

Semiclassical Propagation of Coherent States for the Hartree Equation

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Abstract. In this paper we consider the nonlinear Hartree equation in presence of a given external potential, for an initial coherent state. Under suitable smoothness assumptions, we approximate the solution in terms of a time dependent coherent state, whose phase and amplitude can be determined by a classical flow. The error can be estimated in L^2 by $C\sqrt{\varepsilon}$, ε being the Planck constant. Finally we present a full formal asymptotic expansion.

1. Introduction

Let us consider the Hartree equation in \mathbb{R}^d :

$$\begin{aligned}i\varepsilon\partial_t\Psi^\varepsilon(x,t) &= -\frac{\varepsilon^2}{2}\Delta\Psi^\varepsilon(x,t) + (V(x,t) + U(x,t))\Psi^\varepsilon(x,t), \\ \Psi^\varepsilon(x,0) &= \Psi_0^\varepsilon(x),\end{aligned}\tag{1}$$

where

$$V(x,t) = \int \phi(|x-y|)|\Psi^\varepsilon(y,t)|^2 dy\tag{2}$$

is a self-consistent potential given by a smooth two-body interaction, $\phi:\mathbb{R}\rightarrow\mathbb{R}$, even, and $U(\cdot,t):\mathbb{R}^d\rightarrow\mathbb{R}$ for all $t\geq 0$, is a smooth external potential (see the next section for our precise assumptions on ϕ and U . See, e.g. [6] for a well-posedness study).

The Hartree equation describes the time evolution of a large number of particles in a mean-field regime. In fact, if one considers an N -particle system where the interaction potential is suitably rescaled with N (mean-field model) and the initial datum is (almost) factorized, it turns out that the many-body evolution is approximated, as $N\rightarrow\infty$, by the Hartree dynamics

(1). More precisely, the time evolution of the system, originally ruled by an N -particle (linear) Schrödinger equation, can be described for very large N by the one-particle (nonlinear) Eq. (1), where ϕ is exactly the two-body interaction considered for the many-body dynamics. That is the reason why the radial symmetry assumption arises quite naturally: in the physical systems described by the many-body model the two-body interaction is actually depending only on the particle distance (see references below for a more detailed discussion).

The previous result was originally obtained for sufficiently smooth interactions (see for instance [8, 9, 13, 22]) and then it has been generalized to include Coulomb potentials (see e.g. [2, 3, 7] and, more recently, [14]).

However, here we are not going to consider the case of singular interactions since, as is usual in dealing with (strong) semiclassical asymptotics (see e.g. [19, 20]), the techniques we are going to use require ϕ to verify suitable smoothness assumptions (see below).

In a recent paper [1] the authors of the present one considered the semiclassical limit of the version of the Hartree equation corresponding to mixed states for initial data whose Wigner functions do not concentrate at the classical limit.

The problem we deal with in the present paper is the semiclassical asymptotics for (1) when the initial state is a coherent state centered around the point q, p of the classical phase space, namely

$$\Psi_0^\varepsilon(x) = \varepsilon^{-\frac{d}{4}} a_0 \left(\frac{x - q}{\sqrt{\varepsilon}} \right) e^{i \frac{p \cdot (x - q)}{\varepsilon}} := \psi_{qp}^{\alpha_0}(x). \tag{3}$$

This problem was studied in [15] in the kinetic (Wigner) picture, see Théorème IV.2 therein. There it is shown that, under appropriate conditions, the solution W^ε of the Wigner equation corresponding to the dynamics (1), namely

$$\begin{aligned} & \partial_t W^\varepsilon + k \cdot \partial_x W^\varepsilon \\ &= \frac{i}{\varepsilon(2\pi)^d} \int \int e^{i\xi y} \left(V \left(x + \frac{\varepsilon y}{2}, t \right) - V \left(x - \frac{\varepsilon y}{2}, t \right) \right) dy W^\varepsilon(x, k - \xi) d\xi \\ &+ \frac{i}{\varepsilon(2\pi)^d} \int \int e^{i\xi y} \left(U \left(x + \frac{\varepsilon y}{2}, t \right) - U \left(x - \frac{\varepsilon y}{2}, t \right) \right) dy W^\varepsilon(x, k - \xi) d\xi, \end{aligned} \tag{4}$$

where $V(x, t)$ is the same as in (1) equivalently written as

$$V(x, t) = \int \phi(|x - y|) W^\varepsilon(y, k, t) dk dy, \tag{5}$$

converges, in weak*-sense, to the solution of the (classical) Vlasov equation

$$\begin{aligned} & \partial_t f + k \cdot \partial_x f - \partial_x V_0(x, t) \cdot \partial_k f - \partial_x U(x, t) \cdot \partial_k f = 0, \\ & f(x, k, t)|_{t=0} = f_0(x, k), \end{aligned} \tag{6}$$

where

$$V_0(x, t) = \int \phi(|x - y|) f(y, k, t) dk dy,$$

and $U(x, t)$ is the same as in (1). The initial condition for (6) is given by $f_0 = w - * \lim_{\varepsilon \rightarrow 0} W_0^\varepsilon$. It is easy to check that the conditions of Théorème IV.2 in [15] are satisfied for $W_0^\varepsilon(x, v) = W^\varepsilon[\Psi_0^\varepsilon](x, v)$, Ψ_0^ε as in Eq. (3). In that case (under appropriate assumptions on the pair-interaction potential ϕ and the external potential U) it can be seen that the Wigner measure of the wave function verifies

$$W^\varepsilon[\Psi^\varepsilon](x, k, t) \rightharpoonup \delta(x - X(t))\delta(k - K(t)), \quad \text{as } \varepsilon \rightarrow 0,$$

where

$$\dot{X}(t) = K(t), \quad \dot{K}(t) = -\nabla U(X(t), t), \quad X(0) = q, \quad K(0) = p.$$

In that sense, the semiclassical limit of the problem (1) is known to be the Vlasov dynamics (6), since it is easy to recognize that, due to the smoothness of the potentials, the limiting measure $\delta(x - X(t))\delta(k - K(t))$ is the unique (weak) solution of the Vlasov equation with initial datum $\delta(x - q)\delta(k - p)$.

The goal of the present work is to strengthen this approximation. First of all, we construct L^2 approximations, as opposed to the weak- $*$ limit, and this yields an explicit control of the error in ε which allows to recover the shape with which W^ε concentrates to a δ in phase-space.

2. Main Result

We will consider the Hartree equation in \mathbb{R}^d :

$$\begin{aligned} i\varepsilon \partial_t \Psi^\varepsilon(x, t) &= -\frac{\varepsilon^2}{2} \Delta \Psi^\varepsilon(x, t) + (V(x, t) + U(x, t)) \Psi^\varepsilon(x, t), \\ \Psi^\varepsilon(x, 0) &= \Psi_0^\varepsilon(x), \end{aligned} \tag{7}$$

where

$$V(x, t) = \int \phi(|x - y|) |\Psi^\varepsilon(y, t)|^2 dy. \tag{8}$$

The initial condition will be of the form

$$\Psi_0^\varepsilon(x) = \varepsilon^{-\frac{d}{4}} a_0 \left(\frac{x - q}{\sqrt{\varepsilon}} \right) e^{i \frac{p \cdot (x - q)}{\varepsilon}} := \psi_{qp}^{a_0}$$

and we will make the following assumptions on a_0 , ϕ and U :

Assumption 1.

$$\|a_0\|_{L^2} = \|\Psi_0^\varepsilon\|_{L^2} = 1,$$

$$x^A \partial_x^B a_0(x) \in L^2 \text{ for any pair } A, B \in \mathbb{N}^d \text{ with } |A| + |B| \leq 3,$$

$$\int x_i |a_0(x)|^2 dx = 0, \quad \forall i = 1 \dots d. \tag{9}$$

$$\int k_i |\widehat{a}_0(k)|^2 dk = 0, \quad \forall i = 1 \dots d. \tag{10}$$

Assumption 2.

$$C_b^3(\mathbb{R}) \ni \phi \text{ even}$$

Assumption 3.

$$U \in C^1(\mathbb{R}_t^+, C_b^3(\mathbb{R}^d_x)).$$

We will denote by $C_b^k(\mathbb{R}^m)$ the set of real-valued functions on \mathbb{R}^m which have continuous and uniformly bounded derivatives of order 0 up to k .

