ON THE ASYMPTOTIC BEHAVIOUR OF A QUANTUM TWO-BODY SYSTEM IN THE SMALL MASS RATIO LIMIT

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Abstract. We consider a quantum system of two particles in dimension three interacting via a smooth potential. We characterize the asymptotic dynamics in the limit of small mass ratio for an initial state given in product form, with an explicit control of the error. An application to the decoherence effect produced on the heavy particle is also discussed.

1. Introduction and main result

The analysis of the asymptotic dynamics of a quantum system composed by heavy and light particles for small value of the mass ratio is of considerable relevance in many physical applications.

In particular in molecular physics one is interested in the case in which the light particles, at time zero, are in a bound state corresponding to some energy level $E_n(R_1, \ldots, R_k)$ produced by the interaction potential with the heavy ones considered in the fixed positions $R_1, \ldots, R_k$. Exploiting the Born-Oppenheimer approximation one can show that, for small values of the mass ratio, the slow motion of the heavy particles is well described by a semiclassical evolution while the rapid motion of the light particles produces a persistent effect on the motion of the heavy ones, described by the effective potential $E_n(R_1, \ldots, R_k)$ (see e.g. [H], [HJ] and references therein).

The situation is qualitatively different if there are no bound states of the light particles and only scattering processes between light and heavy particles can take place.

The analysis of such kind of problems if particularly relevant, for instance, in the study of the mechanism of decoherence induced on one heavy particle by multiple scattering by many light ones (see e.g. [JZ], [GF], [HS], [GJKKSZ], [BGJKS] and references therein).

The starting point of the analysis is the two-body interaction between a heavy and a light particle which, at least at a qualitative level, has been clearly described by Joos and Zeh ([JZ]). The idea is that, for small mass ratio, there is a separation of two characteristic time scales, a slow one for the dynamics of the heavy particle and a fast one for the light particle. Therefore, for an initial state of the form $\varphi(R)\chi(r)$, where φ and χ are the initial wave functions of the heavy and the light particle respectively, the evolution of the system is described via the instantaneous transition

$$\varphi(R)\chi(r) \to \varphi(R) \left(S^R\chi\right)(r) \tag{1.1}$$

where S^R is the scattering operator corresponding to the heavy particle fixed at the position R.
The transition (1.1) simply means that the final state is computed in a zero-th order adiabatic approximation, with the light particle instantaneously scattered far away by the heavy one considered as a fixed scattering center.
Formula (1.1) gives a simple and clear description of the process but it is based on a too crude approximation in the sense that time zero for the heavy particle corresponds to infinite time for the light one and then the evolution in time of the system is completely neglected.
In fact, after the consideration of the effect of many scattering events, in [JZ] the formula is further modified introducing, by hand, the internal dynamics of the heavy particle and then restoring the complete time evolution of the system.
It should be remarked that, while for the standard Born-Oppenheimer approximation a detailed mathematical treatment has been developed, in the case where the basic process is the scattering event, as the one described by Joos and Zeh, a complete rigorous analysis seems to be lacking.
Our aim in this paper is to give such a rigorous analysis for a two-particle system in $\mathbb{R}^3$, interacting via a generic potential V.
Starting from the Schrödinger equation of the system and an initial state given in product form, we shall derive the asymptotic form of the wave function for small values of the mass ratio and with an explicit control of the error.
The result can be considered as a rigorous derivation of the formula (1.1), modified taking into account the internal motion of the heavy particle.
Furthermore, we shall exploit the asymptotic form of the wave function to briefly outline how the decoherence effect produced on the heavy particle can be explicitely computed.
It is worth mentioning that a more satisfactory derivation of the decoherence effect would require the consideration of a large number of light particles, along the line of [JZ] and, more recently, of [HS]. In such a case the mathematical treatment of the model is considerably more complicated and it will be not considered here.
We notice that the description of the two particles process is the crucial point for understanding recent experimental works (see e.g. [HUBHAZ] and references therein), where the decoherence effect of a rarefied gas of light particles on the interference fringes in a two slit experiment for macromolecules is measured.
The analysis presented here generalizes a previous result obtained in [DFT], where a one dimensional two-particle system was considered with an interaction given by a repulsive δ-potential. The proof in [DFT] relies on the explicit knowledge of the time dependent propagator for the hamiltonian of the system (see e.g. [S]) and it cannot be extended to the case of a generic interaction.
In the proof presented here the main technical ingredient is a standard dispersive estimate for the solutions of the Schrödinger equation, in the form given by Yajima ([Y]).
In order to formulate our main result, summarized in theorem 1.1 below, we shall introduce some notation and assumptions.
The hamiltonian of the two-particle system reads

$$\hat{H} = -\frac{\hbar^2}{2M}\Delta_R - \frac{\hbar^2}{2m}\Delta_r + \lambda_0 V(r-R) \tag{1.2}$$

where $R, r \in \mathbb{R}^3$ denote respectively the coordinates of the heavy and the light particle, m, M are the corresponding masses, V is the interaction potential and $\lambda_0 > 0$ is a dimensionless coupling constant.
To simplify the notation we fix $M = \hbar = 1$ and denote $\varepsilon \equiv m$ and $\lambda = \varepsilon\lambda_0$ so that the hamiltonian takes the form

$$\hat{H}^\varepsilon = -\frac{1}{2}\Delta_R + \frac{1}{\varepsilon}\left(-\frac{1}{2}\Delta_r + \lambda V(r-R)\right) \tag{1.3}$$

We are interested in the asymptotic behaviour for $\varepsilon \to 0$ and λ fixed of the solution $\Psi^\varepsilon(t)$ of the Schrödinger equation

$$i\frac{\partial \Psi^\varepsilon(t)}{\partial t} = \hat{H}^\varepsilon \Psi^\varepsilon(t) \tag{1.4}$$

$$\Psi^\varepsilon(0; R, r) \equiv \Psi_0(R, r) = \varphi(R)\chi(r) \tag{1.5}$$

Notice that the choice of the initial state in the form of a product state means that no correlation is assumed between the positions of the two particles at time zero.
Moreover let us introduce the one-particle hamiltonians in $L^2(\mathbb{R}^3)$

$$H = -\frac{1}{2}\Delta + \lambda V \tag{1.6}$$

$$H(x) = -\frac{1}{2}\Delta + \lambda V(\cdot - x), \quad x \in \mathbb{R}^3 \tag{1.7}$$

$$H_0 = -\frac{1}{2}\Delta \tag{1.8}$$

and denote by $\mathcal{S}(\mathbb{R}^3)$ the Schwartz space, by $L^2(\mathbb{R}^3)_{ac}$ the absolutely continuous subspace of H and let $< x >= (1 + |x|^2)^{1/2}$.
We shall consider the following technical assumptions on the potential and the initial state

- (A1) the potential V is Hölder-continuous and there exists a constant $C > 0$ such that $|V(x)| \le C < x >^{-\delta}$, $\delta > 5$;
- (A2) zero is not an eigenvalue nor a resonance for H;
- (A3) $\varphi, \chi \in \mathcal{S}(\mathbb{R}^3)$, $\chi \in L^2(\mathbb{R}^3)_{ac}$.

