 3 that the two-body density operator ρ_ε is the solution to the operator equation

$$i\partial_t\rho_\varepsilon(t)=[H_\varepsilon,\rho_\varepsilon(t)]$$

with initial data

$$\rho_\varepsilon(0) \;=\; \rho^M(0)\otimes|U(-\varepsilon^{-\gamma})\chi\rangle\langle U(-\varepsilon^{-\gamma})\chi| \;=\; \sum_j \lambda_j|\psi_{j,\varepsilon}(0)\rangle\langle\psi_{j,\varepsilon}(0)|,$$
$$|\psi_{j,\varepsilon}(0)\rangle := |\varphi_j\rangle|U_0(\varepsilon^{-\gamma})\chi\rangle,$$

where we applied the decomposition in (6.15). Therefore,

$$\rho_\varepsilon(t) = \sum_j \lambda_j|\psi_{j,\varepsilon}(t)\rangle\langle\psi_{j,\varepsilon}(t)|,$$

where $\psi_{j,\varepsilon}(t)$ is the solution to equation (1.1) with initial data $\psi_{j,\varepsilon}(0)$.
Analogously, the two-body density operator ρ^a_ε is the solution to

$$i\partial_t\rho^a_\varepsilon(t) = [H^f_\varepsilon, \rho^a_\varepsilon(t)],$$

with initial data

$$\rho^a_\varepsilon(0) = \mathcal{S}_\varepsilon\left[\rho^M(0)\otimes|\chi\rangle\langle\chi|\right]\mathcal{S}^*_\varepsilon = \sum_j \lambda_j|\psi^a_{j,\varepsilon}(0)\rangle\langle\psi^a_{j,\varepsilon}(0)|,$$
$$|\psi^a_{j,\varepsilon}(0)\rangle := |\varphi_j\rangle|U_0(\varepsilon^{-\gamma})S^X\chi\rangle,$$

where we applied decomposition (6.15). Then,

$$\rho^a_\varepsilon(t) = \sum_j \lambda_j|\psi^a_{j,\varepsilon}(t)\rangle\langle\psi^a_{j,\varepsilon}(t)|,$$

where $\psi^a_{j,\varepsilon}(t)$ is the solution to equation (1.1) with initial data $\psi^a_{j,\varepsilon}(0)$.
Let us estimate the distance between $\rho_\varepsilon(t)$ and ρ^a_ε. We get

$$\begin{aligned}\|\rho_\varepsilon(t)-\rho^a_\varepsilon(t)\|_{\mathcal{L}^1} &\le \sum_j \lambda_j\Big\||\psi_{j,\varepsilon}(t)\rangle\langle\psi_{j,\varepsilon}(t)| - |\psi^a_{j,\varepsilon}(t)\rangle\langle\psi^a_{j,\varepsilon}(t)|\Big\|_{\mathcal{L}^1}\\ &\le 2\sum_j \lambda_j\big\|\psi_{j,\varepsilon}(t)-\psi^a_{j,\varepsilon}(t)\big\|_2,\end{aligned}$$

where we have used the fact that for any ζ_1,ζ_2 in $L^2(\mathbb{R}^{2d})$ with $\|\zeta_1\|_2=\|\zeta_2\|_2=1$

$$\mathrm{Tr}\big||\zeta_1\rangle\langle\zeta_1| - |\zeta_2\rangle\langle\zeta_2|\big| \le\; 2\|\zeta_1-\zeta_2\|_2.$$

It remains to sum up the error bounds given by Theorem 3.2. One gets

$$\begin{aligned}\frac{1}{2}\|\rho_\varepsilon(t)-\rho^a_\varepsilon(t)\|_{\mathcal{L}^1} &\le \sum_j \lambda_j\|e^{-itH_\varepsilon}|\varphi_j\rangle|U_0(-\varepsilon^{-\gamma})\chi\rangle - U^f_\varepsilon(t)|\varphi_j\rangle|U_0(-\varepsilon^{-\gamma})S^X\chi\rangle\|\\ &\le 2\sqrt{2}\|\Delta\chi\|_2\varepsilon^{1-\gamma} + \sqrt{2}C_s\varepsilon\|\chi\|_{H^{s+1}}\\ &\qquad + \sum_j \lambda_j\left[C_{1,j}\left(\tfrac{1+\varepsilon}{\varepsilon}t-\varepsilon^{-\gamma},\varepsilon^{-\gamma}\right) + C_{2,j}\varepsilon + C_{3,j}\varepsilon^{1-\gamma}\right], \quad (6.16)\end{aligned}$$

where

$$C_{1,j}(\tau,\tau') := \|\varphi_j\,[S(\tau,\tau')-S]\,\chi(\cdot-X)\|_2, \quad (6.17)$$
$$C_{2,j} := 2\sqrt{2}\big(\|\nabla\varphi_j\|_2\|\,|x|\chi\|_2 + \|X\varphi_j\|_2\|\nabla\chi\|_2 + \|\,|X|\nabla\varphi_j\|_2 + \|\,|x|\nabla\chi\|_2\big)$$

$$+C_s\|\nabla\varphi_j\|_2\|\chi\|_{H^s}, \qquad (6.18)$$

$$C_{3,j} := 2\sqrt{2}\|\nabla\varphi_j\|_2\|\nabla\chi\|_2. \qquad (6.19)$$

Summing up in all constants with respect to j and using Cauchy–Schwarz inequality leads to the error bounds given by Theorem 3.2. For instance,