Theorem 2.1. *Under Assumptions 1, 2 and 3 there exists a constant C such that, $\forall t \geq 0$,*

$$\|\Psi^\varepsilon(\cdot, t) - e^{i\frac{\mathcal{L}(t)}{\varepsilon} + i\gamma(t)} \psi_{q(t)p(t)}^{\beta_t}\|_{L^2} \leq C e^{Cte^{C\varepsilon}} \cdot \sqrt{\varepsilon}. \tag{11}$$

where β_t is the solution of

$$i\partial_t \beta_t(x) = \left(-\frac{\Delta}{2} + \frac{\phi''(0)x^2}{2} + \frac{\langle x, H(U(q(t)), t)x \rangle}{2} \right) \beta_t(x), \tag{12}$$

$$\beta_0(x) = a_0(x), \tag{13}$$

$$\gamma(t) = -\frac{\phi''(0)}{2} \int_0^t \int \eta^2 |\beta_s(\eta)|^2 d\eta ds, \tag{14}$$

$(q(t), p(t))$ is the Hamiltonian flow associated with $\frac{p^2}{2} + U(q, t) + \phi(0)$ issued from (q, p) ,

$$\mathcal{L}(t) := \int_0^t (p(s)^2/2 - U(q(s), s) - \phi(0)) ds$$

(the Lagrangian action along such Hamiltonian flow).

Remarks. • As shown in the proof of the Theorem, the constant C depends only on $d, \|U\|_{W^{3,\infty}}, \|\phi\|_{W^{3,\infty}}$ and $\sup_{|A|+|B|\leq 3} \|x^B \partial_x^A a_0\|_{L^2}$.

- Note that in the classical flow the nonlinear potential enters only via the inessential constant $\phi(0)$. Indeed, due to the symmetry and smoothness of ϕ , we have $\phi'(0) = 0$ so that, in the limit $\varepsilon \rightarrow 0$, the self-consistent field ∇V vanishes.
- A similar problem for $\phi''(0) \geq 0$ has been faced in [4] in a semirigorous way. Here, we treat the case $\phi''(0) \leq 0$ as well and present an explicit control of momenta and derivatives of the solutions (see Lemma 2.3 below) which allow us to estimate the error in L^2 .
- For a related result (Gross–Pitaevskii equation with a different scaling), see [5].
- Assumption 1 can be relaxed by dismissing Eq. (9). Indeed, even if (9) does not hold one can always make a change of variables $x \mapsto x - \int x|a_0(x)|^2 dx$. However, in that case one would have to adjust appropriately the external potential, which of course is not translation invariant.

3. Proofs

3.1. A Lemma

We first prove the following

Lemma 3.1. $b_t(x) := e^{i\gamma(t)}\beta_t(x)$ as defined by (12), (13), (14) is the unique solution of the initial value problem:

$$\begin{aligned} \left(i\partial_t + \frac{1}{2}\Delta\right) b_t(x) &= \frac{\phi''(0)}{2} \int |x - \eta|^2 |\beta_t(\eta)|^2 d\eta b_t(x) \\ &\quad + \frac{\langle x, H(U(q(t)), t)x \rangle}{2} b_t(x), \\ b_0(x) &= a_0(x). \end{aligned} \tag{15}$$

Proof.

$$i\partial_t b_t(x) = -\gamma'(t)b_t(x) + e^{i\gamma(t)}i\partial_t\beta_t(x). \tag{16}$$

By virtue of Eqs. (12), (13) and (14) we find

$$\begin{aligned} i\partial_t b_t(x) &= \frac{\phi''(0)}{2} \int \eta^2 |\beta_t(\eta)|^2 d\eta b_t(x) + e^{i\gamma(t)} \left(-\frac{\Delta}{2} \beta_t(x) + \frac{\phi''(0)}{2} x^2 \beta_t(x) \right) \\ &\quad + e^{i\gamma(t)} \left(\frac{\langle x, H(U(q(t)), t)x \rangle}{2} \beta_t(x) \right) \end{aligned} \tag{17}$$

$$b_0(x) = a_0(x),$$

namely

$$\begin{aligned} i\partial_t b_t(x) &= -\frac{\Delta}{2} b_t(x) + \frac{\phi''(0)}{2} x^2 b_t(x) + \frac{\phi''(0)}{2} \int \eta^2 |\beta_t(\eta)|^2 d\eta b_t(x) \\ &\quad + \frac{\langle x, H(U(q(t)), t)x \rangle}{2} b_t(x) \\ b_0(x) &= a_0(x). \end{aligned} \tag{18}$$

We first notice that Eq. (12) for $\beta_t(x)$ is a linear Schrödinger equation with an harmonic potential; therefore, the solution $\beta_t(x)$ of the initial value problem (12)–(13) is uniquely determined in $L^2(\mathbb{R}^d)$ and

$$\|\beta_t\|_{L^2} = \|a_0\|_{L^2} = 1, \quad \forall t \in \mathbb{R}. \tag{19}$$

As a consequence of that, it turns out that the initial value problem (18) can be rewritten as

$$\begin{aligned} i\partial_t b_t(x) &= -\frac{\Delta}{2} b_t(x) + \frac{\phi''(0)}{2} \int x^2 |\beta_t(\eta)|^2 d\eta b_t(x) \\ &\quad + \frac{\phi''(0)}{2} \int \eta^2 |\beta_t(\eta)|^2 d\eta b_t(x) + \frac{\langle x, H(U(q(t)), t)x \rangle}{2} b_t(x). \\ b_0(x) &= a_0(x). \end{aligned} \tag{20}$$

Furthermore, it is easy to check that if

$$x a_0(x), \partial_x a_0(x) \in L^2(\mathbb{R}^d), \tag{21}$$

then

$$x\beta_t(x), \partial_x\beta_t(x) \in L^2(\mathbb{R}^d), \quad \text{for all } t, \tag{22}$$

(see Observation 4.3 below).

Condition (21) is satisfied under Assumption 1, so the property (22) holds and, in particular, there exists a bound $C = C(t)$, finite for any time t , such that

$$\int |\eta|^2 |\beta_t(\eta)|^2 d\eta < C(t), \quad \forall t \in \mathbb{R}. \tag{23}$$

Thus, by virtue of (23) and of Assumptions 1, 2 and 3, it follows that the initial value problem (20) is guaranteed to have a unique solution in L^2 and, clearly, $\|b_t\|_{L^2} = \|a_0\|_{L^2} = 1, \quad \forall t$. In fact, the equation for $b_t(x)$ has turned out to be a linear Schrödinger equation with an harmonic potential (and all constants appearing in the potential terms are finite thanks to Assumptions 2 and 3 and Eq. (23)).

Now, it remains only to recognize that (20) is exactly the same as (15). To this end it is sufficient to observe that, since the Eq. (12) for $\beta_t(x)$ is a linear Schrödinger equation with an harmonic potential, and conditions (9) and (10) are satisfied at time $t = 0$, it is guaranteed that

$$\int \eta |\beta_t(\eta)|^2 d\eta = 0, \quad \forall t. \tag{24}$$

Thus, by virtue of (24), it follows that (20) can be rewritten as

$$\begin{aligned} i\partial_t b_t(x) = & -\frac{\Delta}{2} b_t(x) + \frac{\phi''(0)}{2} \int |x - \eta|^2 |\beta_t(\eta)|^2 d\eta b_t(x) \\ & + \frac{\langle x, H(U(q(t)), t)x \rangle}{2} b_t(x). \end{aligned} \tag{25}$$

Finally, it is clear, by the definition of $b_t(x)$, that $|\beta_t(x)| = |b_t(x)|$ for any x and t . Therefore, (25) turns to be exactly the same as (15). \square

3.2. Proof of Theorem 2.1

As is standard when working with coherent states, see, e.g. [11–13, 17, 18], we seek an approximate solution to Eq. (1) of the form

$$\Psi^\varepsilon(x, t) = \varepsilon^{-\frac{d}{4}} a \left(\frac{x - q(t)}{\sqrt{\varepsilon}}, t \right) e^{i\frac{p(t) \cdot (x - q(t))}{\varepsilon}} e^{i\frac{\mathcal{L}(t)}{\varepsilon}}, \tag{26}$$

where

$$\dot{q}(t) = p(t), \quad \dot{p}(t) = -\nabla U(q(t), t). \tag{27}$$

By inserting the ansatz (26) in Eq. (1) we get

$$\begin{aligned} i\varepsilon\partial_t \Psi^\varepsilon(x, t) = & \varepsilon^{-\frac{d}{4}} \left[i\varepsilon\partial_t a \left(\frac{x - q(t)}{\sqrt{\varepsilon}}, t \right) - i\sqrt{\varepsilon}\nabla a \left(\frac{x - q(t)}{\sqrt{\varepsilon}}, t \right) \cdot \dot{q}(t) \right. \\ & \left. - \mathcal{L}'(t)a \left(\frac{x - q(t)}{\sqrt{\varepsilon}}, t \right) - (\dot{p}(t)(x - q(t)) - p(t)\dot{q}(t)) a \left(\frac{x - q(t)}{\sqrt{\varepsilon}}, t \right) \right] \\ & \times e^{i\frac{p(t) \cdot (x - q(t))}{\varepsilon}} e^{i\frac{\mathcal{L}(t)}{\varepsilon}}, \end{aligned} \tag{28}$$

and

$$-\frac{\varepsilon^2}{2}\Delta\Psi^\varepsilon(x,t) = \varepsilon^{-\frac{d}{4}} \left[-\frac{\varepsilon}{2}\Delta a\left(\frac{x-q(t)}{\sqrt{\varepsilon}},t\right) + \frac{p^2(t)}{2}a\left(\frac{x-q(t)}{\sqrt{\varepsilon}},t\right) - i\sqrt{\varepsilon}\nabla a\left(\frac{x-q(t)}{\sqrt{\varepsilon}},t\right) \cdot p(t) \right] e^{i\frac{p(t)\cdot(x-q(t))}{\varepsilon}} e^{i\frac{\mathcal{L}(t)}{\varepsilon}}. \tag{29}$$