The assumptions on V guarantee that all the hamiltonians defined above are selfadjoint operators, bounded below, in the corresponding Hilbert spaces and that the following wave operators in $L^2(\mathbb{R}^3)$ parametrized by $x \in \mathbb{R}^3$

$$\Omega^x_\pm = \mathrm{s} - \lim_{\tau \to \pm\infty} e^{i\tau H(x)} e^{-i\tau H_0} \tag{1.9}$$

exist and are complete. In the following we shall simply write $\Omega_\pm$ instead of $\Omega^0_\pm$.
In what follows we will denote by $\|\cdot\|$ the norm in $L^2(\mathbb{R}^6)$ and by $\|\cdot\|_p$ the norm in $L^p(\mathbb{R}^3)$, with $p \in [1, +\infty]$.
We can now state our main result

Theorem 1.1. *Under the assumptions (A1),(A2),(A3) and for any fixed $\lambda > 0$ and $t > 0$ one has*

$$\|\Psi^\varepsilon(t) - \Psi^a(t)\| \leq \frac{A}{\sqrt{t}}\sqrt{\varepsilon} + B\varepsilon \tag{1.10}$$

where

$$\Psi^a(t) = e^{-it\hat{H}_0^\varepsilon}\Psi_0^a \tag{1.11}$$

$$\hat{H}_0^\varepsilon = -\frac{1}{2}\Delta_R - \frac{1}{2\varepsilon}\Delta_r \tag{1.12}$$

$$\Psi_0^a(R,r) = \varphi(R)\left[\left(\Omega_+^R\right)^{-1}\chi\right](r) \tag{1.13}$$

and the two positive constants A, B depend only on the initial state and on the interaction potential.

Notice that the action of $(\Omega_+^R)^{-1}$ on a state of a particle localized in position very far away and moving towards the scattering center is close to the action of the scattering operator S^R (see e.g. [T]). In this sense theorem 1.1 gives the Joos and Zeh formula modified for the presence of the internal motion of the heavy particle.
As it was mentioned above, in the proof we exploit dispersive estimates for the solutions of the Schrödinger equation. More precisely, using assumptions (A1),(A2) it is shown in [Y] that the wave operators (1.9) are bounded operators in L^p and in Sobolev spaces. Then a direct application of the intertwining property of the wave operators gives the estimates

$$\|e^{-itH}\xi\|_\infty \leq \frac{C}{t^{3/2}}\|\xi\|_1, \quad \sup_{t\geq 0}\|e^{-itH}\xi\|_\infty \leq C\|(H+\mathbb{I})\xi\|_2 \tag{1.14}$$

which will be the key ingredients of our proof (see lemma 2.2). In this way only smoothness assumptions are needed on the initial state. On the other hand we have to make restrictive hypotheses on the potential, especially assumption (A2), and only a rate of convergence $\sqrt{\varepsilon}$ can be proven.
An alternative strategy would be to consider an initial state χ compactly supported away from the origin in the spectral representation of H. Following the methods of time-dependent scattering theory one could prove theorem 1.1 without assuming (A2) and with a rate of convergence of order ε.

2. Proof of theorem 1.1

The proof of theorem 1.1 will be obtained through the proof of the three lemmas below.
The first step consists in finding an approximation of order ε on the initial datum; due to the unitarity of the time evolution such an approximation holds at any time.

Lemma 2.1. *There exists a constant $C_1 > 0$ such that, for any $t \in \mathbb{R}$ one has*

$$\|\Psi^\varepsilon(t) - \Psi_1^\varepsilon(t)\| \leq C_1\varepsilon \tag{2.1}$$

where we defined

$$\Psi_1^\varepsilon(t; R, r) \equiv \int_{\mathbb{R}^6} dx'\, dy'\, e^{-i\frac{t}{1+\varepsilon}H_0}\left(\frac{R+\varepsilon r}{1+\varepsilon} - x'\right)\varphi(x')e^{-i\frac{t(1+\varepsilon)}{\varepsilon}H^\varepsilon}(r-R, y')\chi(y'+x') \tag{2.2}$$

with

$$H^\varepsilon = -\frac{1}{2}\Delta + \frac{\lambda}{1+\varepsilon}V \tag{2.3}$$

Proof. The proof follows the same line of Lemma 1 in [DFT].
First, one considers the transformation T^ε which gives the description of the system in terms of the relative and the center of mass coordinates. For a generic square integrable Ψ such a transformation reads

$$(T^\varepsilon\Psi)(x, y) \equiv \Psi\left(x - \frac{\varepsilon}{1+\varepsilon}y; x + \frac{y}{1+\varepsilon}\right) \tag{2.4}$$

where the coordinate $x \equiv \frac{R+\varepsilon r}{1+\varepsilon}$ denotes the position of the center of mass of the system, while $y \equiv r - R$ is the coordinate of the relative motion.
Exploiting the factorization of the dynamics in the coordinates (x, y), one can write the time evolution of the initial datum $\Psi_0 = \varphi \otimes \chi$ in the following way

$$\begin{aligned}(T^\varepsilon\Psi^\varepsilon)(t; x, y) \equiv& (T^\varepsilon\Psi^\varepsilon(t))(x, y)\\ =& \int_{\mathbb{R}^6} dx'dy'\, e^{-i\frac{t}{1+\varepsilon}H_0}(x - x')e^{-i\frac{1+\varepsilon}{\varepsilon}tH^\varepsilon}(y, y')[T^\varepsilon(\varphi\otimes\chi)](x', y')\end{aligned} \tag{2.5}$$