$$\begin{aligned}\sum_j \lambda_j C_{1,j}(\tau,\tau') &= \sum_j \lambda_j \left\|\varphi_j\left[S^X(\tau,\tau') - S^X\right]\chi\right\| \\ &\leq \left(\sum_j \lambda_j\right)^{\frac{1}{2}} \left(\sum_j \lambda_j \left\|\varphi_j\left[S^X(\tau,\tau') - S^X\right]\chi\right\|^2\right)^{\frac{1}{2}} \\ &= \left(\operatorname{Tr}\left[\sum_j \lambda_j \left|\varphi_j\left[S^X(\tau,\tau') - S^X\right]\chi\right\rangle\left\langle\varphi_j\left[S^X(\tau,\tau') - S^X\right]\chi\right|\right]\right)^{\frac{1}{2}} \\ &= 2\left\|\rho^M(0)|[S(\tau,\tau') - S]\chi(\cdot - X')\rangle\langle[S(\tau,\tau') - S]\chi(\cdot - X)\right\|_{\mathcal{L}^1}^{\frac{1}{2}},\end{aligned}$$

and analogously

$$\begin{aligned}\sum_j \lambda_j \|X\cdot\nabla\varphi_j\|_2 &\leq \left(\sum_j \lambda_j\right)^{\frac{1}{2}} \left(\sum_j \lambda_j \||X|\nabla\varphi_j\|_2^2\right)^{\frac{1}{2}} \\ &\leq \left[\operatorname{Tr}\big(|X|\, i\nabla\rho^M(0)\, i\nabla |X|\big)\right]^{\frac{1}{2}}.\end{aligned}$$

The others terms may be handled analogously. Due to (3.12) the same estimate as (6.16) holds for $\|\rho_\varepsilon^M - \rho_\varepsilon^{M,a}\|_{\mathcal{L}^1}$. It only remains to recall that $\rho_\varepsilon^{M,a} = U_0(t)\rho^M(0)U_0(-t)$ is indeed independent of ε.

The dynamics of the density operator $\rho_\varepsilon^{M,a}$. From the fact that ρ_ε^a is the solution to $i\partial_t\rho_\varepsilon^a := [H_\varepsilon^f, \rho_\varepsilon^a]$, using the notation $\bar{t}(\varepsilon) := \frac{1+\varepsilon}{\varepsilon}t$, we get

$$\rho_\varepsilon^a(t) = [U_0(t)\otimes U_0(\bar{t}(\varepsilon))]\rho_\varepsilon^a(0)[U_0(-t)\otimes U_0(-\bar{t}(\varepsilon))].$$

Choosing a basis $(\chi_i)_{i\in\mathbb{N}}$ of $L^2(\mathbb{R}^d)$ one gets by definition of the partial trace

$$\begin{aligned}\rho_\varepsilon^a(t) &= \sum_i \langle U_0(\bar{t}(\varepsilon))\chi_i|\rho_\varepsilon^a(t)|U_0(\bar{t}(\varepsilon))\chi_i\rangle \\ &= \sum_i \langle U_0(\bar{t}(\varepsilon))\chi_i|[U_0(t)\otimes U_0(\bar{t}(\varepsilon))]\rho_\varepsilon^a(0)[U_0(-t)\otimes U_0(-\bar{t}(\varepsilon))]|U_0(\bar{t}(\varepsilon))\chi_i\rangle \\ &= \sum_i \langle\chi_i|[U_0(t)\otimes\mathbb{I}]\rho_\varepsilon^a(0)[U_0(-t)\otimes\mathbb{I}]|\chi_i\rangle \\ &= U_0(t)\Big[\sum_i \langle\chi_i|\rho_\varepsilon^a(0)|\chi_i\rangle\Big]U_0(-t) \\ &= U_0(t)\rho_\varepsilon^{M,a}(0)U_0(-t).\end{aligned}$$

This implies that $\rho_\varepsilon^{M,a}$ is a solution to the free transport equation. Then, it remains to identify the initial condition. One finds

$$\rho_\varepsilon^a(0) := [\mathbb{I}\otimes U_0(-\varepsilon^{-\gamma})]\widehat{\mathcal{S}}\rho^M(0)\otimes|\chi\rangle\langle\chi\widehat{\mathcal{S}}^*[\mathbb{I}\otimes U_0(+\varepsilon^{-\gamma})],$$

$$\begin{aligned}\rho_\varepsilon^{M,a}(0) &= \mathrm{Tr}\big[\widehat{\mathcal{S}}\big(\rho^M(0)\otimes|\chi\rangle\langle\chi|\big)\widehat{\mathcal{S}}^*\big]\\ &= \mathrm{Tr}\big[\rho^M(0)\otimes|S^X\chi\rangle\langle S^{X'}\chi|\big].\end{aligned}$$

In terms of kernels, the last identity can be expressed as

$$\rho_\varepsilon^{M,a}(0,X,X') = \rho^M(0,X,X')\langle S^X\chi|S^{X'}\chi\rangle = \rho^M(0,X,X')I_\chi(X,X').$$