With regard to the potential terms in (1), we find

$$\begin{aligned} &(V(x,t) + U(x,t))\Psi^\varepsilon(x,t) \\ &= \varepsilon^{-d/4} \left(\int \phi(|x-y|)\varepsilon^{-d/2} \left| a\left(\frac{y-q(t)}{\sqrt{\varepsilon}},t\right) \right|^2 dy + U(x,t) \right) \\ &\quad \times a\left(\frac{x-q(t)}{\sqrt{\varepsilon}},t\right) e^{i\frac{p(t)\cdot(x-q(t))}{\varepsilon}} e^{i\frac{\mathcal{L}(t)}{\varepsilon}}. \end{aligned} \tag{30}$$

By (28), (29) and (30) we get that the amplitude a solves the following initial value problem:

$$\begin{aligned} \left(i\partial_t + \frac{1}{2}\Delta\right)a(\mu,t) &= \frac{1}{\varepsilon}V_\varepsilon(\mu,t)a(\mu,t) \\ &\quad + \frac{1}{\varepsilon} [U(q(t) + \sqrt{\varepsilon}\mu,t) - U(q(t),t) \\ &\quad - \sqrt{\varepsilon}\nabla U(q(t),t) \cdot \mu] a(\mu,t), \\ a(\mu,0) &= a_0(\mu), \end{aligned} \tag{31}$$

where

$$V_\varepsilon(\mu,t) = \int (\phi(\sqrt{\varepsilon}|\mu - \eta|) - \phi(0)) |a(\eta,t)|^2 d\eta, \tag{32}$$

$q(t), p(t)$ are as in the claim of Theorem 2.1 and we have used the rescaling $\mu = \frac{x-q(t)}{\sqrt{\varepsilon}}$.

Note that we should have

$$V_\varepsilon(\mu,t) = \int \phi(\sqrt{\varepsilon}|\mu - \eta|) |a(\eta,t)|^2 d\eta - \phi(0), \tag{33}$$

instead of (32) in Eq. (31). However, Eq. (31) with potential (33) is a Hartree equation which preserves the L^2 norm so that we can replace (33) by (32).

Since $\phi \in C_b^3(\mathbb{R})$ is even, $\phi'(0) = 0$ and therefore the Taylor expansion yields

$$\begin{aligned} \phi(\sqrt{\varepsilon}|\mu - \eta|) - \phi(0) &= \frac{\varepsilon|\mu - \eta|^2}{2}\phi''(0) + \varepsilon^{\frac{3}{2}}R(|\mu - \eta|), \\ |R(|\mu - \eta|)| &\leq C\|\phi'''\|_{L^\infty}|\mu - \eta|^3, \end{aligned} \tag{34}$$

while for the terms involving U we find

$$\begin{aligned}
 &U(q(t) + \sqrt{\varepsilon}\mu, t) - U(q(t), t) - \sqrt{\varepsilon}\nabla U(q(t), t) \cdot \mu \\
 &= \varepsilon \left\langle \mu, \frac{H(U(q(t)), t)}{2} \mu \right\rangle + \varepsilon^{\frac{3}{2}} R_U(\mu, t), \\
 &|R_U(\mu, t)| \leq C \sup_{\alpha \in \mathbb{N}^d: |\alpha|=3} |\nabla^\alpha U(q(t), t)| |\mu|^3,
 \end{aligned} \tag{35}$$

where $H(f)_{ij} := (\partial_{x_i} \partial_{x_j} f)$.

The core of the proof is to estimate the two remainders $\varepsilon^{\frac{3}{2}} R(|\mu - \eta|)$ and $\varepsilon^{\frac{3}{2}} R_U(\mu, t)$ so that we can substitute $(\phi(\sqrt{\varepsilon}|\mu - \eta|) - \phi(0))$ by $\frac{\varepsilon|\mu - \eta|^2}{2} \phi''(0)$ (as in (34)) and $U(q(t) + \sqrt{\varepsilon}\mu, t) - U(q(t), t) - \sqrt{\varepsilon}\nabla U(q(t), t) \cdot \mu$ by $\varepsilon \langle \mu, \frac{H(U(q(t)), t)}{2} \mu \rangle$ (as in (35)).

The idea of course has general similarities to the linear case [11–13, 17, 18]; however, we give a completely self-contained proof here.

Denote $a_t(\mu) := a(\mu, t)$ and

$$h_t(\mu) = b_t(\mu) - a_t(\mu). \tag{36}$$

By straightforward substitution we get that $h_0(\mu) = 0$ (see (15)) and

$$\begin{aligned}
 &\left(i\partial_t + \frac{1}{2}\Delta - \underbrace{\left(\frac{\phi''(0)}{2} \int |\mu - \eta|^2 |b_t(\eta)|^2 d\eta + \left\langle \mu, \frac{H(U(q(t)), t)}{2} \mu \right\rangle \right)}_{V_Q(\mu, t)} \right) h_t(\mu) \\
 &= \frac{\phi''(0)}{2} \underbrace{\int |\mu - \eta|^2 (|b_t(\eta)|^2 - |a_t(\eta)|^2) d\eta}_{I_1(\mu, t)} a_t(\mu) \\
 &\quad - \underbrace{\sqrt{\varepsilon} \int R(|\mu - \eta|) |a_t(\eta)|^2 d\eta}_{I_2(\mu, t)} a_t(\mu) - \sqrt{\varepsilon} R_U(\mu, t) a_t(\mu).
 \end{aligned} \tag{37}$$

By standard manipulations it turns out that

$$\|h_t\|_{L^2} \frac{d}{dt} \|h_t\|_{L^2} \leq \frac{|\phi''(0)|}{2} |\langle I_1, h_t \rangle| + \sqrt{\varepsilon} |\langle I_2, h_t \rangle| + \sqrt{\varepsilon} |\langle R_U(\cdot, t) a_t, h_t \rangle|. \tag{38}$$

Moreover, the term involving I_1 can be estimated as follows:

$$\begin{aligned}
 |\langle I_1, h \rangle| &\leq \left| \int_{\mu} \int_{\eta} |\mu - \eta|^2 (|b_t(\eta)|^2 - |a_t(\eta)|^2) d\eta \bar{a}_t(\mu) h_t(\mu) d\mu \right| \\
 &= \left| \int_{\mu} \int_{\eta} |\mu - \eta|^2 (|b_t(\eta)| - |a_t(\eta)|) (|b_t(\eta)| + |a_t(\eta)|) d\eta \bar{a}_t(\mu) h_t(\mu) d\mu \right|
 \end{aligned}$$

$$\begin{aligned} &\leq \left| \int_{\mu} \int_{\eta} |\mu - \eta|^2 |h_t(\eta)| (|b_t(\eta)| + |a_t(\eta)|) d\eta \bar{a}_t(\mu) h_t(\mu) d\mu \right| \\ &\leq 2 \|h_t\|_{L^2}^2 \int (1 + |\mu|^2)^2 [|a_t(\mu)| + |b_t(\mu)|]^2 d\mu, \end{aligned} \tag{39}$$

while, thanks to (34), the term involving I_2 is estimated by

$$\begin{aligned} |\langle I_2, h \rangle| &\leq C \|\phi'''\|_{L^\infty} \left| \int_{\mu} \int_{\eta} |\mu - \eta|^3 |a_t(\eta)|^2 d\eta \bar{a}_t(\mu) h(\mu, t) d\mu \right| \\ &\leq C \|\phi'''\|_{L^\infty} \left(\left(\int d\eta |\eta|^3 |a_t(\eta)|^2 \right) \|a_t\|_{L^2} \|h_t\|_{L^2} \right. \\ &\quad \left. + 3 \left(\int d\eta |\eta|^2 |a_t(\eta)|^2 \right)^{3/2} \|h_t\|_{L^2} + 3 \left(\int d\mu |\mu|^4 |a_t(\mu)|^2 \right)^{1/2} \right. \\ &\quad \left. \times \left(\int d\eta |\eta| |a_t(\eta)|^2 \right) \|h_t\|_{L^2} + \left(\int d\mu |\mu|^6 |a_t(\mu)|^2 \right)^{1/2} \|a_t\|_{L^2}^2 \|h_t\|_{L^2} \right). \end{aligned} \tag{40}$$

One should observe here that $\int d\eta |\eta| |a_t(\eta)|^2 \leq (\int d\eta (1 + |\eta|^2) |a_t(\eta)|^2)$.