Unitarity of T^ε and of the time evolution implies

$$\begin{aligned}\|\Psi^\varepsilon(t) - \Psi_1^\varepsilon(t)\|^2 &= \|T^\varepsilon\Psi^\varepsilon(t) - T^\varepsilon\Psi_1^\varepsilon(t)\|^2\\ = \|T^\varepsilon(\varphi\otimes\chi) - T^0(\varphi\otimes\chi)\|^2 &= \int_{\mathbb{R}^6} dxdy \left|\varphi\left(x - \frac{\varepsilon y}{1+\varepsilon}\right)\chi\left(x + \frac{y}{1+\varepsilon}\right) - \varphi(x)\chi(x+y)\right|^2\\ &= \int_{\mathbb{R}^6} dxdy \left|F\left(x - \frac{\varepsilon y}{1+\varepsilon}, y\right) - F(x, y)\right|^2\end{aligned} \tag{2.6}$$

where we defined $F(x, y) \equiv \varphi(x)\chi(x + y)$. Denoting

$$\tilde{F}(k, y) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3} dx\, e^{-ik\cdot x}\, F(x, y) \tag{2.7}$$

and using elementary properties of the Fourier transform, it is easily seen that

$$\begin{aligned} \|\Psi^\varepsilon(t) - \Psi_1^\varepsilon(t)\|^2 &= \int_{\mathbb{R}^6} dk\, dy \left| \tilde{F}(k,y) \left(e^{-i\frac{\varepsilon}{1+\varepsilon} y\cdot k} - 1 \right) \right|^2 \\ &\le \left(\frac{\varepsilon}{1+\varepsilon} \right)^2 \int_{\mathbb{R}^6} dx\, dy\, |y \cdot k\, F(k,y)|^2 \\ &\le \varepsilon^2 \int_{\mathbb{R}^6} dx\, dy\, |y|^2 \left| \nabla_x \left(\varphi(x)\chi(x+y) \right) \right|^2 \end{aligned} \tag{2.8}$$

Defining

$$C_1^2 \equiv \int_{\mathbb{R}^6} dx\, dy\, |y|^2 \left| \nabla_x \left(\varphi(x)\chi(x+y) \right) \right|^2 \tag{2.9}$$

the proof is complete. □

¿From formula (2.2) it is clear that for the light particle the limit $\varepsilon \to 0$ is equivalent to a large time asymptotics, i.e. to a scattering regime.
The only technical point is that the corresponding generator (2.3) also depends on ε and then the standard scattering estimates cannot be directly used.

Lemma 2.2. *There exist two constants $C_2, C_3 > 0$ such that for any $t > 0$ one has*

$$\|\Psi_2^\varepsilon(t) - \Psi_1^\varepsilon(t)\|_2 \le C_2 \varepsilon + C_3 \sqrt{\frac{\varepsilon}{t}} \tag{2.10}$$

where

$$\Psi_2^\varepsilon(t; R, r) \equiv \int_{\mathbb{R}^3} dx'\, e^{-i\frac{t}{1+\varepsilon}H_0} \left(\frac{R+\varepsilon r}{1+\varepsilon} - x' \right) \varphi(x') \int_{\mathbb{R}^3} dy'\, e^{-i\frac{1+\varepsilon}{\varepsilon}tH_0}(r-R-y') \left[\Omega_+^{-1} \chi(\cdot + x') \right](y') \tag{2.11}$$

Proof. In the following we will denote $\chi(x+y)$ by $\chi_x(y)$.
Due to unitarity of the transformation T^ε defined in (2.4), one has

$$\|\Psi_2^\varepsilon(t) - \Psi_1^\varepsilon(t)\| = \|T^\varepsilon \Psi_2^\varepsilon(t) - T^\varepsilon \Psi_1^\varepsilon(t)\| \tag{2.12}$$

where from definitions (2.2) and (2.11) one yields

$$T^\varepsilon \Psi_1^\varepsilon(t; x, y) = \int_{\mathbb{R}^3} dx'\, e^{-i\frac{t}{1+\varepsilon}H_0}(x - x')\varphi(x') \int_{\mathbb{R}^3} dy'\, e^{-i\frac{1+\varepsilon}{\varepsilon}tH^\varepsilon}(y, y')\chi_{x'}(y') \tag{2.13}$$

$$T^\varepsilon \Psi_2^\varepsilon(t; x, y) = \int_{\mathbb{R}^3} dx'\, e^{-i\frac{t}{1+\varepsilon}H_0}(x - x')\varphi(x') \int_{\mathbb{R}^3} dy'\, e^{-i\frac{1+\varepsilon}{\varepsilon}tH_0}(y - y') \left(\Omega_+^{-1} \chi_{x'} \right)(y') \tag{2.14}$$

Therefore a straightforward computation gives

$$\begin{aligned}\|\Psi_2^\varepsilon(t)-\Psi_1^\varepsilon(t)\| &= \left[\int_{\mathbb{R}^6} dx\,dy\,|\varphi(x)|^2\left|\left(e^{-i\frac{1+\varepsilon}{\varepsilon}tH^\varepsilon}\chi_x\right)(y)-\left(e^{-i\frac{1+\varepsilon}{\varepsilon}tH_0}\Omega_+^{-1}\chi_x\right)(y)\right|^2\right]^{\frac12}\\ &\le \sup_{x\in\mathbb{R}^3}\|e^{-i\frac{1+\varepsilon}{\varepsilon}tH^\varepsilon}\chi_x-e^{-i\frac{1+\varepsilon}{\varepsilon}tH_0}\Omega_+^{-1}\chi_x\|_2\\ &= \sup_{x\in\mathbb{R}^3}\|e^{i\frac{1+\varepsilon}{\varepsilon}tH_0}e^{-i\frac{1+\varepsilon}{\varepsilon}tH^\varepsilon}\chi_x-\Omega_+^{-1}\chi_x\|_2 \qquad (2.15)\end{aligned}$$