6.3. Proof of Theorem 5.1. First, we can cut the error into three parts

$$\begin{aligned}&\|\rho^{M,a}(0,X,X')-\rho^{M,b}(0,X,X')\|_{\mathcal{L}_1}\\ \le&\|(i\Gamma_\chi(X)-i\Gamma_\chi(X'))\rho^M(0,X,X')\|_{\mathcal{L}_1}\\ &+\|(\Theta^{app}_{\sigma,p}(X-X')-\Theta_\chi(X-X'))\rho^M(0,X,X')\|_{\mathcal{L}_1}\\ &+\|(1-\Theta^{app}_{\sigma,p}(X-X'))\rho^M(0,X,X')-\rho^{M,b}(0,X,X')\|_{\mathcal{L}_1}\\ \le&(\mathrm{I})+(\mathrm{II})+(\mathrm{III}).\end{aligned}$$

The terms (I) and (II) are easily estimated using Proposition 4.3. We get

$$(\mathrm{I})\le 2e^{-2\sigma^2p^2} \quad \text{and} \quad (\mathrm{II})\le\sqrt{\frac{2}{\pi\sigma^2}}\left\|\frac{d|r_k|^2}{dk}\right\|_\infty. \tag{6.20}$$

It remains to estimate (III). Denoting $\widetilde{\varphi}_\pm(X):=e^{2ipX}\varphi_\pm(X)$, we may separate (III) into

$$\begin{aligned}(\mathrm{III}) =& \left\||r_p|^2e^{2ip(X-X')-\frac{(X-X')^2}{2\sigma^2}}\rho^M(0,X,X')-\frac{|r_p|^2}{2}\left[\widetilde{\varphi}_-(X)\overline{\widetilde{\varphi}_-(X')}-\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}\right]\right\|_{\mathcal{L}_1}\\ \le& \frac{|N^2-1|}{2}|r_p|^2\left\|e^{2ip(X-X')-\frac{(X-X')^2}{2\sigma^2}}(\varphi_+(X)+\varphi_-(X'))(\overline{\varphi_+(X')}+\overline{\varphi_-(X')})\right\|_{\mathcal{L}_1}\\ &+\frac{|r_p|^2}{2}\left\|\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}\left(1-e^{-\frac{(X-X')^2}{2\sigma^2}}\right)\right\|_{\mathcal{L}_1}\\ &+\frac{|r_p|^2}{2}\left\|\widetilde{\varphi}_-(X)\overline{\widetilde{\varphi}_-(X')}\left(1-e^{-\frac{(X-X')^2}{2\sigma^2}}\right)\right\|_{\mathcal{L}_1}\\ &+\frac{|r_p|^2}{2}\left\|\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_-(X')}e^{-\frac{(X-X')^2}{2\sigma^2}}\right\|_{\mathcal{L}_1}+\frac{|r_p|^2}{2}\left\|\widetilde{\varphi}_-(X)\overline{\widetilde{\varphi}_+(X')}e^{-\frac{(X-X')^2}{2\sigma^2}}\right\|_{\mathcal{L}_1}\\ =&(\mathrm{III.a})+(\mathrm{III.b})+(\mathrm{III.c})+(\mathrm{III.d})+(\mathrm{III.e}).\end{aligned}$$

To estimate (III.a), we use $|1-N^{-2}|\le e^{-\frac{X_0^2}{2\sigma_H^2}}$, and notice that

$$\left\|e^{2ip(X-X')-\frac{(X-X')^2}{2\sigma^2}}(\varphi_+(X)+\varphi_-(X'))(\overline{\varphi_+(X')}+\overline{\varphi_-(X')})\right\|_{\mathcal{L}_1}=\frac{2}{N^2}.$$

Indeed, by the identity

$$e^{-\frac{(X-X')^2}{2\sigma^2}} = \frac{\sqrt{2}}{\sqrt{\pi}\sigma}\int_{\mathbb{R}}e^{-\frac{(X-\lambda)^2}{\sigma^2}}e^{-\frac{(X'-\lambda)^2}{\sigma^2}}\,d\lambda \tag{6.21}$$

one immediately has

$$\begin{aligned}&e^{2ip(X-X')-\frac{(X-X')^2}{2\sigma^2}}(\varphi_+(X)+\varphi_-(X))(\overline{\varphi_+(X')}+\overline{\varphi_-(X')})\\ =&\frac{\sqrt{2}}{\sqrt{\pi}\sigma}\int_{\mathbb{R}}\left(e^{2ipX}e^{-\frac{(x-\lambda)^2}{\sigma^2}}(\varphi_+(X)+\varphi_-(X))\right)\left(e^{-2ipX'}e^{-\frac{(X'-\lambda)^2}{\sigma^2}}(\overline{\varphi_+(X')}+\overline{\varphi_-(X')})\right)d\lambda.\end{aligned}$$

Therefore the operator to be estimated is positive and its trace norm can be computed by integrating the integral kernel on the diagonal $X=X'$, which obtains $\frac{2}{N^2}$. Summarizing, one obtains

$$\text{(III.a)} \le e^{-\frac{X_0^2}{2\sigma_H^2}}. \tag{6.22}$$

Let us estimate (III.b). Denoting $\widetilde{\gamma}(X,X'):=e^{-\frac{(X-X')^2}{2\sigma^2}}\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}$, one has

$$\text{(III.b)}=\frac{|r_p|^2}{2}\left\|\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}-\widetilde{\gamma}(X,X')\right\|_{\mathcal{L}_1}.$$

