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Semiclassical wave packets for weakly nonlinear Schrödinger equations with rotation

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Abstract. We consider semiclassically scaled, weakly nonlinear Schrödinger equations with external confining potentials and additional angular-momentum rotation term. This type of model arises in the Gross–Pitaevskii theory of trapped, rotating quantum gases. We construct asymptotic solutions in the form of semiclassical wave packets, which are concentrated in both space and in frequency around an classical Hamiltonian phase-space flow. The rotation term is thereby seen to alter this flow, but not the corresponding classical action.

1. Introduction

Semiclassical wave packets are a well-known tool in the approximate description of quantum mechanics as $\varepsilon \simeq \hbar \to 0$. The latter represents a singular limiting regime which leads to highly oscillatory solutions in the corresponding Schrödinger dynamics, cf. [5] for a general introduction. In an attempt to overcome this issue, one seeks a representation for the exact quantum mechanical wave function ψ^ε via

$$\psi^\varepsilon(t,x) \underset{\varepsilon\to 0}{\sim} \varepsilon^{-d/4} v\Big(t, \frac{x-q(t)}{\sqrt{\varepsilon}}\Big) e^{i(S(t)+p(t)\cdot(x-q(t)))/\varepsilon}, \quad x \in \mathbb{R}^d. \tag{1.1}$$

Here, $q(t) \in \mathbb{R}^d$ and $p(t) \in \mathbb{R}^d$ denote the mean position and momentum at time $t \in \mathbb{R}$, whereas $S(t) \in \mathbb{R}$ is a purely time-dependent phase proportional to the classical action. Finally, the amplitude function $v(t,y) \in \mathbb{C}$ describes slowly varying changes due to dispersive effects within the dynamics. The right hand side of (1.1) corresponds to a wave function which is well-localized (at scale $\sqrt{\varepsilon}$) both in space and in frequency (or momentum). In particular, for wave functions of the form (1.1) the following three quantities

$$\|\psi^\varepsilon(t)\|_{L^2(\mathbb{R}^d)}, \quad \left\|\Big(\sqrt{\varepsilon}\nabla - i\frac{p(t)}{\sqrt{\varepsilon}}\Big)\psi^\varepsilon(t)\right\|_{L^2(\mathbb{R}^d)}, \quad \text{and} \quad \left\|\frac{x-q(t)}{\sqrt{\varepsilon}}\psi^\varepsilon(t)\right\|_{L^2(\mathbb{R}^d)}$$

are all of order $\mathcal{O}(1)$, as $\varepsilon \to 0$.

It is known that the amplitude v satisfies a homogenized, i.e., ε-independent, Schrödinger-type equation with an effective quadratic potential (see the derivation below). A popular ansatz for the solution v of this homogenized equation is that of a Gaussian function, which can be shown to be propagated exactly. In this case, wave packets of the form (1.1) comprise semiclassically scaled coherent states which minimize the Heisenberg uncertainty relation, cf. [16]. Coherent states allow to approximately describe the full quantum dynamics of ψ^ε via a system of ordinary differential equations for q, p, and the matrices

Ⓑ Birkhäuser

used to parametrize the Gaussian function v, see [10,11]. This makes this type of approximation particularly interesting for numerical simulations, where one seeks to represent general states $\psi^\varepsilon(t, \cdot) \in L^2(\mathbb{R}^d)$ by a (well chosen) superposition of such Gaussian wave packets, see [15,19] for a general overview of this topic. One should note, however, that the derivation of the aforementioned ordinary differential equations can be rather involved, in particular if the Hamiltonian operator governing the dynamics of ψ^ε has a complicated expression.