Let us denote $\tau\equiv\frac{1+\varepsilon}{\varepsilon}t$. Then

$$\begin{aligned}e^{i\tau H_0}e^{-i\tau H^\varepsilon}\chi_x-\Omega_+^{-1}\chi_x &= \left(e^{i\tau H_0}e^{-i\tau H^\varepsilon}\chi_x-e^{i\tau H_0}e^{-i\tau H}\chi_x\right)\;+\;\left(e^{i\tau H_0}e^{-i\tau H}\chi_x-\Omega_+^{-1}\chi_x\right)\\ &\equiv (I)+(II) \qquad (2.16)\end{aligned}$$

First we estimate (I). Notice that

$$(I)=e^{i\tau H_0}\left(e^{-i\tau H^\varepsilon}e^{i\tau H}-\mathbb{I}\right)e^{-i\tau H}\chi_x \qquad (2.17)$$

By Duhamel's formula we have

$$e^{-i\tau H^\varepsilon}e^{i\tau H}-\mathbb{I} \;=\; \int_0^\tau ds\,\frac{d}{ds}e^{-isH^\varepsilon}e^{isH} \;=\; i\frac{\varepsilon}{1+\varepsilon}\lambda\int_0^\tau ds\,e^{-isH^\varepsilon}\,V\,e^{isH} \qquad (2.18)$$

Therefore

$$(I)=i\frac{\varepsilon}{1+\varepsilon}\lambda\,e^{i\tau H_0}\int_0^\tau ds\,e^{-i(\tau-s)H^\varepsilon}\,V\,e^{-isH}\chi_x \qquad (2.19)$$

Separating the small and the large time contributions in equation (2.19) we obtain

$$\begin{aligned}\|(I)\|_2 &\le \frac{\varepsilon}{1+\varepsilon}|\lambda|\int_0^\tau ds\|Ve^{-isH}\chi_x\|_2\\ &\le \frac{\varepsilon}{1+\varepsilon}|\lambda|\|V\|_2\left[\int_0^1 ds\,\|e^{-isH}\chi_x\|_\infty+\int_1^\infty ds\,\|e^{-isH}\chi_x\|_\infty\right] \qquad (2.20)\end{aligned}$$

The first integral in the r.h.s. of (2.20) is estimated using the second inequality in (1.14), the intertwining properties of the wave operators and the Fourier transform

$$\begin{aligned}\|e^{-itH}\chi_x\|_\infty &= \|\Omega_+e^{-itH_0}\Omega_+^{-1}\chi_x\|_\infty \;\le\; C\|e^{-itH_0}\Omega_+^{-1}\chi_x\|_\infty \;\le\; C\;\|\mathcal{F}\left(\Omega_+^{-1}\chi_x\right)\|_1\\ &\le C\left(\int_{\mathbb{R}^3}\frac{dk}{(k^2+1)^2}\right)^{\frac12}\left(\int_{\mathbb{R}^3}dk\,(k^2+1)^2\left|\mathcal{F}\left(\Omega_+^{-1}\chi_x\right)(k)\right|^2\right)^{\frac12}\\ &\le C\|\Omega_+^{-1}(H+\mathbb{I})\chi_x\|_2 \;\le\; C\|(H+\mathbb{I})\chi_x\|_2 \qquad (2.21)\end{aligned}$$

For the second integral in the r.h.s. of (2.20) one can use the first estimate in (1.14), namely

$$\|e^{-itH}\chi_x\|_\infty\le\frac{C}{t^{3/2}}\|\chi_x\|_1 \qquad (2.22)$$

¿From formulas (2.20), (2.21), (2.22), we finally obtain

$$\begin{aligned}\|(I)\|_2 &\leq C\frac{\varepsilon}{1+\varepsilon}\lambda\|V\|_2\left(\|(H+\mathbb{I})\chi_x\|_2+\|\chi\|_1\right)\\ &\leq C\frac{\varepsilon}{1+\varepsilon}\lambda\|V\|_2\left(\|\chi\|_{H^2(\mathbb{R}^3)}+\|V\|_\infty\|\chi\|_2+\|\chi\|_1\right)\end{aligned} \tag{2.23}$$

In order to estimate the term (II) in (2.16), we proceed analogously. Since

$$e^{i\tau H_0}e^{-i\tau H}\chi_x-\Omega_+^{-1}\chi_x=i\lambda\int_\tau^\infty ds\, e^{isH_0}Ve^{-isH}\chi_x \tag{2.24}$$

we can exploit the second inequality in (1.14)

$$\begin{aligned}\|(II)\|_2 &\leq \lambda\int_\tau^\infty ds\,\|Ve^{-isH}\chi_x\|_2 \leq \lambda\|V\|_2\int_\tau^\infty ds\,\|e^{-isH}\chi_x\|_\infty \leq C\lambda\|V\|_2\|\chi\|_1\int_\tau^\infty\frac{ds}{s^{3/2}}\\ &\leq C\lambda\|V\|_2\|\chi\|_1\sqrt{\frac{\varepsilon}{t}}\end{aligned} \tag{2.25}$$

¿From equations (2.15), (2.16), (2.23), (2.25), we have

$$\|\Psi_2^\varepsilon(t)-\Psi_1^\varepsilon(t)\| \leq C\lambda\|V\|_2\left[\varepsilon\left(\|\chi\|_{H^2(\mathbb{R}^3)}+\|V\|_\infty\|\chi\|_2\right)+\left(\varepsilon+\sqrt{\frac{\varepsilon}{t}}\right)\|\chi\|_1\right] \tag{2.26}$$

so the proof is complete. □

Let us notice that performing the change of variables

$$x'=\frac{\varepsilon r'+R'}{1+\varepsilon},\quad y'=r'-R' \tag{2.27}$$

in the integral in definition (2.11) and using the identity

$$e^{-i\frac{t}{1+\varepsilon}H_0}\left(\frac{\varepsilon(r-r')+(R-R')}{1+\varepsilon}\right)e^{-i\frac{1+\varepsilon}{\varepsilon}tH_0}(r-r'-(R-R'))=e^{-itH_0}(R-R')e^{-i\frac{t}{\varepsilon}H_0}(r-r') \tag{2.28}$$

we obtain

$$\Psi_2^\varepsilon(t;r,R)=\int_{\mathbb{R}^6}dr'\,dR'\,e^{-itH_0}(R-R')e^{-i\frac{t}{\varepsilon}H_0}(r-r')\,f^\varepsilon(r',R') \tag{2.29}$$

with

$$f^\varepsilon(r,R)\equiv\varphi\left(\frac{\varepsilon r+R}{1+\varepsilon}\right)\left[\Omega_+^{-1}\chi\left(\frac{\varepsilon r+R}{1+\varepsilon}+\cdot\right)\right](r-R),\ \varepsilon\geq 0 \tag{2.30}$$

Moreover, definitions (1.11), (1.12) and (1.13) yield

$$\Psi^a(t;r,R)=\int dr'\,dR'\,e^{-itH_0}(R-R')\varphi(R')e^{-i\frac{t}{\varepsilon}H_0}(r-r')\left[\left(\Omega_+^{R'}\right)^{-1}\chi\right](r') \tag{2.31}$$

¿From (2.29), (2.30) and (2.31), it is clear that the proof of theorem 1.1 is complete if we show that f^ε can be replaced by f^0 with an error of order ε.