Proceeding as was done for (III.a), we see that $\widetilde{\gamma}$ is a positive operator with trace one. To go on, we follow [24, Remark 1.4]. Setting $A(X,X')=\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}-\widetilde{\gamma}(X,X')$, we see that A (seen now as an operator) can have only one positive eigenvalue, denoted λ_+ (otherwise there would exist a space of dimension two where A is positive, but this is impossible because $\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}$ is the kernel of a rank one projection). Since A has zero trace, it must be $\mathrm{Tr}|A|=2\lambda_+$ and $\|A\|_{\mathcal{L}^1}=2\|A\|\le 2\|A\|_{\mathcal{L}^2}$, where $\mathcal{L}_2$ denotes the Hilbert–Schmidt norm and the norm without index is the usual operator norm. This fact allows one to bound (III.b) by

$$\text{(III.b)}\le |r_p|^2\left\||\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}-\widetilde{\gamma}(X,X')\right\|_{\mathcal{L}_2}$$

and the Hilbert–Schmidt norm can easily be computed as the L^2-norm of the corresponding integral kernel, namely

$$\begin{aligned}\left\||\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}-\widetilde{\gamma}(X,X')\right\|^2_{\mathcal{L}_2} &= \int_{\mathbb{R}^2}\left|\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}\left(1-e^{-\frac{(X-X')^2}{2\sigma^2}}\right)\right|^2 dX\,dX' \\ &\le \frac{1}{2\pi\sigma_H^2}\int_{\mathbb{R}^2} e^{-\frac{X^2+(X')^2}{2\sigma_H^2}}\left(1-e^{-\frac{(X-X')^2}{2\sigma^2}}\right)dX\,dX' \\ &=1-\frac{1}{\pi}\int_{\mathbb{R}^2} e^{-(X^2+(X')^2)}e^{-\frac{\sigma_H^2}{\sigma^2}(X-X')^2}\,dX\,dX'.\end{aligned}$$

In the last line we rescaled variables as $X\to\sqrt{2}\sigma_H X$ and $X'\to\sqrt{2}\sigma_H X'$. Now, observe that

$$e^{-\frac{\sigma_H^2}{\sigma^2}(X-X')^2}\ge e^{-\frac{2\sigma_H^2}{\sigma^2}(X^2+(X')^2)},$$

so the integral decouples and one obtains

$$\left\||\widetilde{\varphi}_+(X)\overline{\widetilde{\varphi}_+(X')}-\widetilde{\gamma}(X,X')\right\|^2_{\mathcal{L}_2}\le 1-\frac{1}{\pi}\left(\int e^{-\frac{\sigma^2+2\sigma_H^2}{\sigma^2}X^2}\,dX\right)^2\le 2\frac{\sigma_H^2}{\sigma^2},$$

and finally

$$\text{(III.b)} \le \sqrt{2}|r_p|^2\frac{\sigma_H}{\sigma}. \tag{6.23}$$

The term (III.c) may be bounded by the same quantity. Let us focus on (III.d). In order to estimate it, we make use of the identity (6.21) and obtain

$$\text{(I.d)}=\frac{|r_p|^2}{\sigma\sqrt{2\pi}}\left\|\int_{\mathbb{R}}\widetilde{\varphi}_+(X)e^{-\frac{(X-\lambda)^2}{\sigma^2}}e^{-\frac{(X'-\lambda)^2}{\sigma^2}}\overline{\widetilde{\varphi}_-(X')}\,d\lambda\right\|_{\mathcal{L}_1}$$

$$\leq \frac{|r_p|^2}{\sigma\sqrt{2\pi}} \int_{\mathbb{R}} \left\| \widetilde{\varphi}_+(X) e^{-\frac{(X-\lambda)^2}{\sigma^2}} e^{-\frac{(X'-\lambda)^2}{\sigma^2}} \overline{\widetilde{\varphi}_-(X')} \right\|_{\mathcal{L}_1} d\lambda$$
$$= \frac{|r_p|^2}{\sigma\sqrt{2\pi}} \int_{\mathbb{R}} \left\| \widetilde{\varphi}_+(X) e^{-\frac{(X-\lambda)^2}{\sigma^2}} \right\|_2 \left\| e^{-\frac{(X'-\lambda)^2}{\sigma^2}} \overline{\widetilde{\varphi}_-(X')} \right\|_2 d\lambda.$$

By a direct computation,

$$\left\| e^{2ipX} \varphi_\pm(X) e^{-\frac{(X-\lambda)^2}{\sigma^2}} \right\|_2^2 = \frac{\sigma}{\sqrt{4\sigma_H^2 + \sigma^2}} e^{-\frac{(\lambda \mp X_0)^2}{2\sigma_H^2 + \frac{\sigma^2}{2}}}$$

so that

$$\text{(III.d)} \leq \frac{|r_p|^2}{\sqrt{2\pi}\sqrt{4\sigma_H^2+\sigma^2}} \int_{\mathbb{R}} e^{-\frac{(\lambda - X_0)^2}{4\sigma_H^2+\sigma^2}} e^{-\frac{(\lambda + X_0)^2}{4\sigma_H^2+\sigma^2}} d\lambda = \frac{|r_p|^2}{2\sqrt{2}} e^{-\frac{X_0^2}{2\sigma_H^2 + \frac{\sigma^2}{2}}}.$$

Term (III.e) can be estimated in the same way. Finally, putting everything together, we get the requested bound.