Finally, due to (35), the term involving $R_U(\mu, t)$ is controlled as follows:

$$\begin{aligned} &|\langle R_U(\cdot, t) a_t, h_t \rangle| \\ &\leq C \sup_{\alpha: |\alpha|=3} |\nabla^\alpha U(q(t), t)| \left(\int d\mu |\mu|^3 |a_t(\mu)| |h_t(\mu)| \right) \\ &\leq C \sup_t \sup_{\alpha: |\alpha|=3} |\nabla^\alpha U(q(t), t)| \left(\int d\mu |\mu|^6 |a_t(\mu)|^2 \right)^{1/2} \|h_t\|_{L^2}. \end{aligned} \tag{41}$$

Making use of Lemma 4.2 and Eq. (70) below, one can estimate the terms of the form $\| |\cdot|^m a_t \|_{L^2} = (\int d\eta |\eta|^{2m} |a_t(\eta)|^2)^{1/2}$, for $m \leq 3$, and $\| |\cdot|^m b_t \|_{L^2} = (\int d\eta |\eta|^{2m} |b_t(\eta)|^2)^{1/2}$, for $m \leq 2$, in terms of the same quantities evaluated at time $t = 0$. Now, by summing up the previous estimates it readily follows that there are ε -independent functions $C_1(t), C_2(t)$ such that

$$\frac{d}{dt} \|h_t\|_{L^2} \leq \sqrt{\varepsilon} C_1(t) + C_2(t) \|h_t\|_{L^2}. \tag{42}$$

In particular, $C_1(t), C_2(t)$ depend on the potentials ϕ and U and on the L^2 -norm of moments and derivatives of a_0 (up to the order 3). With regard to the time dependence, $C_1(t), C_2(t)$ are double exponentials $Ce^{Ce^{Ct}}$, following Lemma 4.2 and observations 4.3, 4.4.

The conclusion follows by application of the Gronwall lemma. □

4. Auxiliary Results

Observation 4.1. *Observe that under our assumptions the nonlinear Eq. (31) can be shown to have, for any $T > 0$, a unique solution in $C^1([0, T], L^2(\mathbb{R}^d))$*

(see, e.g. [6]). Therefore, it follows (see, e.g. [21]) that the corresponding time-dependent linear problem

$$\begin{aligned} \left(i\partial_t + \frac{1}{2}\Delta\right) u(\mu, t) &= \frac{1}{\varepsilon} \int (\phi(\sqrt{\varepsilon}|\mu - \eta|) - \phi(0)) |a(\eta, t)|^2 d\eta u(\mu, t) \\ &+ \frac{1}{\varepsilon} (U(q(t) + \sqrt{\varepsilon}\mu, t) - U(q(t), t) - \sqrt{\varepsilon}\nabla U(q(t), t) \cdot \mu) u(\mu, t), \quad (43) \\ u(x, 0) &= u_0(x), \quad u_0 \in L^2(\mathbb{R}^d) \quad \|u_0\|_{L^2} = 1, \end{aligned}$$

has a unique and well-defined L^2 propagator.

Lemma 4.2. (Propagation of Moments and derivatives for $a(x, t)$). *Let $a(x, t)$ be the solution of the initial value problem (31). Suppose that for some $m \in \mathbb{N}$ there exists an ε -independent constant $M_m > 0$ such that*

$$\|x^A \partial_x^B a_0\|_{L^2} \leq M_m \tag{44}$$

for all $A, B \in \mathbb{N}^d$ such that $|A| + |B| \leq m$.

If moreover $\phi \in C_b^m(\mathbb{R})$ and $U \in C^1(\mathbb{R}_t^+, C_b^m(\mathbb{R}_x^d))$, there exists a (finite) ε -independent constant C_m such that

$$\|x^A \partial_x^B a(t)\|_{L^2} \leq C_m e^{C_m e^{C_m t}} M_m, \tag{45}$$

for all $A, B \in \mathbb{N}^d$ such that $|A| + |B| \leq m$.

For $m = 1$ inequality (45) holds by assuming $\phi \in C_b^2(\mathbb{R})$ and $U \in C^1(\mathbb{R}_t^+, C_b^2(\mathbb{R}_x^d))$, while in the case $m = 0$ formula (45) becomes an equality and holds with unitary constant (for all t) by simply assuming $\phi \in C_b^0(\mathbb{R})$ and $U \in C^1(\mathbb{R}_t^+, C_b^1(\mathbb{R}_x^d))$.

Remarks. • The proof makes no use of an energy conservation argument, and this is the reason why the Lemma can be established for both signs of $\phi''(0)$.

- ϕ is the same as in Sect. 2; see there for the full assumptions.

Proof. Denote

$$\psi^{A,B}(x, t) = x^B \partial_x^A a(x, t), \tag{46}$$

e.g. $\psi^{0,0}(x, t) := a(x, t)$.

It is straightforward to check that

$$\begin{aligned}
 & \left(i\partial_t + \frac{1}{2}\Delta - \frac{1}{\varepsilon}V_\varepsilon(x, t) - \frac{1}{\varepsilon}U(q(t) + \sqrt{\varepsilon}x, t) \right. \\
 & \quad \left. + \frac{1}{\varepsilon}U(q(t), t) + \frac{1}{\sqrt{\varepsilon}}\nabla U(q(t), t) \cdot x \right) \psi^{A,B} \\
 &= \sum_{k=1}^d \left[\frac{B_k(B_k - 1)}{2} \psi^{A, B-2e_k} + B_k \psi^{A+e_k, B-e_k} \right] \\
 & \quad + \frac{1}{\varepsilon} \sum_{0 \leq l < A} \prod_{k=1}^d \binom{A_k}{l_k} \partial_x^{A-l} V_\varepsilon(x, t) \psi^{l,B} \\
 & \quad + \frac{1}{\varepsilon} \sum_{0 \leq l < A} \prod_{k=1}^d \binom{A_k}{l_k} \partial_x^{A-l} U(q(t) + \sqrt{\varepsilon}x, t) \psi^{l,B} \\
 & \quad - \frac{1}{\sqrt{\varepsilon}} \sum_{\substack{0 \leq l \leq A \\ |l|=1}} \prod_{k=1}^d \binom{A_k}{l_k} \partial_x^l (\nabla U(q(t), t) \cdot x) \psi^{A-l,B} \tag{47}
 \end{aligned}$$

where $B = (B_1, \dots, B_k, \dots, B_d), l = (l_1, \dots, l_k, \dots, l_d), A = (A_1, \dots, A_k, \dots, A_d)$ and $0 \leq l < A$ means that $0 \leq l_k < A_k$ for any $k = 1, 2, \dots, d$. The initial data for (47) are defined consistently by

$$\psi^{A,B}(x, 0) = x^B \partial_x^A a_0(x),$$

and in particular $\psi^{0,0}(x, 0) := a_0(x)$.

Some remarks with regard to our notation are in order; it is clear for example that if $B_k = 0$ or $B_k = 1$, then the first term on the right-hand side yields no contribution and similarly for $B_k = 0$ in the second term and $|A| = 0$ for the remaining terms, respectively.

The derivation of (47) is straightforward by induction.

Denote by $P(t, \tau)$ the propagator associated with the left-hand side of Eq. (47), which is known to be uniquely well defined in L^2 (see Observation 4.1). As a consequence, for $m = 0$, the result claimed by Lemma 4.2 follows from the existence of the propagator. We will proceed for $m \in \mathbb{N}$ by induction.

We will work with vectors including all the moments and derivatives, namely, $\vec{\Psi} = \{\psi^{A,B}\}_{A,B:|A|+|B|\leq m} \in X_m$ and

$$\|\vec{\Psi}\|_{X_m} = \sum_{0 \leq |A|+|B|\leq m} \|\psi^{A,B}\|_{L^2},$$

where $X_0 := L^2(\mathbb{R}^d)$.