Lemma 2.3. *There exists a constant $C_3 > 0$ such that for any $t \in \mathbb{R}$ one has*

$$\|\Psi_2^\varepsilon(t) - \Psi^a(t)\| \le C_4 \varepsilon \tag{2.32}$$

Proof. Following the same line of lemma 1 and using regularity properties of wave operators ([Y]) we have

$$\begin{aligned} \|f^\varepsilon - f^0\|^2 &= \|T^\varepsilon f^\varepsilon - T^\varepsilon f^0\|^2 = \int_{\mathbb{R}^6} dx\, dy \left| T^\varepsilon f^\varepsilon(x,y) - T^\varepsilon f^\varepsilon\left(x - \frac{\varepsilon}{1+\varepsilon} y, y\right)\right|^2 \\ &\le \varepsilon^2 \int_{\mathbb{R}^6} dx\, dy\, |y|^2 \left|\nabla_x \left[\varphi(x) \Omega_+^{-1} \chi_x(y)\right]\right|^2 \\ &\le 9\varepsilon^2 \sum_{j,k=1}^{3} \int_{\mathbb{R}^6} dx\, dk \left| \partial_{x_i} \partial_{k_j} \varphi(x) \widehat{\Omega_+^{-1}\chi_x}(k)\right|^2 \end{aligned} \tag{2.33}$$

where $\widehat{\Omega_+^{-1}\chi_x}$ is the Fourier transform of $\Omega_+^{-1}\chi_x$.
Let us prove that the integral in (2.33) is finite. ¿From stationary scattering theory (see e.g.[I], [RSIII]) it is well-known that

$$\widehat{\Omega_+^{-1}\chi_x}(k) = (2\pi)^{-\frac{3}{2}} \int_{\mathbb{R}^3} dz\, \overline{\Phi_+(z,k)} \chi_x(z) \tag{2.34}$$

where $\Phi_+(z,k)$ is a classical solution of the time-independent Schrödinger equation

$$-\frac{1}{2}\Delta_z \Phi_+(z,k) + V(z)\Phi_+(z,k) = \frac{|k|^2}{2}\Phi_+(z,k) \tag{2.35}$$

Therefore, from (2.34) and (2.35)

$$\widehat{\Omega_+^{-1}\chi_x}(k) = \frac{1}{(2\pi)^{\frac{3}{2}}(|k|^2+1)} \int_{\mathbb{R}^3} dz\, \overline{\Phi_+(z,k)} (2H+1)\chi_x(z) \tag{2.36}$$

where the regularity of χ allowed us to transfer the action of H from Φ_+ to χ_x. A straightforward computation gives

$$\left|\partial_{k_j} \widehat{\Omega_+^{-1}\chi_x}(k)\right|^2 \le \pi^{-3}(|k|^2+1)^{-2} \left[\xi_0^2 \|(2H+1)\chi_x\|_1^2 + \xi_1^2 \left(\int_{\mathbb{R}^3} dz\, (1+|z|)|(2H+1)\chi_x(z)|\right)^2\right] \tag{2.37}$$

where we introduced

$$\xi_0 \equiv \sup_{x,k\in\mathbb{R}^3} |\Phi_+(x,k)| \tag{2.38}$$

$$\xi_1 \equiv \sup_{x\in\mathbb{R}^3, k\in\mathbb{R}^3\setminus\{0\}} \left|\frac{\partial_{k_j}\Phi_+(x,k)}{1+|x|}\right| \tag{2.39}$$

In proposition 2.5 of [TDM-B] it is proven that ξ_0 and ξ_1 are finite.

In order to proceed with the estimate of the r.h.s. of (2.37) we observe that

$$\|(2H+1)\chi_x\|_1 \ \leq \ \|\Delta\chi\|_1 + 2\|V\|_2\|\chi\|_2 + \|\chi\|_1 \tag{2.40}$$

and moreover

$$\begin{aligned}\int_{\mathbb{R}^3} dz\,(1+|z|)|(2H+1)\chi_x(z)| \ &\leq \ \int_{\mathbb{R}^3} dz'(1+|z'|+|x|)|-\Delta\chi(z')+2V(z'-x)\chi(z')+\chi(z')| \\ &\leq \ |x|\left(\|\Delta\chi\|_1 + 2\|V\|_2\|\chi\|_2 + \|\chi\|_1\right) \\ &\quad +\|(1+|\cdot|)\Delta\chi\|_1 + 2\|V\|_2\|(1+|\cdot|)\chi\|_2 + \|(1+|\cdot|)\chi\|_1\end{aligned} \tag{2.41}$$

¿From estimates (2.37), (2.40) and (2.41) we obtain

$$\left|\partial_{k_j}\widehat{\Omega_+^{-1}\chi_x}(k)\right|^2 \ \leq \ \pi^{-3}(|k|^2+1)^{-2}\xi^2\left[\gamma_0(V,\chi)+\gamma_1(V,\chi)|x|^2\right] \tag{2.42}$$

where $\xi = \max(\xi_0,\xi_1)$ and

$$\begin{aligned}\gamma_0(V,\chi) \ &\equiv \ 9\|\Delta\chi\|_1^2 + 36\|V\|_2^2\|\chi\|_2^2 + 9\|\chi\|_1^2 \\ \gamma_1(V,\chi) \ &\equiv \ 6\|(1+|\cdot|)\Delta\chi\|_1^2 + 24\|V\|_2^2\|(1+|\cdot|)\chi\|_2^2 + 6\|(1+|\cdot|)\chi\|_1^2\end{aligned} \tag{2.43}$$