Appendix A.

A.1. The Dirac's delta potential in dimension one. Assume that the potential is a Dirac's delta with strength α, i.e. $V = \alpha\delta_0$.

The operator $-\frac{1}{2}\Delta_x + \alpha\delta_0 : D(H_\alpha) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is defined on the domain

$$D(H_\alpha) := \{\psi \in H^2(\mathbb{R}^-) \cap H^2(\mathbb{R}^+) \text{ s.t. } \psi(0^+) = \psi(0^-) \text{ and } \psi'(0^+) - \psi'(0^-) = 2\alpha\psi(0^+)\} \tag{A.1}$$

by the action

$$\left(-\frac{1}{2}\Delta_x + \alpha\delta_0\right)\psi(x) = -\frac{1}{2}\psi''(x), \qquad x \neq 0,$$

and is a self-adjoint operator in $L^2(\mathbb{R})$.

The propagator

$$U_\alpha(t) := \exp\left[-it\left(-\frac{1}{2}\Delta_x + \alpha\delta_0\right)\right]$$

is explicitly known (see [5, 15]). In order to express it, we shall use the following operators:

$$\begin{aligned} \text{the symmetry operator} \quad & \mathcal{R}\chi := \frac{1}{2}[\chi + \chi(-\cdot)], \\ \text{the projection on positive positions} \quad & \mathcal{P}_x^+\chi := \mathbb{1}_{\mathbb{R}^+}\chi, \\ \text{the projection on positive momenta} \quad & \mathcal{P}_k^+\chi := \mathcal{F}^{-1}(\mathbb{1}_{\mathbb{R}^+}\widehat{\chi}), \\ \text{the translation by } u \quad & \theta_u\chi := \chi(\cdot - u), \end{aligned}$$

where $\mathcal{F}^{-1}$ denotes the inverse Fourier transform. The projection on negative positions $\mathcal{P}_x^-$ and on negative momenta $\mathcal{P}_k^-$ are defined in a similar way. Remark that all these operators on $L^2(\mathbb{R})$ have norm equal to 1, and that $\mathcal{R}$, $\mathcal{P}_k^+$, $\mathcal{P}_k^-$, and θ_u commute with the free evolution group $U_0(\tau)$.

PROPOSITION A.1. *Given $\alpha>0$, for any $t\in\mathbb{R}\setminus\{0\}$ the propagator $U_\alpha(t)$ can be expressed as*

$$U_\alpha(t)=U_0(t)-4\alpha\mathcal{R}\mathcal{P}_x^+\left(\int_0^{+\infty}e^{-\alpha u}\theta_{-u}\,du\right)U_0(t)\mathcal{P}_x^-\mathcal{R}. \tag{A.2}$$

Proof. From [5, 15] we know that $U_\alpha(t)$ is the integral operator defined by the kernel

$$U_\alpha(t,x,x'):=U_0(t,x-x')-\alpha\int_0^\infty e^{-\alpha u}U_0(t,u+|x|+|x'|)\,du, \tag{A.3}$$

where U_0 denotes the propagation kernel of the free Schrödinger equation

$$U_0(t,y):=\frac{1}{\sqrt{2i\pi t}}e^{\frac{i}{2t}y^2}. \tag{A.4}$$

In order to obtain (A.2) it suffices to notice

$$\begin{aligned}\int_{\mathbb{R}}U_0(t,u+|x|+|x'|)\chi(x')\,dx&=\int_{\mathbb{R}}U_0(t,u+|x|+|x'|)\,\mathcal{R}\chi(x')\,dx'\\&=2\int_{\mathbb{R}}U_0(t,u+|x|-x')\,\mathbb{1}_{\mathbb{R}^-}(x')\,\mathcal{R}\chi(x')\,dx'\\&=4\mathcal{R}\,\mathbb{1}_{\mathbb{R}^+}(x)\int_{\mathbb{R}}U_0(t,u+x-x')\,\mathcal{P}_x^-\mathcal{R}\chi(x')\,dx'\\&=4\mathcal{R}\mathcal{P}_x^+\theta_{-u}U_0(t)\mathcal{P}_x^-\mathcal{R}\chi(x).\end{aligned}$$

and the proof is complete. ∎

The following proposition gives the convergence rate to the scattering operator needed in order to obtain Corollary 3.2 from Theorem 3.2 and 3.4.