For $m = 1$ we have

$$\begin{aligned}
 & \left(i\partial_t + \frac{1}{2}\Delta - \frac{1}{\varepsilon}V_\varepsilon(x, t) - \frac{1}{\varepsilon}U(q(t) + \sqrt{\varepsilon}x, t) \right. \\
 & \quad \left. + \frac{1}{\varepsilon}U(q(t), t) + \frac{1}{\sqrt{\varepsilon}}\nabla U(q(t), t) \cdot x \right) \psi^{e_j, 0}(x, t) \\
 & = \frac{1}{\varepsilon} \partial_{x_j} V_\varepsilon(x, t) \psi^{0, 0}(x, t) + \frac{1}{\varepsilon} \partial_{x_j} U(q(t) + \sqrt{\varepsilon}x, t) \psi^{0, 0}(x, t) \\
 & \quad - \frac{1}{\sqrt{\varepsilon}} \partial_{z_j} U(z, t)|_{z=q(t)} \psi^{0, 0}(x, t),
 \end{aligned} \tag{48}$$

and

$$\begin{aligned}
 & \left(i\partial_t + \frac{1}{2}\Delta - \frac{1}{\varepsilon}V_\varepsilon(x, t) - \frac{1}{\varepsilon}U(q(t) + \sqrt{\varepsilon}x, t) + \frac{1}{\varepsilon}U(q(t), t) \right. \\
 & \quad \left. + \frac{1}{\sqrt{\varepsilon}}\nabla U(q(t), t) \cdot x \right) \psi^{0, e_j}(x, t) = \psi^{e_j, 0}(x, t)
 \end{aligned} \tag{49}$$

By virtue of the Duhamel formula we get

$$\begin{aligned}
 \psi^{e_j, 0}(x, t) & = P(t, 0)\psi^{e_j, 0}(x, 0) + \int_0^t d\tau P(t, \tau) \left[\frac{1}{\varepsilon} \partial_{x_j} V_\varepsilon(x, \tau) \psi^{0, 0}(x, \tau) \right] \\
 & \quad + \int_0^t d\tau P(t, \tau) \left[\frac{1}{\varepsilon} \partial_{x_j} U(q(\tau) + \sqrt{\varepsilon}x, \tau) \psi^{0, 0}(x, \tau) \right. \\
 & \quad \left. - \frac{1}{\sqrt{\varepsilon}} \partial_{z_j} U(q(\tau), \tau) \psi^{0, 0}(x, \tau) \right]
 \end{aligned} \tag{50}$$

and

$$\psi^{0, e_j}(x, t) = P(t, 0)\psi^{0, e_j}(x, 0) + \int_0^t d\tau P(t, \tau) [\psi^{e_j, 0}(x, \tau)]. \tag{51}$$

Then, by recalling that $P(t, \tau)$ is L^2 -norm preserving, we find

$$\begin{aligned}
 \|\psi^{e_j, 0}(t)\|_{L^2} & \leq \|\psi^{e_j, 0}(0)\|_{L^2} + \int_0^t d\tau \left\| \frac{1}{\varepsilon} \partial_{x_j} V_\varepsilon(x, \tau) \psi^{0, 0}(\tau) \right\|_{L^2} \\
 & \quad + \int_0^t d\tau \left\| \left(\frac{1}{\varepsilon} \partial_{x_j} U(q(\tau) + \sqrt{\varepsilon}x, \tau) - \frac{1}{\sqrt{\varepsilon}} \partial_{z_j} U(q(\tau), \tau) \right) \psi^{0, 0}(\tau) \right\|_{L^2}
 \end{aligned} \tag{52}$$

and

$$\|\psi^{0, e_j}(t)\|_{L^2} \leq \|\psi^{0, e_j}(0)\|_{L^2} + \int_0^t d\tau \|\psi^{e_j, 0}(\tau)\|_{L^2}. \tag{53}$$

Now, taking into account the terms involving U in (52), we get

$$\begin{aligned} & \frac{1}{\varepsilon} \partial_{x_j} U(q(\tau) + \sqrt{\varepsilon}x, \tau) - \frac{1}{\sqrt{\varepsilon}} \partial_{z_j} U(q(\tau), \tau) \\ &= \frac{1}{\sqrt{\varepsilon}} \partial_{z_j} U(z, \tau)|_{z=q(\tau)+\sqrt{\varepsilon}x} - \frac{1}{\sqrt{\varepsilon}} \partial_{z_j} U(z, \tau)|_{z=q(\tau)} \\ &= \left[\partial_{z_j}^2 U(z, \tau)|_{z=q(\tau)+\sqrt{\delta}x} \right] x_j, \quad \text{for some } \delta \in (0, \varepsilon); \end{aligned} \tag{54}$$

therefore,

$$\begin{aligned} & \left\| \left(\frac{1}{\varepsilon} \partial_{x_j} U(q(\tau) + \sqrt{\varepsilon}x, \tau) - \frac{1}{\sqrt{\varepsilon}} \partial_{z_j} U(q(\tau), \tau) \right) \psi^{0,0}(\tau) \right\|_{L^2} \\ &= \left\| \left[\partial_{z_j}^2 U(z, \tau)|_{z=q(\tau)+\sqrt{\delta}x} \right] x_j \psi^{0,0}(\tau) \right\|_{L^2} \\ &= \left\| \left[\partial_{z_j}^2 U(z, \tau)|_{z=q(\tau)+\sqrt{\delta}x} \right] \psi^{0,e_j}(\tau) \right\|_{L^2} \\ &\leq \sup_{\tau \in [0,t]} \|\partial^2 U(\cdot, \tau)\|_{L^\infty} \|\psi^{0,e_j}(\tau)\|_{L^2}. \end{aligned} \tag{55}$$

On the other side, with regard to the term involving V_ε in (52), we have

$$\begin{aligned} & \left| \frac{1}{\varepsilon} \partial_{x_j} V_\varepsilon(x, \tau) \right| = \left| \int d\eta \partial_{x_j} \frac{1}{\varepsilon} \phi(\sqrt{\varepsilon}|x - \eta|) |\psi^{0,0}(\eta, \tau)|^2 \right| \\ &\leq \int d\eta \left| \frac{\phi'(\sqrt{\varepsilon}|x - \eta|)}{\sqrt{\varepsilon}} \right| |\psi^{0,0}(\eta, \tau)|^2 \leq L \int d\eta |x - \eta| |\psi^{0,0}(\eta, \tau)|^2, \end{aligned} \tag{56}$$

where L is the global Lipschitz constant of ϕ' (the L^∞ -norm of ϕ'') that is known to be finite since $\phi \in C_b^2(\mathbb{R}^d)$.

Here and henceforth, in order to simplify the notation, we will use freely the conventions $\psi^{\alpha,\beta} := \psi^{\alpha,\beta}(\tau)$ and $\psi_\tau^{\alpha,\beta}(x) := \psi^{\alpha,\beta}(x, \tau)$, for any α, β .

Then, by (56) we get that

$$\begin{aligned} & \left\| \frac{1}{\varepsilon} \partial_{x_j} V_\varepsilon(x, \tau) \psi_\tau^{0,0} \right\|_{L^2}^2 \\ &\leq L^2 \int dx \int d\eta |x - \eta| |\psi_\tau^{0,0}(\eta)|^2 \int d\eta' |x - \eta'| |\psi_\tau^{0,0}(\eta')|^2 |\psi_\tau^{0,0}(x)|^2 \\ &\leq L^2 \int |x|^2 |\psi_\tau^{0,0}(x)|^2 dx + 3L^2 \left(\int |\eta| |\psi_\tau^{0,0}(\eta)|^2 d\eta \right)^2 \\ &\leq L^2 \| |x| \psi_\tau^{0,0} \|_{L^2}^2 + 3L^2 \| |x| \psi_\tau^{0,0} \|_{L^2}^2, \end{aligned} \tag{57}$$

where we made use of the fact that $\|\psi_\tau^{0,0}\|_{L^2} = \|\psi_0^{0,0}\|_{L^2} = \|a_0\|_{L^2} = 1$, for any time τ .

At this point we observe that

$$\| |x| \psi_\tau^{0,0} \|_{L^2}^2 = \| |x| a(\tau) \|_{L^2}^2 = \sum_j \|\psi^{0,e_j}(\tau)\|_{L^2}^2.$$

Therefore, we have just proven that there exists a constant $C > 0$ depending only on the L^∞ -norm of the second derivative of ϕ , such that

$$\left\| \frac{1}{\varepsilon} \partial_{x_j} V_\varepsilon(x, \tau) \psi^{0,0}(\tau) \right\|_{L^2} \leq C \sqrt{\sum_j \|\psi^{0,e_j}(\tau)\|_{L^2}^2} = \|\psi^{0,1}(\tau)\|_{L^2}. \tag{58}$$

Now, by using (55) and (58) in (52), we obtain

$$\|\psi^{e_j,0}(t)\|_{L^2} \leq \|\psi^{e_j,0}(0)\|_{L^2} + C \int_0^t d\tau \|\psi^{0,1}(\tau)\|_{L^2} + C \int_0^t d\tau \|\psi^{0,e_j}(\tau)\|_{L^2}, \tag{59}$$

where C is not the same constant of formula (58)—we denoted it by the same symbol just for the sake of simplicity.