Similarly, noticing that

$$\partial_{x_i}\widehat{\Omega_+^{-1}\chi_x}(k) \ = \ \widehat{\Omega_+^{-1}(\partial_{x_i}\chi)_x}(k) \tag{2.44}$$

we have

$$\left|\partial_{x_i}\partial_{k_j}\widehat{\Omega_+^{-1}\chi_x}(k)\right|^2 \ \leq \ \pi^{-3}(|k|^2+1)^{-2}\xi^2\left[\beta_0(V,\chi)+\beta_1(V,\chi)|x|^2\right] \tag{2.45}$$

where

$$\begin{aligned}\beta_0(V,\chi) \ &\equiv \ 9\|\Delta\nabla\chi\|_1^2 + 36\|V\|_2^2\|\nabla\chi\|_2^2 + 9\|\nabla\chi\|_1^2 \\ \beta_1(V,\chi) \ &\equiv \ 6\|(1+|\cdot|)\Delta\nabla\chi\|_1^2 + 24\|V\|_2^2\|(1+|\cdot|)\nabla\chi\|_2^2 + 6\|(1+|\cdot|)\nabla\chi\|_1^2\end{aligned} \tag{2.46}$$

¿From (2.42) and (2.45) it is easily seen that

$$\begin{aligned}\left|\partial_{x_i}\partial_{k_j}\varphi(x)\widehat{\Omega_+^{-1}\chi_x}(k)\right|^2 \ \leq \ & 2\pi^{-3}(|k|^2+1)^{-2}\xi^2\left\{|\partial_{x_i}\varphi(x)|^2\left[\gamma_0(V,\chi)+\gamma_1(V,\chi)|x|^2\right]\right. \\ & \left.+|\varphi(x)|^2\left[\beta_0(V,\chi)+\beta_1(V,\chi)|x|^2\right]\right\}\end{aligned} \tag{2.47}$$

Since, by hypothesis, φ belongs to the Schwarz space, the last integral in (2.47) is bounded. Finally, standard commutation rules between the hamiltonian and the translation operator provide the following identity

$$\left[\Omega_+^{-1}\chi(R+\cdot)\right](r-R) = \left[\left(\Omega_+^R\right)^{-1}\chi\right](r) \tag{2.48}$$

¿From equations (2.29), (2.33) and (2.48) the result is proven. □

Proof of theorem 1.1. Lemmas 2.1, 2.2, 2.3 give the result with $A = C_3$ and $B = C_1 + C_2 + C_4$.

In the proof of lemma 2.3 we established that the moment of inertia of $\Omega_+^{-1}\chi$ was finite. Iterating the method, we can generalize the result to moments of any order.

Proposition 2.1. *Let the potential V satisfy hypotheses (A1), (A2), (A3), let ξ be an element of $H^2(\mathbb{R}^3)$, $m \in \mathbb{N}$ such that $\int_{\mathbb{R}^3} dy\,(1+|y|)^m\,|[(2H+1)\xi](y)| < \infty$ and $V = O(|x|^{-m-2})$ for $|x| \to \infty$. Then we have*

$$\int_{\mathbb{R}^3} dr\,|r|^{2m}\left|\left(\Omega_+^{-1}\xi\right)(r)\right|^2 < \infty \tag{2.49}$$

Proof. In the Fourier space we have

$$\int_{\mathbb{R}^3} dr\,|r|^{2m}\left|\left(\Omega_+^{-1}\xi\right)(r)\right|^2 \leq m\sum_{i=1}^{3}\int_{\mathbb{R}^3} dk\left|\partial_{k_i}^m\left[\frac{1}{|k|^2+1}\,\Omega_+^{-1}\widehat{(2H+1)}\xi(k)\right]\right|^2 \tag{2.50}$$

where we exploited the intertwining properties of the wave operators.
Furthermore,

$$\begin{aligned}
&\left|\partial_{k_i}^m\left[\frac{1}{|k|^2+1}\,\Omega_+^{-1}\widehat{(2H+1)}\xi(k)\right]\right| \\
= &\left|\sum_{j=0}^{m}\frac{m!}{j!(m-j)!}\left(\partial_{k_i}^{m-j}\frac{1}{|k|^2+1}\right)\left[\partial_{k_i}^{j}\Omega_+^{-1}\widehat{(2H+1)}\xi(k)\right]\right| \\
\leq\; & M\left|\sum_{j=0}^{m}\frac{m!}{j!(m-j)!}\partial_{k_i}^{j}\Omega_+^{-1}\widehat{(2H+1)}\xi(k)\right|
\end{aligned} \tag{2.51}$$

where we introduced $M \equiv \max_{k\in\mathbb{R}^3, j\in\{0,\ldots,m\}}\left|\partial_{k_i}^{j}\Omega_+^{-1}\widehat{(2H+1)}\xi(k)\right|$.
¿From the integral expression of the wave operators we have

$$\partial_{k_i}^{(j)}\Omega_+^{-1}\widehat{(2H+1)}\xi(k) = (2\pi)^{-\frac{3}{2}}\int_{\mathbb{R}^3} dy\,\partial_{k_i}^{(j)}\overline{\Phi_+(y,k)}[(2H+1)\xi](y) \tag{2.52}$$

Using the estimates of $\partial_{k_i}^{(j)}\Phi_+(y,k)$ obtained in [TDM-B] we have

$$\left|\partial_{k_i}^{(j)}\Omega_+^{-1}\widehat{(2H+1)}\xi(k)\right| \leq \frac{C}{(2\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3} dy\,(1+|y|)^m\,|[(2H+1)\xi](y)| \tag{2.53}$$