PROPOSITION A.2. *If $V=\alpha\delta_0$, with $\alpha>0$, then the scattering operator S_α for the Hamiltonian $-\frac{1}{2}\Delta+V$ is well defined and given by*

$$S_\alpha=\mathrm{Id}-4\alpha\mathcal{R}\mathcal{P}_k^+\left(\int_0^{+\infty}e^{-\alpha u}\theta_{-u}\,du\right)\mathcal{R}. \tag{A.5}$$

The associated scattering matrix is defined as usual by the following transmission and reflection amplitudes

$$r_k=-\frac{\alpha}{\alpha-i|k|},\qquad t_k=-\frac{i|k|}{\alpha-i|k|}. \tag{A.6}$$

Moreover, there exists a constant C_2 such that, for any $\chi\in L^2(\mathbb{R})$ satisfying $\langle\cdot\rangle^2\chi\in L^2(\mathbb{R})$, one has

$$\|[S_\alpha(\tau,\tau')-S_\alpha]\chi\|_2\le C_2\left(3\|\langle x\rangle^2\chi\|_2+\frac{2}{\alpha^2}\right)\min(\tau,\tau')^{-\frac{1}{4}}. \tag{A.7}$$

The key ingredient of the proof is the stationary phase estimate (A.11), see Lemma A.1, which is proven in the next section.

Proof. (Proof of Proposition A.2.)

Step 1. Identifying the limit. We need to study the limit of $U_0(-\tau)U'_\alpha(\tau+\tau')U_0(-\tau')$ as $\tau,\tau'\to+\infty$. Using formula (A.2) and the fact that $\mathcal{R}$ and U_0 commute, one gets

$$\begin{aligned}&U_0(-\tau)U'_\alpha(\tau+\tau')U_0(-\tau')\\ =&\mathrm{Id}-4\alpha\mathcal{R}U_0(-\tau)\mathcal{P}_x^+\left(\int_0^{+\infty}e^{-\alpha u}\theta_{-u}\,du\right)U_0(\tau+\tau')\mathcal{P}_x^-U_0(-\tau')\mathcal{R}.\end{aligned}$$

Roughly speaking, for large negative times the component of the wave function lying in the negative half-line approximately coincides with the component of the wave function that travels with positive speed. It seems then natural to replace, for large τ', $\mathcal{P}_x^-U_0(-\tau')$ by $U_0(-\tau')\mathcal{P}_k^+$. Using the fact that $U_0(t)$, θ_u, and $\mathcal{P}_k^+$ commute with one another at any t, one obtains

$$\begin{aligned}&U_0(-\tau)U'_\alpha(\tau+\tau')U_0(-\tau')\\ =&\mathrm{Id}-4\alpha\mathcal{R}U_0(-\tau)\mathcal{P}_x^+U_0(\tau)\mathcal{P}_k^+\left(\int_0^{+\infty}e^{-\alpha u}\theta_{-u}\,du\right)\mathcal{R}+\eta_1(\tau,\tau'),\\ &\text{with}\quad \|\eta_1(\tau,\tau')\chi\|_2\le 4\left\|[\mathcal{P}_x^-U_0(-\tau')-U_0(-\tau')\mathcal{P}_k^+]\mathcal{R}\chi\right\|_2.\end{aligned}\tag{A.8}$$

In the last estimate we used the fact that all concerned operators have norm one, and a factor α^{-1} comes by the integral in u. The next step consists in erasing the operator $\mathcal{P}_x^+$ in the r.h.s. of (A.8). Indeed, it acts after the operator $\mathcal{P}_k^+$, and therefore everything should move to the left for positive times anyway. We obtain

$$\begin{aligned}U_0(-\tau)U_\alpha(\tau+\tau')U_0(-\tau')&=\mathrm{Id}-S'_\alpha+\eta_2(\tau,\tau')+\eta_1(\tau,\tau')\\ \text{with}\quad S'_\alpha&:=4\alpha\mathcal{R}\mathcal{P}_k^+\left(\int_0^{+\infty}e^{-\alpha u}\theta_{-u}\,du\right)\mathcal{R}\end{aligned}\tag{A.9}$$

$$\text{and, defined}\ \chi_\alpha:=\alpha\int_0^{+\infty}e^{-\alpha u}\theta_{-u}\mathcal{R}\chi\,du,\quad \|\eta_2(\tau,\tau')\chi\|_2\le 4\left\|\mathcal{P}_x^-U_0(\tau)\mathcal{P}_k^+\chi_\alpha\right\|_2,\tag{A.10}$$

where in the last line, we used $\mathcal{P}_x^++\mathcal{P}_x^-=\mathrm{Id}$. The operator $S_\alpha=\mathrm{Id}-\alpha S'_\alpha$ can be explicitly written in Fourier variables. Indeed, for all $\chi\in L^2$, using that $\mathcal{R}$ commutes with the Fourier transform $\mathcal{F}$, one has

$$\begin{aligned}\widehat{S'_\alpha\chi}(k)&=\mathcal{F}\left[4\mathcal{R}\mathcal{P}_k^+\left(\alpha\int_0^{+\infty}e^{-\alpha u}\theta_{-u}\,du\right)\mathcal{R}\chi\right](k)\\ &=2\mathcal{F}\left[\alpha\left(\int_0^{+\infty}e^{-\alpha u}\theta_{-u}\,du\right)\mathcal{R}\chi\right](|k|)=2\alpha\int_0^{+\infty}e^{-\alpha u}\mathcal{F}[\theta_{-u}\mathcal{R}\chi](|k|)\,du\\ &=2\alpha\int_0^{+\infty}e^{-(\alpha-i|k|)u}\mathcal{F}[\mathcal{R}\chi](|k|)\,du=\frac{2\alpha}{\alpha-i|k|}\mathcal{R}\widehat{\chi}(|k|)\\ &=\alpha\frac{\widehat{\chi}(k)+\widehat{\chi}(-k)}{\alpha-i|k|}.\end{aligned}$$

Owing to (A.3), the scattering operator S_α is given by

$$\widehat{S_\alpha\chi}(k):=\widehat{\chi}(k)-\frac{\alpha}{\alpha-i|k|}(\widehat{\chi}(k)+\widehat{\chi}(-k))$$

$$= \frac{-i|k|}{\alpha - i|k|}\widehat{\chi}(k) - \frac{\alpha}{\alpha - i|k|}\widehat{\chi}(-k),$$

which, in view of (4.3), provides the transmission and reflection amplitudes.