Now by summing Eqs. (59) and (53) over $j = 1, \dots, d$, we get

$$\|\vec{\Psi}(t)\|_{X_1} \leq \|\vec{\Psi}(0)\|_{X_1} + C \int_0^t d\tau \|\vec{\Psi}(\tau)\|_{X_1}. \tag{60}$$

The conclusion follows by applying the Gronwall lemma, i.e.

$$\|\vec{\Psi}(t)\|_{X_1} \leq \|\vec{\Psi}(0)\|_{X_1} e^{Ct} \leq M_1 e^{Ct}, \tag{61}$$

where M_1 has been defined in (44).

For $m \geq 2$, the previous inductive step from $m = 1$ applies almost verbatim: first, by virtue of the Duhamel formula, we write the solution of Eq. (47) by using the propagator $P(t, \tau)$ associated with the time evolution on the left-hand side. Then, by using the L^2 -control on $P(t, \tau)$, it only remains to show that the “source terms” appearing on the right-hand side of (47) are bounded—uniformly in ε —in terms of $\|\psi^{A,B}\|_{L^2}$ or $\|\vec{\Psi}\|_{X_m}$. The way to do that is by using $\|\psi^{A,B}\|_{L^2}, |A| + |B| < m$ as constants now.

For example, let us look at the term involving the potential V_ε on the right-hand side of (47), i.e.

$$\begin{aligned} & \frac{1}{\varepsilon} \sum_{0 \leq l < A} \prod_{k=1}^d \binom{A_k}{l_k} \partial_x^{A-l} V_\varepsilon(x, t) \psi^{l,B}(x, t) \\ &= \frac{1}{\varepsilon} \sum_{\substack{0 \leq l < A \\ |A-l|=1}} \prod_{k=1}^d \binom{A_k}{l_k} \partial_x^{A-l} V_\varepsilon(x, t) \psi^{l,B}(x, t) \\ &+ \frac{1}{\varepsilon} \sum_{\substack{0 \leq l < A \\ |A-l|>1}} \prod_{k=1}^d \binom{A_k}{l_k} \partial_x^{A-l} V_\varepsilon(x, t) \psi^{l,B}(x, t). \end{aligned} \tag{62}$$

The estimation for any of the terms in the last sum reads

$$\begin{aligned}
 & \left\| \partial_x^{A-l} \int \frac{1}{\varepsilon} \phi(\sqrt{\varepsilon}|x-\eta|) |\psi^{0,0}(\eta, t)|^2 d\eta \psi^{l,B}(x, t) \right\|_{L^2}^2 \\
 & \leq \left(\varepsilon^{\frac{|A-l|-2}{2}} \|\phi^{(A-l)}\|_{L^\infty} \right)^2 \left\| \int |x-\eta| |\psi^{0,0}(\eta, t)|^2 d\eta \psi^{l,B}(x, t) \right\|_{L^2}^2 \\
 & \leq 2D \|\eta|\psi_t^{0,0}\|_{L^2} \|\psi_t^{l,B}\|_{L^2} \|x|\psi_t^{l,B}\|_{L^2} + D \|\eta|\psi_t^{0,0}\|_{L^2} \|\psi_t^{l,B}\|_{L^2}^2 \\
 & \quad + D \|x|\psi_t^{l,B}\|_{L^2}^2 \\
 & = 2D \|\psi_t^{0,1}\|_{L^2} \|\psi_t^{l,B}\|_{L^2} \|\psi_t^{l,B+1}\|_{L^2} + D \|\psi_t^{0,1}\|_{L^2}^2 \|\psi_t^{l,B}\|_{L^2}^2 \\
 & \quad + D \|\psi_t^{l,B+1}\|_{L^2}^2, \tag{63}
 \end{aligned}$$

where D is a constant only depending on $\|\phi^{(A-l)}(x)\|_{L^\infty}$ (that is finite under our assumptions since $A-l \leq m$). Furthermore, it is clear that, by construction, we are guaranteed that the exponent $\frac{|A-l|-2}{2}$ for ε is non negative.

On the other side, the estimate for any of the terms in the first sum on the right-hand side of (62) is given by

$$\begin{aligned}
 & \|\partial_x^{A-l} \int \frac{1}{\varepsilon} \phi(\sqrt{\varepsilon}|x-\eta|) |\psi^{0,0}(\eta, t)|^2 d\eta \psi^{l,B}(x, t)\|_{L^2}^2 \\
 & \leq L \|\int |x-\eta| |\psi^{0,0}(\eta, t)|^2 d\eta \psi^{l,B}(x, t)\|_{L^2}^2 \\
 & \leq 2L \|\eta|\psi_t^{0,0}\|_{L^2} \|\psi_t^{l,B}\|_{L^2} \|x|\psi_t^{l,B}\|_{L^2} + L \|\eta|\psi_t^{0,0}\|_{L^2} \|\psi_t^{l,B}\|_{L^2}^2 \\
 & \quad + L \|x|\psi_t^{l,B}\|_{L^2}^2 \\
 & = 2L \|\psi_t^{0,1}\|_{L^2} \|\psi_t^{l,B}\|_{L^2} \|\psi_t^{l,B+1}\|_{L^2} + L \|\psi_t^{0,1}\|_{L^2}^2 \|\psi_t^{l,B}\|_{L^2}^2 \\
 & \quad + L \|\psi_t^{l,B+1}\|_{L^2}^2, \tag{64}
 \end{aligned}$$

where L is the global Lipschitz constant of ϕ' (see (56)), which is guaranteed to be finite since $\phi \in C_b^m(\mathbb{R}^d)$, with $m \geq 2$.

Now, by virtue of the estimate we proved for $m=1$ (see (60)), from (63) and (64) we find that

$$\begin{aligned}
 & \|\partial_x^{A-l} \int \frac{1}{\varepsilon} \phi(\sqrt{\varepsilon}|x-\eta|) |\psi^{0,0}(\eta, t)|^2 d\eta \psi^{l,B}(x, t)\|_{L^2}^2 \\
 & \leq KM_1 e^{Ct} \|\psi^{l,B}(t)\|_{L^2} \|\psi^{l,B+1}(t)\|_{L^2} + KM_1 e^{Ct} \|\psi^{l,B}(t)\|_{L^2}^2 \\
 & \quad + K \|\psi^{l,B+1}(t)\|_{L^2}^2, \tag{65}
 \end{aligned}$$

where $K = \max\{D, L\}$ and we recall that $|l| + |B| \leq |A| - 1 + |B| \leq m - 1$ and $|l| + |B| + 1 \leq |A| - 1 + |B| + 1 \leq m$. Thus,

$$\begin{aligned}
 & \|\partial_x^{A-l} \int \frac{1}{\varepsilon} \phi(\sqrt{\varepsilon}|x-\eta|) |\psi^{0,0}(\eta, t)|^2 d\eta \psi^{l,B}(x, t)\|_{L^2}^2 \\
 & \leq K(M_1 e^{Ct} + 1) \|\vec{\Psi}(t)\|_{X_m}^2. \tag{66}
 \end{aligned}$$

Concerning the terms involving the potential U on the right-hand side of (47), the idea is quite similar. In fact, we observe that

$$\begin{aligned}
 & \frac{1}{\varepsilon} \sum_{0 \leq l < A} \prod_{k=1}^d \binom{A_k}{l_k} \partial_x^{A-l} U(q(t) + \sqrt{\varepsilon}x, t) \psi^{l,B}(x, t) \\
 & \quad - \frac{1}{\sqrt{\varepsilon}} \sum_{\substack{0 \leq l \leq A, \\ |l|=1}} \prod_{k=1}^d \binom{A_k}{l_k} \partial_x^l (\nabla U(q(t), t) \cdot x) \psi^{A-l,B}(x, t) \\
 & = \sum_{\substack{0 \leq l \leq A, \\ |l|=1}} C_{A,l,B} \left(\frac{1}{\varepsilon} \partial_x U(q(t) + \sqrt{\varepsilon}x, t) \psi^{A-l,B}(x, t) \right. \\
 & \quad \left. - \frac{1}{\sqrt{\varepsilon}} \partial_x (\nabla U(q(t), t) \cdot x) \psi^{A-l,B}(x, t) \right) \\
 & \quad + \frac{1}{\varepsilon} \sum_{\substack{0 \leq l < A, \\ |A-l| > 1}} \prod_{k=1}^d \binom{A_k}{l_k} \partial_x^{A-l} U(q(t) + \sqrt{\varepsilon}x, t) \psi^{l,B}(x, t), \tag{67}
 \end{aligned}$$

where we made a discrete change of variable $l \mapsto A - l$ in the first term of the left-hand side.