Motivated by the mean-field description of trapped rotating quantum gases, the aim of this paper is to show how to use semi-classical wave packets in the context of (weakly nonlinear) Schrödinger equations with external scalar potential and additional angular momentum rotation term. To this end, we consider the following Gross–Pitaevskii equation with rotation

$$i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V(x)\psi^\varepsilon + \lambda\varepsilon^\alpha|\psi^\varepsilon|^2\psi + \varepsilon(\Omega \cdot L)\psi^\varepsilon, \quad \psi^\varepsilon_{|t=0} = \psi^\varepsilon_0. \tag{1.2}$$

Here $(t, x) \in \mathbb{R} \times \mathbb{R}^d$ with $d = 2$ or 3, respectively, $\lambda \in \mathbb{R}$ denotes a coupling constant, which allows for both focusing and defocusing nonlinearities, and $\alpha = \alpha(d) > 0$ is a parameter used to ensure the critical strength of the nonlinearity (see below). The operator $\Omega \cdot L$ describes the rotation around a given axis $\Omega \in \mathbb{R}^d$, where

$$L = -ix \wedge \nabla,$$

is the quantum mechanical angular momentum operator. In addition, $V(x)$ denotes some external potential, for which we shall impose:

Assumption 1.1. The potential $V \in C^\infty(\mathbb{R}^d; \mathbb{R})$ is smooth and sub-quadratic, i.e.,

$$\partial_x^\alpha V \in L^\infty(\mathbb{R}^d) \quad \forall|\alpha| \geq 2.$$

A typical example, for such a potential is that of a harmonic confinement, i.e., $V(x) = \frac{1}{2}|x|^2$, which is often used to describe the electromagnetic trapping of experimental Bose-Einstein condensates.

We further assume that the initial data ψ^ε_0 is given in the form of a localized wave packet, i.e.,

$$\psi^\varepsilon_0(x) = \varepsilon^{-d/4}v_0\left(\frac{x - q_0}{\sqrt{\varepsilon}}\right)e^{i(x-q_0)\cdot p_0/\varepsilon}, \quad q_0, p_0 \in \mathbb{R}^d, \tag{1.3}$$

where $v_0 \in \Sigma^3$, but not necessarily Gaussian. Here, and in the following we shall denote the natural energy space associated with (1.2) by

$$\Sigma^k = \left\{f \in L^2(\mathbb{R}^d): \quad \|f\|_{\Sigma^k} := \sum_{|\alpha|+|\beta|\leqslant k}\|x^\alpha\partial_x^\beta f\|_{L^2(\mathbb{R}^d)} < \infty\right\}. \tag{1.4}$$

In the next two sections, we shall show how to rigorously derive the dynamical equations needed to construct an approximation of the solution to (1.2) in the form (1.1), first in the linear case $\lambda = 0$, and second in the case of a critical nonlinearity, i.e., $\lambda \neq 0$ and $\alpha = \alpha_{\mathrm{crit}}$, where

$$\alpha_{\mathrm{crit}} = \begin{cases} 2 & \text{for } d = 2, \\ \frac{5}{2} & \text{for } d = 3. \end{cases}$$

The assumption $\alpha = \alpha_{\mathrm{crit}}$ thereby ensures that nonlinear effects are present in the dynamics of the slowly varying amplitude v, while for $\alpha > \alpha_{\mathrm{crit}}$ the problem becomes effectively linearizable. Of course, $\alpha_{\mathrm{crit}} > 0$ means that the nonlinearity in (1.2) formally vanishes in the limit $\varepsilon \to 0$, which is why we call it a weakly nonlinear regime. As we shall see, the approximation in the linear case will hold up to Ehrenfest time-scales $t \sim \mathcal{O}(\ln\frac{1}{\varepsilon})$, whereas in the (weakly) nonlinear case, we will need to restrict ourselves to time-scales $t \sim \mathcal{O}(1)$. In the case $\lambda = 0$ and v_0 given by a Gaussian, we shall show how to adapt the system of ordinary differential equations governing such wave packets to the case with rotation.