Step 2. Control of the error terms $\eta_1(\tau,\tau')\chi$ and $\eta_2(\tau,\tau')\chi$. For the control of $\eta_1(\tau,\tau')\chi$ one first observes

$$\begin{aligned}\mathcal{P}_x^- U_0(-\tau') - U_0(-\tau')\mathcal{P}_k^+ &= \mathcal{P}_x^- U_0(-\tau')[\mathcal{P}_k^- + \mathcal{P}_k^+] - [\mathcal{P}_x^- + \mathcal{P}_x^+]U_0(-\tau')\mathcal{P}_k^+ \\ &= \mathcal{P}_x^- U_0(-\tau')\mathcal{P}_k^- - \mathcal{P}_x^+ U_0(-\tau')\mathcal{P}_k^+,\end{aligned}$$

so that a bound on $\|\eta_1(\tau,\tau')\chi\|_2$ follows from two applications of Lemma A.1, to be proven in the next section. Thus, for any $n \geq 2$

$$\|\eta_1(\tau,\tau')\chi\|_2 \leq 2C_2\,\|\langle x\rangle^2\chi\|_2\,(\tau')^{-\frac{1}{4}}.$$

Next, a bound on $\|\eta_2(\tau,\tau')\chi\|_2$ follows by Lemma A.1, with χ_α as initial data, and by noticing that the moments of χ_α are related to those of χ. Precisely,

$$\begin{aligned}\|\langle x\rangle^2\chi_\alpha\|_2 &:= \alpha\left\|\int_0^{+\infty} e^{-\alpha u}\langle x\rangle^2\theta_{-u}\mathcal{R}\chi\,du\right\|_2 \leq \alpha\int_0^{+\infty} e^{-\alpha u}\left\|\langle x-u\rangle^2\mathcal{R}\chi\right\|_2 du \\ &\leq 2\alpha\int_0^{+\infty} e^{-\alpha u}\left(\left\|\langle x\rangle^2\chi\right\|_2 + \langle u\rangle^2\|\chi\|_2\right) du \\ &\leq 2\left\|\langle x\rangle^{n+1}\chi\right\|_2 + \frac{2}{\alpha^2}.\end{aligned}$$

Therefore,

$$\|\eta_2\chi\|_2 \leq C_2\,\|\langle x\rangle^{n+1}\chi_\alpha\|_2\,\tau^{-\frac{1}{4}} \leq C_2\left[\left\|\langle x\rangle^2\chi\right\|_2 + \frac{2}{\alpha^2}\right]\tau^{-\frac{1}{4}}.$$

□

A.2. A stationary phase estimate. Here we give a stationary phase lemma. It is crucial in order to prove the convergence of the scattering operator for the Dirac's delta potential in dimension one, as stated in Proposition A.2.

LEMMA A.1. *There exists a constant C_2 such that the following estimate holds*

$$\forall\tau\in\mathbb{R}^+, \qquad \|\mathcal{P}_x^- U(\tau)\mathcal{P}_k^+\chi\|_2 \leq C_2\,\|\langle x\rangle^2\chi\|_2\,\tau^{-\frac{1}{4}}. \tag{A.11}$$

The same estimates are also valid for $\mathcal{P}_x^+U(\tau)\mathcal{P}_k^-$, $\mathcal{P}_x^+U(-\tau)\mathcal{P}_k^+$, and $\mathcal{P}_x^-U(-\tau)\mathcal{P}_k^-$, always with positive τ.

Proof. (Proof of Lemma A.1.) We follow the classical argument used to obtain stationary phase estimates. The first step consists in separating low frequencies from high ones in χ. We choose a smooth function $g:\mathbb{R}\to[0,1]$ such that $g=1$ on $(-\infty,1]$, $g=0$ on $[2,+\infty)$. We introduce a scale $\eta<1$ to be fixed more precisely later, and the associated function $g_\eta(k) := g\left(\frac{k}{\eta}\right)$. We shall use the decomposition

$$\chi = \chi_l + \chi_h, \quad \text{with}\,\widehat{\chi}_l = \widehat{\chi}g_\eta, \quad \widehat{\chi}_h = \widehat{\chi}(1-g_\eta). \tag{A.12}$$