¿From formulas (2.50), (2.51), (2.53) we conclude that

$$\begin{aligned} & \int_{\mathbb{R}^3} dr\, |r|^{2m} \left| \left(\Omega_+^{-1} \xi \right)(r) \right|^2 \\ \leq \; & \frac{3}{(2\pi)^3} m^2 M^2 C^2 \sum_{j=0}^{m} \left(\frac{m!}{j!(m-j)!} \right)^2 \left(\int_{\mathbb{R}^3} dy\, (1+|y|)^m \, |[(2H+1)\xi](y)| \right)^2 \\ < \; & \infty \end{aligned} \tag{2.54}$$

and the proof is complete. □

3. Application to decoherence

It is well known that interference effects observed in the quantum system prepared in a superposition state are extremely sensible to the interaction with the environment.
Stressing this aspect one can define decoherence as the mechanism of irreversible diffusion in the environment of the spatial correlations present in a micro sub-system initially in a superposition state.
Here we consider the simplest situation where the system and the environment consist of a heavy and a light particle respectively.
In this case the mechanism of decoherence is originated by the scattering of the light particle from the heavy one and it is described in [JZ] starting from formula (1.1).
In fact, if the initial state of the heavy particle is a coherent superposition of two well separated wave packets, exploiting the linearity of the evolution in (1.1), one sees that the two wave packets act as independent scatterers producing two different scattered waves for the light particle.
The scalar product of these two scattered waves is strictly less than one and this is the origin of the decoherence effect on the heavy particle.
We shall describe this mechanism exploiting the result of theorem 1.1 and then imposing suitable assumptions on the initial state and the strength of the interaction.
In particular, in order to describe the dynamics of the heavy particle in presence of the light one, we introduce the reduced density matrix, defined as the positive, trace class operator $\rho^\varepsilon(t)$ in $L^2(\mathbb{R}^3)$ with $\mathrm{Tr}\,\rho^\varepsilon(t) = 1$ and integral kernel given by

$$\rho^\varepsilon(t; R, R') = \int_{\mathbb{R}^3} dr\, \Psi^\varepsilon(t; R, r) \overline{\Psi^\varepsilon}(t; R', r) \tag{3.1}$$

As a consequence of theorem 1.1 one easily obtains the asymptotic dynamics of the heavy particle in the small mass ratio limit.

Corollary 3.1. *Under the same assumptions of theorem 1.1 one has*

$$\lim_{\varepsilon \to 0} \mathrm{Tr}\, |\rho^\varepsilon(t) - \rho^a(t)| = 0 \tag{3.2}$$

where

$$\rho^a(t) = e^{-itH_0}\rho_0^a e^{itH_0} \tag{3.3}$$

and ρ_0^a is a density matrix whose integral kernel is

$$\rho_0^a(R,R') = \varphi(R)\overline{\varphi}(R')\mathcal{I}(R,R') \tag{3.4}$$

$$\mathcal{I}(R,R') = ((\Omega_+^R)^{-1}\chi, (\Omega_+^{R'})^{-1}\chi) \tag{3.5}$$

It should be stressed that the asymptotic dynamics of the heavy particle described by $\rho^a(t)$ is a free evolution and the only effect of the interaction is to induce a sudden change of the initial state from $\varphi(R)\overline{\varphi}(R')$ to $\varphi(R)\overline{\varphi}(R')\mathcal{I}(R,R')$.
Notice that $\mathcal{I}(R,R') = \overline{\mathcal{I}}(R',R)$ and $|\mathcal{I}(R,R')| \leq 1$.
It is easily seen that $\lim_{R'\to\infty} \|(\Omega_+^{R'})^{-1}\chi - \chi\| = 0$ and $|((\Omega_+^R)^{-1}\chi, \chi)| < 1$ for any fixed $R \in \mathbb{R}^3$ and any χ such that $\chi \neq (\Omega_+^R)^{-1}\chi$.
Then there exist $K, K' > 0$ such that $|\mathcal{I}(R,R')| < 1$ for $|R| < K$ and $|R'| > K'$ and this in particular implies that $\mathrm{Tr}(\rho^a(t))^2 = \mathrm{Tr}(\rho_0^a)^2 < 1$, i.e. the asymptotic dynamics of the heavy particle is described by a mixed state.
We can also describe the behaviour of $\mathcal{I}(R,R')$ for small values of $|R-R'|$.
In fact $\mathcal{I}(R,R') = 1 + ((\Omega_+^R)^{-1}\chi, ((\Omega_+^{R'})^{-1} - (\Omega_+^R)^{-1})\chi)$ and the last scalar product can be estimated as follows

Proposition 3.2. *If $V \in H^1(\mathbb{R}^3)$ then for any $R, R' \in \mathbb{R}^3$ one has*

$$\left\|(\Omega_+^R)^{-1}\chi - (\Omega_+^{R'})^{-1}\chi\right\|_2 \leq C_5\lambda\|\nabla V\|_2|R-R'| \tag{3.6}$$

where C_5 does not depend on R, R'.

Proof. We follow the line of the proof of lemma 2.2, formulas (2.16)-(2.26), to obtain

$$\begin{aligned}
\left[(\Omega_+^R)^{-1} - (\Omega_+^{R'})^{-1}\right]\chi &= \lim_{t\to\infty} e^{itH_0}\left[e^{-itH(R)}e^{itH(R')} - \mathbb{I}\right]e^{-itH(R')}\chi \\
&= \lim_{t\to\infty} e^{itH_0}\int_0^t ds\,\frac{d}{ds}\left(e^{-isH(R)}e^{isH(R')}\right)e^{-itH(R')}\chi \\
&= i\lambda\lim_{t\to\infty} e^{itH_0}e^{itH(R)}\int_0^t d\sigma\, e^{-i\sigma H(R)}\left(V^{R'} - V^R\right)e^{i\sigma H(R')}\chi
\end{aligned} \tag{3.7}$$

where V^x acts as the multiplication by the function $V(\cdot - x)$ and we performed the change of variable $\sigma = t - s$. Thus one has

$$\left\|\left[(\Omega_+^R)^{-1} - (\Omega_+^{R'})^{-1}\right]\chi\right\|_2 \leq \lambda\|V^R - V^{R'}\|_2\int_0^\infty d\sigma\,\|e^{i\sigma H^{R'}}\chi\|_\infty \tag{3.8}$$

Still following the proof of lemma 2.2 we use the dispersive estimates (1.14) to obtain

$$\left\| \left[(\Omega_+^R)^{-1} - (\Omega_+^{R'})^{-1} \right] \chi \right\|_2 \leq C\lambda \left(\|\chi\|_{H^2(\mathbb{R}^3)} + \|V\|_\infty \|\chi\|_2 + \|\chi\|_1 \right) \|V^R - V^{R'}\|_2 \tag{3.9}$$