Now, with regard to first term of the right-hand side, the estimation that has to be used is exactly the one we did in (55); thus one finds, $\forall l : |l| = 1$

$$\begin{aligned}
 & \left\| \frac{1}{\varepsilon} \partial_x U(q(t) + \sqrt{\varepsilon}x, t) \psi^{A-l,B}(t) - \frac{1}{\sqrt{\varepsilon}} \partial_x (\nabla U(q(t), t) \cdot x) \psi^{A-l,B}(t) \right\|_{L^2} \\
 & \leq \sup_t \|\partial^2 U(\cdot, t)\|_{L^\infty} \|\psi^{A,B}(t)\|_{L^2} \leq \sup_t \|\partial^2 U(\cdot, t)\|_{L^\infty} \|\vec{\Psi}(t)\|_{X_m} \tag{68}
 \end{aligned}$$

(the adjustment for $l = 0$ is obvious).

Now, for the last term in (67) we have

$$\begin{aligned}
 & \left\| \frac{1}{\varepsilon} \partial_x^{A-l} U(q(t) + \sqrt{\varepsilon}x, t) \psi^{l,B}(x, t) \right\|_{L^2} \\
 & \leq \varepsilon^{\frac{|A-l|-2}{2}} \sup_t \|\partial^{(A-l)} U(\cdot, t)\|_{L^\infty} \|\psi^{l,B}(t)\|_{L^2} \\
 & \leq \sup_t \|\partial^{(m)} U(\cdot, t)\|_{L^\infty} \|\vec{\Psi}(t)\|_{X_m}, \tag{69}
 \end{aligned}$$

where we used that $A - l \leq A \leq m, |A - l| - 2 \geq 0$ and $l + B < A + B \leq m$.

Similar (simpler, in fact) estimates can be shown for the other terms on the right-hand side of (47). □

Observation 4.3 (Propagation of moments and derivatives for $\beta_t(x)$). $\beta_t(x)$ was defined in Eqs. (12), (13). Under the assumptions of Lemma 4.2, regularity estimates for $\beta_t(x)$ analogous to Lemma 4.2 for $a(x, t)$ hold, i.e. for any $t > 0$

$$\|x^B \partial_x^A \beta_t\|_{L^2} \leq C_m(t) \sum_{|A'|+|B'| \leq m} \|x^{B'} \partial_x^{A'} a_0\|_{L^2}, \quad \forall A, B \in \mathbb{N}^d : |A| + |B| \leq m.$$

Remarks • The proof is in fact simpler than the one of Lemma 4.2. It can easily be checked that, due to the fact that we have to deal with harmonic potentials, the terms that arise from the differentiation of the potentials turn to be exactly of the form $x\beta_t(x)$.

- As a consequence of Observation 4.3, there exists a ε -independent constant $C > 0$ depending on the L^∞ -norm of the second x -derivative of $U(x, t)$ and on $|\phi''(0)|$, such that

$$\int dx |x|^2 |\beta_t(x)|^2 < \left(\int dx |x|^2 |a_0(x)|^2 \right) e^{Ct} < \infty, \quad \forall t.$$

We remind that this is exactly what we need to make the proof of Theorem 2.1 work successfully (see (23)).

Observation 4.4 (Propagation of Moments and derivatives for $b_t(x)$). *Although apparently $b_t(x)$ solves a nonlinear equation, it can be obtained as the solution of a linear Schrödinger equation with an harmonic potential whose coefficients are determined by the L^2 -norm of the first moment of $\beta_t(x)$, by $\phi''(0)$ and $H(U)$ (see (25) and Lemma 3.1).*

Therefore, as a consequence of Observation 4.3, it follows that, as long as $U \in C^1(\mathbb{R}_t^+, C_b^m(\mathbb{R}_x^d))$ and $\phi''(0)$ is finite, we can get a result for $b_t(x)$, e.g. analogous to Lemma 4.2 for $a(x, t)$, i.e.

$$x^B \partial_x^A b_t \in L^2, \quad \forall A, B \in \mathbb{N}^d : |A| + |B| \leq m \quad \forall t,$$

under the same assumption (44) on the (common) initial datum $a_0(x)$.

In particular, there is a bound $C(t) < \infty$, independent of ε , such that

$$\int dx |x|^{2m} |b_t(x)|^2 < C(t), \quad \forall t, \quad m \leq 3. \tag{70}$$

We observe that (70), for $m = 2$, is exactly what we need to make the proof of Theorem 2.1 work successfully (see (39), (40) and (41)).

5. Higher Order Approximations

On the basis of the above results, it seems natural to ask whether it is possible to go beyond the $\sqrt{\varepsilon}$ -approximation discussed previously (see (11)) and to find higher order corrections $a_t^{(k)}(\mu)$ to the amplitude $a_t^{(0)}(\mu) := b_t(\mu)$ so that the right-hand side of (11) is of size ε^m for arbitrarily large m , as this is the case for the linear Schrödinger equation [17, 18]. Although we will not present all the (tedious) details of the construction, we claim that one can determine a semiclassical expansion

$$a_t^\varepsilon(\mu) = a_t^{(0)}(\mu) + \sqrt{\varepsilon} a_t^{(1)}(\mu) + \varepsilon a_t^{(2)}(\mu) + \dots + \varepsilon^{k/2} a_t^{(k)}(\mu) + \dots, \tag{71}$$

with

$$a_0^{(k)}(\mu) = \delta_{k,0} a_0(\mu), \tag{72}$$

such that

$$\Psi^\varepsilon(x, t) = e^{i\frac{L(t)}{\varepsilon} + i\gamma(t)} \psi_{q(t)p(t)}^{\beta_t} + O(\varepsilon^\infty).$$

In order to determine the equations governing the evolution for each coefficient $a_t^{(k)}(\mu)$ we need to look at the expansion for the potential terms appearing in (31). With regard to the nonlinear part involving the pair interaction ϕ , we get

$$\begin{aligned} \frac{1}{\varepsilon} (\phi(\sqrt{\varepsilon}|\mu - \eta|) - \phi(0)) &= \frac{|\mu - \eta|}{\sqrt{\varepsilon}} \phi'(0) + \frac{|\mu - \eta|^2}{2} \phi''(0) + \frac{\sqrt{\varepsilon}|\mu - \eta|^3}{3!} \phi'''(0) \\ &+ \dots + \frac{(\sqrt{\varepsilon})^k |\mu - \eta|^k}{k!} \phi^{(k)}(0) + \dots \end{aligned} \tag{73}$$

In Theorem 2.1 we were assuming $\phi \in C_b^3(\mathbb{R})$. Clearly, if we want to go to higher orders in the approximation we need more smoothness on ϕ and on the external potential U . Therefore, here and henceforth we assume

$$\phi \in C_b^\infty(\mathbb{R}), \text{ and } \phi \text{ even} \tag{74}$$

so that we have

$$\begin{aligned} \frac{1}{\varepsilon} (\phi(\sqrt{\varepsilon}|\mu - \eta|) - \phi(0)) \\ = \frac{|\mu - \eta|^2}{2} \phi''(0) + \dots + (\sqrt{\varepsilon})^{2n-1} \frac{|\mu - \eta|^{2n}}{(2n)!} \phi^{(2n)}(0) + \dots \quad n \geq 2 \end{aligned} \tag{75}$$

Observation 5.1. *Assumption (74) is actually too strong if one wants to deal with an approximation up to a certain order k .*

With regard to the linear terms in (31) involving the external potential U , we get

$$\begin{aligned} \frac{1}{\varepsilon} (U(q(t) + \sqrt{\varepsilon}\mu, t) - U(q(t), t) - \sqrt{\varepsilon}\nabla U(q(t), t) \cdot \mu) \\ = \left\langle \mu, \frac{H(U(q(t), t))}{2} \mu \right\rangle + \dots + (\sqrt{\varepsilon})^{n-1} \frac{\nabla^n U(q(t), t)}{n!} \cdot \mu^n + \dots \end{aligned} \tag{76}$$

where of course $n \geq 3$. Here we are using the notation

$$\nabla^n U \cdot \mu^n = \sum_{\substack{\alpha_1 \dots \alpha_d: \\ \sum \alpha_i = n}} \frac{\partial^n U}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}} \mu^{\alpha_1} \dots \mu^{\alpha_d}. \tag{77}$$