2. The linear case

In this section, we shall study the case $\lambda = 0$, i.e., we consider

$$i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V(x)\psi^\varepsilon + \varepsilon(\Omega \cdot L)\psi^\varepsilon, \quad \psi^\varepsilon_{|t=0} = \psi^\varepsilon_0, \tag{2.1}$$

where ψ^ε_0 is given in the form (1.3). In order to understand how the rotation term influences the dynamics, we first notice that the linear Hamiltonian H can be seen as the ε-quantization of the following classical Hamiltonian phase-space function $H : \mathbb{R}^{2d} \to \mathbb{R}$:

$$H(x,\xi) = \frac{1}{2}|\xi|^2 + V(x) + \Omega \cdot (x \wedge \xi).$$

The corresponding Hamiltonian trajectories for a particle with position $q(t) \in \mathbb{R}^d$ and momentum $p(t) \in \mathbb{R}^d$ are therefore given by

$$\begin{cases} \dot{q} = \nabla_p H(q,p) = p + \Omega \wedge q, & q(0) = q_0, \\ \dot{p} = -\nabla_q H(q,p) = -\nabla V(q) + \Omega \wedge p, & p(0) = p_0. \end{cases} \tag{2.2}$$

Lemma 2.1. (Classical dynamics) *Let $(q_0, p_0) \in \mathbb{R}^d \times \mathbb{R}^d$ and V satisfy Assumption 1.1. Then, (2.2) has a unique global, smooth solution $(q,p) \in C^\infty(\mathbb{R}; \mathbb{R}^d)^2$, which grows at most exponentially.*

Proof. The local well-posedness of the solution can be inferred from the fact that V is smooth. From (2.2), we see that q solves the following ordinary differential equation:

$$\ddot{q} = -\nabla V(q) + 2\Omega \wedge \dot{q} - \Omega \wedge (\Omega \wedge q).$$

Multiply both sides by $\dot{q}$,

$$\frac{d}{dt}H(q,p) \equiv \frac{d}{dt}\left(\frac{1}{2}|\dot{q}|^2 - \frac{1}{2}|\Omega \wedge q|^2 + V(q)\right) = 0.$$

We can see that $|\Omega \wedge q|^2 \lesssim \langle q \rangle^2$, and $V(q) \lesssim \langle q \rangle^2$ by Assumption 1.1, so

$$\dot{q} \lesssim \langle q \rangle,$$

which shows that

$$|q(t)| \lesssim e^{c_0 t}.$$

Plugging this into (2.2) yields the same estimate for $p(t)$. $\qquad\qquad\square$

Remark 2.2. The system (2.2) has already been studied in [2] in the case of a purely harmonic, but not necessarily isotropic, confinement potential $V(x) = \sum_{j=1}^d \gamma_j x_j^2$. It is shown that in this case there are indeed initial data for which the solution grows exponentially forward or backward in time, and thus the classical dynamics is no longer trapped within a bounded phase-space region.

Next, we compute the Lagrangian $L(q,p)$ corresponding to $H(q,p)$, via

$$L(q,p) = p \cdot \dot{q} - H(q,p)$$

$$= p \cdot (p + \Omega \wedge q) - \frac{1}{2}|p|^2 - V(q) - \Omega \cdot (q \wedge p)$$

$$= \frac{1}{2}|p|^2 - V(q),$$

using the fact that $\Omega \cdot (q \wedge p) = p \cdot (\Omega \wedge q)$. One can see that $L(q,p)$ is indeed of the same form as in the case without rotation. In particular, we shall define the associated action function to be as usual, i.e.,

$$S(t) = \int_0^t \frac{1}{2}|p(s)|^2 - V(q(s))\, ds. \tag{2.3}$$

The latter will be used to determine the purely t-dependent part of the phase of our wave packets.

Remark 2.3. An alternative way to express the Hamiltonian dynamics with rotation is to introduce the canonical momentum $\pi(t) := p(t) + \Omega \wedge q(t)$, and compute

$$\begin{aligned}
\dot{\pi} &= \dot{p} + \Omega \wedge \dot{q} \\
&= -\nabla V(q) + \Omega \wedge p + \Omega \wedge \pi \\
&= -\nabla V(q) + 2\Omega \wedge \pi - \Omega \wedge (\Omega \wedge q).
\end{aligned}$$

Using this, (2.2) can be rewritten in the following form:

$$\begin{cases} \dot{q} = \pi, \\ \dot{\pi} = -\nabla V(q) + 2\Omega \wedge \pi - \Omega \wedge (\Omega \wedge q). \end{cases} \tag{2.4}$$

This system has been used to describe rotating solutions of mean-field models for self-gravitating classical particles, see [18].