The contribution of χ_l is bounded by

$$\|\mathcal{P}_x^- U(\tau)\mathcal{P}_k^+\chi_l\|_2 \leq \|\mathcal{P}_k^+\chi_l\|_2 = \|\mathbb{1}_{\mathbb{R}^+}\widehat{\chi}_l\|_2 \leq \sqrt{2\eta}\,\|\widehat{\chi}_l\|_\infty$$

$$\leq \sqrt{2\eta \|\widehat{\chi}_l\|_2 \|\partial_k \widehat{\chi}_l\|_2} \leq C \|\langle x\rangle \chi\|_2 \sqrt{\eta}, \tag{A.13}$$

where we have used a Gagliardo–Nirenberg–Sobolev inequality.
The contribution of χ_h can be controlled by using stationary phase methods. In fact, denoting, for some fixed τ, $\chi_h^* = \mathcal{P}_x^- U(\tau)\mathcal{P}_k^+ \chi_h$, for any $x<0$ we get

$$\begin{aligned} \chi_h^*(x) &= \int e^{ikx} \widehat{\chi_h^*}(k) \frac{dk}{\sqrt{2\pi}} = \int e^{ikx} \widehat{U(\tau)\mathcal{P}_k^+}\chi_h(k) \frac{dk}{\sqrt{2\pi}} \\ &= \int_\eta^{+\infty} e^{-i\tau\left(\frac{k^2}{2} - \frac{kx}{\tau}\right)} \widehat{\mathcal{P}_k^+ \chi_h}(k) \frac{dk}{\sqrt{2\pi}}. \end{aligned} \tag{A.14}$$

Introducing the differential operator $\square_y$ defined by

$$[\square_y h](k) = \frac{d}{dk}\left(\frac{h(k)}{k-y}\right), \tag{A.15}$$

and integrating twice by parts, we obtain

$$\begin{aligned} \chi_h^*(\tau y) &= \int e^{-i\tau\left(\frac{k^2}{2} - ky\right)} \widehat{\chi_h}(k)\, dk = -\frac{i}{\tau} \int e^{-i\tau\left(\frac{k^2}{2} - ky\right)} \square_y \widehat{\chi_h}(k)\, dk \\ &= -\frac{1}{\tau^2} \int_\eta^{+\infty} e^{-i\tau\left(\frac{k^2}{2} - ky\right)} \square_y^2 \widehat{\chi_h}(k)\, dk. \end{aligned} \tag{A.16}$$

The quantity $\square_y^2 \widehat{\chi_h}$ may be rewritten as the following sum

$$\square_x^2 \widehat{\chi_h}(k) = \sum_{n_1+n_2+n_3=2} c_{n_1,n_2,n_3} \frac{1}{\eta^{n_2}} \frac{\partial_k^{n_1}\widehat{\chi}(k)}{(k-y)^{2+n_3}} \partial_k^{n_2}\left[1 - g\left(\frac{k}{\eta}\right),\right]$$

where all amplitudes c_{n_1,n_2,n_3} are bounded (in absolute value) by 3. Using this sum in equation (A.16), we can perform some integration on k and get

$$|\chi_h^*(\tau y)| \leq \frac{\|\partial_k^2 \widehat{\chi}\|_2}{\tau^2 (\eta - y)^{3/2}} + \frac{C_2}{\tau^2} \sum_{n_1+n_2+n_3=2, n_1\neq 2} \frac{\|\partial_k^{n_1}\widehat{\chi}\|_\infty}{\eta^{n_2}(\eta-y)^{2+n_3-1}}.$$

The first term in the r.h.s. comes from the term with $n_1=2$, for which we used Cauchy–Schwarz inequality. The constant C_2 depends on $\|\partial^i g\|_\infty$ for $i=1,2$. Remark that for $n_1=0,1$, we may always bound $\|\partial_k^{n_1}\widehat{\chi}\|_\infty$ by $\|\partial_k^2\widehat{\chi}\|_2$ thanks to the Gagliardo–Nirenberg–Sobolev inequality $\|\zeta\|_\infty^2 \leq \|\partial_k \zeta\|_2 \|\zeta\|_2$. In view of this and since $y<0$, the worst term in the sum of the r.h.s. is the one obtained for $n_2=2$. This leads to the bound

$$|\chi_h^*(\tau y)| \leq \frac{C_2 \|\partial_k^2 \widehat{\chi}\|_2}{\tau^2}\left(\frac{1}{(\eta-y)^{3/2}} + \frac{1}{\eta^2(\eta-y)}\right).$$

Taking the square and integrating with respect to $x=\tau y$, we obtain

$$\|\chi_h^*\|_2 \leq \frac{C_2\|\partial_k^2\widehat{\chi}\|_2}{\tau^{3/2}}\left(\frac{1}{\eta} + \frac{1}{\eta^{5/2}}\right) \leq \frac{C_2\|\partial_k^2\widehat{\chi}\|_2}{\tau^{3/2}\eta^{5/2}}, \tag{A.17}$$

when $\eta \leq 1$. Adding (A.13) and (A.17), we finally obtain

$$\|\mathcal{P}_x^- U(\tau)\mathcal{P}_k^+ \chi\|_2 \leq C_2 \|\langle x\rangle^2 \chi\|_2 \left(\sqrt{\eta} + \tau^{-3/2}\eta^{-5/2}\right).$$

The optimal choice for η is then $\eta = \tau^{-1/2}$ which leads to

$$\|\mathcal{P}_x^- U(\tau)\mathcal{P}_k^+ \chi\|_2 \leq C_2 \|\langle x\rangle^2 \chi\|_2 \tau^{-\frac{1}{4}}.$$

□

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