Since V is an element of $H^1(\mathbb{R}^3)$, the following estimate holds

$$\begin{aligned} \|V^R - V^{R'}\|_2^2 &\leq \int_{\mathbb{R}^3} dk \, \left| e^{ik(R-R')} - 1 \right|^2 \left| \hat{V}(k) \right|^2 \\ &\leq |R - R'|^2 \|\nabla V\|_2^2 \end{aligned} \tag{3.10}$$

Inserting the estimate (3.10) in inequality (3.9) the proposition is proven. □

For a concrete analysis of the decoherence effect we fix the initial state of the heavy particle in the form of a superposition of two wave packets

$$\varphi(R) = b^{-1} \left(f_\sigma^1(R) + f_\sigma^2(R) \right), \quad b \equiv \|f_\sigma^1 + f_\sigma^2\|_2 \tag{3.11}$$

$$f_\sigma^j(R) = \frac{1}{\sigma^{3/2}} f\left(\frac{R - R_j}{\sigma} \right) e^{iP_j \cdot R}, \qquad R_j, P_j \in \mathbb{R}^3, \quad j = 1, 2 \tag{3.12}$$

where $f \in \mathcal{S}(\mathbb{R}^3)$ is a real valued function with $\|f\|_2 = 1$.
Furthermore we assume that the potential V is slowly varying on a length scale of the order of the spatial localization of each wave packet, more precisely, we assume $C_5 \lambda \|\nabla V\|_2 \sigma \ll 1$.
Using such assumption and choosing the initial state (3.11) we can see that the state of the entire system at any $t > 0$ can be written in the typical form of a cat-like entangled state.

Corollary 3.3. *If the initial state for the heavy particle is given by (3.11), (3.12) and $V \in H^1(\mathbb{R}^3)$ satisfies the hypotheses (A1), (A2), (A3) then there exists a constant $C > 0$ such that for any $t > 0$ one has*

$$\|\Psi^a(t) - \Psi^e(t)\| \leq C \frac{\lambda}{b} \|\nabla V\|_2 \, \sigma \tag{3.13}$$

where

$$\Psi^e(t) \equiv e^{-it\hat{H}_0^\varepsilon} \Psi_0^e \tag{3.14}$$

and

$$\Psi_0^e(R, r) \equiv \frac{1}{b} f_\sigma^1(R) \left[\left(\Omega_+^{R_1} \right)^{-1} \chi \right](r) + \frac{1}{b} f_\sigma^2(R) \left[\left(\Omega_+^{R_2} \right)^{-1} \chi \right](r) \tag{3.15}$$

Proof. Exploiting proposition (3.2) we have

$$\begin{aligned} &\|\Psi^a(t) - \Psi^e(t)\| = \|\Psi_0^a - \Psi_0^e(t)\| \\ &\leq \frac{1}{b} \sum_{j=1}^2 \left\{ \int dR \, dr \, \left| f_\sigma^j(R) \right|^2 \left| \left[(\Omega_+^R)^{-1} \chi \right](r) - \left[(\Omega_+^{R_j})^{-1} \chi \right](r) \right|^2 \right\}^{\frac{1}{2}} \\ &\leq C_5 \frac{\lambda}{b} \|\nabla V\|_2 \sum_{j=1}^2 \left\{ \int dR \, \left| f_\sigma^j(R) \right|^2 |R - R_j|^2 \right\}^{\frac{1}{2}} \end{aligned} \tag{3.16}$$

Performing the change of variable $\frac{R-R_j}{\sigma}=z$ we conclude the proof. $\square$

¿From corollary 3.3 we have that the reduced density matrix for the heavy particle $\rho^a(t)$ can be further approximated by

$$\rho^e(t) \;=\; e^{-itH_0}\rho_0^e e^{itH_0} \tag{3.17}$$

where ρ_0^e has integral kernel

$$\rho_0^e(R,R') = \frac{1}{b^2}\left|f_\sigma^1(R)\right|^2 + \frac{1}{b^2}\left|f_\sigma^2(R)\right|^2 + \frac{\Lambda}{b^2} f_\sigma^1(R)\overline{f}_\sigma^2(R') + \frac{\overline{\Lambda}}{b^2} f_\sigma^2(R)\overline{f}_\sigma^1(R') \tag{3.18}$$

$$\Lambda \equiv \int_{\mathbb{R}^3} dr\, \overline{\left[\left(\Omega_+^{R_1}\right)^{-1}\chi\right](r)}\left[\left(\Omega_+^{R_2}\right)^{-1}\chi\right](r) \tag{3.19}$$

It is clear from (3.19) that, if the interaction is absent, then $\Lambda = 1$ and (3.18) describes the pure state corresponding to the coherent superposition of f_σ^1 and f_σ^2 evolving according to the free hamiltonian.
Suppose in particular that the free time evolution of f_σ^1 and f_σ^2 show a significant overlapping. In this case the time evolution of the last two terms in (3.18) gives contributions on the diagonal $R = R'$ which are comparable with the time evolution of the first two terms, making possible the typical interference effects.
If the interaction with the light particle is present, one sees that its only effect on the heavy particle is to reduce the non diagonal terms in (3.18) by the factor Λ, whith $|\Lambda| \leq 1$, and this means that the interference effects for the heavy particle are correspondingly reduced.
In this sense we can say that a (partial) decoherence effect on the heavy particle has been induced and, moreover, the effect is completely characterized by the parameter Λ.
It is worth observing that for a comparison of the theoretical prediction with the now available experimental data (see e.g. [HUBHAZ]) a careful evaluation of the parameter Λ is required, which takes into account the specific initial state χ chosen for the light particle.
Such evaluation has been approached in [JZ] and [GF]. A more careful analysis can be found in [HS], where normalized states instead of unphysical "plane waves" are used and, besides, at each step, the approximations made are clearly justified on a physical ground. In particular, it is correctly argued that the replacement of Ω_+^{-1} with the S matrix requires specifical assumptions on the initial state χ.
It would be of interest to give a rigorous derivation of the formulas derived in [HS], with an explicit control of the error made at each step of the approximation. Moreover, using Joos-Zeh formula it would be worth to give a rigorous approach to the focusing effect around classical trajectories induced by the interaction with the environment. In early days of quantum mechanics this effect was analyzed by Mott ([M]) in the attempt to give an explanation, in terms of quantum dynamics, of the particle trajectories observed in a cloud chamber. At the best of our knowledge no new results along this line were obtained since then.
We plan to analyse these problems in further work.

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