Having derived the classical dynamics in the case with rotation, we can now turn to the derivation of the semiclassical approximation. To this end, we first change the unknown ψ^ε into a new function u^ε, via

$$\psi^\varepsilon(t,x) = \varepsilon^{-d/4} u^\varepsilon\Big(t, \frac{x - q(t)}{\sqrt{\varepsilon}}\Big) e^{i(S(t) + p(t)\cdot(x - q(t)))/\varepsilon}, \tag{2.5}$$

where $q(t)$ and $p(t)$ are solutions to (2.2), and $S(t)$ is defined by (2.3). Plugging this ansatz into equation (2.1) and assuming sufficient smoothness, we obtain, after some lengthy computations, that

$$\begin{aligned}
0 &= i\varepsilon\partial_t\psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon - V(x)\psi^\varepsilon - \varepsilon(\Omega \cdot L)\psi^\varepsilon \\
&= \varepsilon^{-d/4} e^{i\phi/\varepsilon}\big(\varepsilon R_1 + \varepsilon^{1/2} R_2 + R_3\big),
\end{aligned}$$

where we denote

$$\phi(t,x) = S(t) + p(t)\cdot(x - q(t)),$$

and we also find

$$\begin{aligned}
R_1 &= i\partial_t u^\epsilon + \frac{1}{2}\Delta u^\epsilon - (\Omega \cdot L)u^\epsilon, \\
R_2 &= i\nabla u^\epsilon \cdot (p - \dot{q} + \Omega \wedge q), \\
R_3 &= \Big(-\sqrt{\epsilon}y\cdot(\dot{p} - \Omega \wedge p) + p\cdot\dot{q} + V(q) - V(q + \sqrt{\epsilon}y) - |p|^2 - \Omega\cdot(q \wedge p)\Big)u^\epsilon.
\end{aligned}$$

In here, the fact that $S(t)$ is given by (2.3) is essential. Recalling that p, q are assumed to be solutions to (2.2), we see that, indeed, $R_2 \equiv 0$, whereas R_3 simplifies to

$$R_3 = u^\varepsilon\Big(\sqrt{\varepsilon}y\cdot\nabla V(q) + V(q) - V(q + \sqrt{\varepsilon}y)\Big).$$

In order for u^ε to be a solution to (2.1), we therefore have to guarantee that

$$\varepsilon R_1 + R_3 = 0,$$

which is equivalent to imposing

$$i\partial_t u^\varepsilon = -\frac{1}{2}\Delta u^\varepsilon + \mathcal{V}^\varepsilon(t,y)u^\varepsilon + (\Omega \cdot L)u^\varepsilon, \quad u^\varepsilon_{|t=0} = v_0. \tag{2.6}$$

Here, v_0 is the initial amplitude induced by (1.3), and $\mathcal{V}^\varepsilon$ is a time-dependent potential given by

$$\mathcal{V}^\varepsilon(t,y) = \frac{1}{\varepsilon}\big(V(q(t) + \sqrt{\varepsilon}y) - V(q(t)) - \sqrt{\varepsilon}y\cdot\nabla V(q(t))\big). \tag{2.7}$$

By formally passing to the limit $\varepsilon \to 0$ in this expression, we observe that

$$\mathcal{V}^\varepsilon(t,y) \underset{\varepsilon \to 0}{\sim} \frac{1}{2} y \cdot Q_V(t) y,$$

i.e., a harmonic potential with $Q_V(t) = \nabla^2 V(q(t))$, the Hessian matrix of V. Note that Assumption 1.1 implies that $Q_V \in C_b^\infty(\mathbb{R}; \mathbb{R}^{2d})$.