Analogously to what we observed for the pair-interaction ϕ , we need more smoothness for U , so that here and henceforth we require

$$U \in C^1(\mathbb{R}_t^+, C_b^\infty(\mathbb{R}_x^d)). \tag{78}$$

Now, inserting (71), (75) and (76) in (31) we readily arrive to a sequence of problems for the coefficients $a_t^{(k)}(\mu)$ of the expansion (71). For $k = 0$ we obviously find

$$\begin{cases} \left(i\partial_t + \frac{\Delta_\mu}{2} + \frac{\phi''(0)}{2} \int d\eta |\mu - \eta|^2 |a_t^{(0)}(\eta)|^2 + \left\langle \mu, \frac{H(U(q(t), t))}{2} \mu \right\rangle \right) \\ a_t^{(0)}(\mu) = 0, \\ a_0^{(0)}(\mu) = a_0^\varepsilon(\mu), \end{cases} \tag{79}$$

namely, the initial value problem that we had for $b_t(\mu)$ in the previous sections (see (15)). Then, for $k = 1$, we find

$$\begin{cases} \left(i\partial_t + \frac{\Delta_\mu}{2} + \frac{\phi''(0)}{2} \int d\eta |\mu - \eta|^2 |a_t^{(0)}(\eta)|^2 + \left\langle \mu, \frac{H(U(q(t),t),t)}{2} \mu \right\rangle \right) a_t^{(1)}(\mu) \\ = \frac{\phi''(0)}{2} \left(\int d\eta |\mu - \eta|^2 2\Re[\bar{a}_t^{(0)}(\eta)a_t^{(1)}(\eta)] \right) a_t^{(0)}(\mu) + \frac{\nabla^3 U(q(t),t)}{3!} \cdot \mu^3 a_t^{(0)}(\mu), \\ a_0^{(1)}(\mu) = 0. \end{cases} \tag{80}$$

This is a linear initial value problem where the left-hand side is known to have a unique well-defined L^2 -propagator $P^{(0)}(t)$ due to the existence and uniqueness in L^2 of the solution $a_t^{(0)}(\mu)$ of the zero-order initial value problem (79) and to the L^2 -control on its first moment (see Observation 4.4 and (70)). Its well-posedness in L^2 follows by the L^2 -control on the source term $\frac{\nabla^3 U(q(t),t)}{3!} \cdot \mu^3 a_t^{(0)}(\mu)$ and on a suitable L^2 -control of the first term on the RHS of (80). Smoothness of U, ϕ and the L^2 -control on $\mu^3 a_0^{(0)}(\mu)$ are sufficient for that by Observation 4.4. In particular, for the first term on the RHS of (80) we have

$$\begin{aligned} & \left\| \frac{\phi''(0)}{2} \left(\int d\eta |\mu - \eta|^2 2\Re[\bar{a}_t^{(0)}(\eta)a_t^{(1)}(\eta)] \right) a_t^{(0)}(\mu) \right\|_{L^2}^2 \\ &= \left(\frac{\phi''(0)}{2} \right)^2 \int d\mu \int d\eta |\mu - \eta|^2 \bar{a}_t^{(0)}(\eta) a_t^{(1)}(\eta) \\ & \quad \times \int d\eta' |\mu - \eta'|^2 \bar{a}_t^{(0)}(\eta') a_t^{(1)}(\eta') |a_t^{(0)}(\mu)|^2 \\ & \quad + \left(\frac{\phi''(0)}{2} \right)^2 \int d\mu \int d\eta |\mu - \eta|^2 a_t^{(0)}(\eta) \bar{a}_t^{(1)}(\eta) \\ & \quad \times \int d\eta' |\mu - \eta'|^2 a_t^{(0)}(\eta') \bar{a}_t^{(1)}(\eta') |a_t^{(0)}(\mu)|^2 \\ & \leq C_{a_t^{(0)}} \left\| a_t^{(1)} \right\|_{L^2}^2, \end{aligned} \tag{81}$$

where $C_{a_t^{(0)}} > 0$ is a constant that depends on the moments of $a_t^{(0)}(\mu)$ up to order 3. By virtue of (81) and the L^2 -control on the term involving U in (80), the Duhamel formula and the Gronwall lemma allow one to conclude that

$$a_t^{(1)} \in L^2(\mathbb{R}^d), \quad \forall t. \tag{82}$$

Moreover, following along same lines as before (see Lemma 4.2, Observation 4.4 and subsequent remarks), it can be easily checked that, by assuming enough regularity for the initial datum $a_0^{(0)}(\mu) = a_0(\mu)$, one can control the derivatives and moments of $a_t^{(1)}(\mu)$ up to any fixed order m , i.e.

$$x^B \partial_x^A a_t^{(1)} \in L^2(\mathbb{R}^d), \quad \forall t, \quad \forall A, B \in \mathbb{N}^d : |A| + |B| \leq m. \tag{83}$$

This will be crucial to go on with the higher order dynamics because, for example, the equation for the second coefficient $a_t^{(2)}(\mu)$ is

$$\begin{cases} \left(i\partial_t + \frac{\Delta_\mu}{2} + \frac{\phi''(0)}{2} \int d\eta |\mu - \eta|^2 |a_t^{(0)}(\eta)|^2 + \left\langle \mu, \frac{H(U(q(t),t),t)}{2} \mu \right\rangle \right) a_t^{(2)}(\mu) \\ = \frac{\phi''(0)}{2} \left(\int d\eta |\mu - \eta|^2 2\Re[\bar{a}_t^{(0)}(\eta) a_t^{(2)}(\eta)] \right) a_t^{(0)}(\mu) + \frac{\nabla^4 U(q(t),t)}{4!} \cdot \mu^4 a_t^{(0)}(\mu) \\ + \frac{\phi^{(4)}(0)}{4!} \left(\int d\eta |\mu - \eta|^4 |a_t^{(0)}(\eta)|^2 \right) a_t^{(0)}(\mu) + \frac{\phi''(0)}{2} \left(\int d\eta |\mu - \eta|^2 |a_t^{(1)}(\eta)|^2 \right) \\ \times a_t^{(0)}(\mu) \\ + \frac{\phi''(0)}{2} \left(\int d\eta |\mu - \eta|^2 2\Re[\bar{a}_t^{(0)}(\eta) a_t^{(1)}(\eta)] \right) a_t^{(1)}(\mu) + \frac{\nabla^3 U(q(t),t)}{3!} \cdot \mu^3 a_t^{(1)}(\mu). \\ a_0^{(2)}(\mu) = 0, \end{cases} \tag{84}$$

So, again, as for the case $k = 1$, we obtained a linear initial value problem where the propagator associated with the left-hand side is $P^{(0)}(t)$ that is known to be well-defined in L^2 . Then, as before, the solution $a_t^{(2)}(\mu)$ can be written through the Duhamel formula, applying the propagator $P^{(0)}(t)$ to the term $\frac{\phi''(0)}{2} \left(\int d\eta |\mu - \eta|^2 2\Re[\bar{a}_t^{(0)}(\eta) a_t^{(2)}(\eta)] \right) a_t^{(0)}(\mu)$ and to the various source terms in (84). The term which is linear in $a_t^{(2)}(\mu)$ is estimated as in (81) while the source terms are controlled in L^2 by virtue of the control on moments and derivatives of $a_t^{(0)}(\mu)$ and $a_t^{(1)}(\mu)$. To the end, by using the Gronwall lemma, we get

$$a_t^{(2)} \in L^2(\mathbb{R}^d), \quad \forall t. \tag{85}$$

and, moreover, by assuming a sufficiently high number of moments and derivatives of the (zero-order) “full” initial datum $a_0^{(0)}(\mu) = a_0(\mu)$ to be controlled in L^2 , we can control as well the derivatives and moments of $a_t^{(2)}(\mu)$ up to any fixed order m , i.e.

$$x^B \partial_x^A a_t^{(2)} \in L^2(\mathbb{R}^d), \quad \forall t, \quad \forall A, B \in \mathbb{N}^d : |A| + |B| \leq m. \tag{86}$$

At this point it is clear how to proceed in general. The equation for $a_t^{(k)}(\mu)$ is a linear Schrödinger equation with a source term involving the coefficients $a_t^{(n)}(\mu)$ with $n < k$, which have been estimated by the previous steps. The L^2 -control of $a_t^{(k)}(\mu)$ follows by the L^2 -control on a sufficiently high number of moments and derivatives of $a_t^{(n)}(\mu)$ with $n < k$.

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