We therefore expect that u^ε is asymptotically close (in an appropriate norm) to v, defined to be the solution of the following, ε-independent effective amplitude equation:

$$i\partial_t v = -\frac{1}{2}\Delta v + \frac{1}{2}\big(y \cdot Q_V(t)y\big)v + (\Omega \cdot L)v, \quad v_{|t=0} = v_0. \tag{2.8}$$

We shall briefly study the existence of solutions v to this equation. The corresponding time-dependent classical Hamiltonian function

$$H(t,y,\xi) := \frac{1}{2}|\xi|^2 + \frac{1}{2}y \cdot Q_V(t)y + \Omega \cdot (y \wedge \xi) \tag{2.9}$$

is smooth and sub-quadratic in $(y,\xi) \in \mathbb{R}^{2d}$ and therefore fits within the framework of [14], where the fundamental solution of the associated Schrödinger propagator is constructed (see also the appendix).

Lemma 2.4. (from [14]) *Let $d = 2, 3$, $v_0 \in \Sigma^k$ and V satisfy Assumption 1.1. Then, for all $k \in \mathbb{N}$, equation (2.8) has a unique global solution $v \in C(\mathbb{R}, \Sigma^k)$, satisfying*

$$\|v(t,\cdot)\|_{L^2(\mathbb{R}^d)} = \|v_0\|_{L^2(\mathbb{R}^d)} \ \forall t \in \mathbb{R}.$$

In addition, there exists a $C_{k,d} > 0$, such that

$$\|v(t,\cdot)\|_{\Sigma^k} \lesssim e^{C_{k,d}\,t}.$$

We can now state the main approximation result of this section.

Proposition 2.5. (Linear wave packets with rotation) *Let $d = 2$ or 3, $v_0 \in \Sigma^3$ and V satisfy Assumption 1.1. Consider the semiclassical wave packet given by*

$$\varphi^\varepsilon(t,x) = \varepsilon^{-d/4} v\Big(t, \frac{x - q(t)}{\sqrt{\varepsilon}}\Big) e^{i(S(t) + p(t)\cdot(x-q(t)))/\varepsilon},$$

where $v \in C(\mathbb{R}, \Sigma^3)$ is a solution to (2.8), $S(t)$ is the action defined in (2.3) and $(q,p) \in C^\infty(\mathbb{R}; \mathbb{R}^d)^2$ solve the Hamiltonian equations (2.2). Then, there exists a constant $C > 0$ and independent of $\varepsilon \in (0,1]$, such that

$$\|\psi^\varepsilon(t,\cdot) - \varphi^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)} \lesssim \sqrt{\varepsilon} e^{Ct}.$$

In particular, there exists $c > 0$ independent of ε, such that, as $\varepsilon \to 0$:

$$\sup_{0 \leqslant t \leqslant c \log \frac{1}{\varepsilon}} \|\psi^\varepsilon(t,\cdot) - \varphi^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)} \longrightarrow 0.$$

Proof. The proof follows along the same as in [7]. We first notice that since V is smooth and sub-quadratic, a Taylor-expansion shows

$$|\Delta_V^\varepsilon(t,y)| = \Big|\mathcal{V}^\varepsilon(t,y) - \tfrac{1}{2}y \cdot Q_V(t)y\Big| \lesssim \sqrt{\varepsilon}|y|^3. \tag{2.10}$$

We can define the error term $r^\varepsilon(t,y) = u^\varepsilon(t,y) - v(t,y)$, and obtain that r^ε solves the following equation

$$i\partial_t r^\varepsilon = -\frac{1}{2}\Delta r^\varepsilon + (\Omega \cdot L)r^\varepsilon + \mathcal{V}^\varepsilon(t,y)r^\varepsilon + \Big(\mathcal{V}^\varepsilon(t,y) - \frac{1}{2}y \cdot Q_V(t)y\Big)v, \tag{2.11}$$

with vanishing initial data $r^\varepsilon(0,y) = 0$. Since the right hand side of (2.11) is given by self-adjoint operators acting on r^ε plus a source term, a standard energy estimate shows that

$$\|r^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)} \leqslant \int_0^t |\Delta_V^\varepsilon(\tau,y)|\,d\tau \lesssim \sqrt{\varepsilon}\int_0^t \||y|^3 v(\tau,\cdot)\|_{L^2(\mathbb{R}^d)}.$$

We note that

$$\||y|^3 v(\tau, \cdot)\|_{L^2(\mathbb{R}^d)} \leqslant \|v(\tau, \cdot)\|_{\Sigma^3} \lesssim e^{C\tau}, \quad \forall \tau \in \mathbb{R},$$

in view of Lemma 2.4. We therefore obtain

$$\|r^\varepsilon(t, \cdot)\|_{L^2(\mathbb{R}^d)} \lesssim \sqrt{\varepsilon} e^{Ct}.$$

The result then follows from the fact that the wave packet rescaling (2.5) leaves the L^2-norm invariant, and thus

$$\|\psi^\varepsilon(t, \cdot) - \varphi^\varepsilon(t, \cdot)\|_{L^2(\mathbb{R}^d)} = \|u^\varepsilon(t, \cdot) - v(t, \cdot)\|_{L^2(\mathbb{R}^d)} \equiv \|r^\varepsilon(t, \cdot)\|_{L^2(\mathbb{R}^d)} \lesssim \sqrt{\varepsilon} e^{Ct}.$$

$\square$

Remark 2.6. The time-scale $t \sim \mathcal{O}(\log \frac{1}{\varepsilon})$ is called the Ehrenfest-time. It is known to be the longest possible time-scale until which one can hope to establish an effective semi-classical approximation, in general, cf. [17]. Under stronger assumptions on v_0, it is possible to generalize the above approximation result to hold in stronger Σ^k norms up to Ehrenfest-time.

A particular class of global solutions v to (2.8) is obtained for (complex-valued) Gaussian initial data. More precisely, by following the ideas of Hagedorn [10], we consider initial data of the form

$$v_0(y) = \frac{1}{(\det A_0)^{1/2}} \exp\left(-\frac{1}{2} y \cdot (B_0 A_0^{-1}) y\right), \tag{2.12}$$

where the matrices A_0 and B_0 satisfy the following properties:

A_0 and B_0 are invertible;

$B_0 A_0^{-1}$ is symmetric; $B_0 A_0^{-1} = M_1 + i M_2$, with M_j symmetric;

$\mathrm{Re}\, B_0 A_0^{-1}$ is strictly positive definite;

$(\mathrm{Re}\, B_0 A_0^{-1})^{-1} = A_0 A_0^*.$ \hfill (2.13)

We shall now show that such Gaussian wave packets are indeed propagated by equation (2.8).

Corollary 2.7. (Gaussian wave packets) *Let $v \in C(\mathbb{R}, \Sigma^k)$ be the solution to* (2.8)*, with v_0 given by* (2.12)–(2.13)*. Then, for all time $t \in \mathbb{R}$, v is given by*

$$v(t, y) = \frac{1}{\left(\det A(t)\right)^{1/2}} \exp\left(-\frac{1}{2} y \cdot (B(t) A(t)^{-1}) y\right), \tag{2.14}$$

provided $A(t)$ and $B(t)$ solve the following ordinary differential equations

$$\begin{cases} \dot{A}(t) = iB(t) - [R_\Omega, A(t)]; \quad A(0) = A_0, \\ \dot{B}(t) = iQ_V(t)A(t) - [R_\Omega, B(t)]; \quad B(0) = B_0, \end{cases} \tag{2.15}$$

where R_Ω is a skewed-symmetric matrix, given by

$$R_\Omega = \begin{bmatrix} 0 & \Omega_3 & -\Omega_2 \\ -\Omega_3 & 0 & \Omega_1 \\ \Omega_2 & -\Omega_1 & 0 \end{bmatrix}.$$

In addition, (2.15) *guarantees that $A(t)$ and $B(t)$ satisfy* (2.13) *for all $t \in \mathbb{R}$.*

Proof. We first assume that A and B satisfy (2.13) for all $t \in \mathbb{R}$ and plug the Gaussian ansatz (2.14) into (2.8). After another lengthy computation we find that v solves (2.8), if and only if the matrices A and B satisfy:

$$\mathrm{Tr}(i\dot{A}A^{-1} + BA^{-1}) +$$
$$y^\top \left(i\dot{B}A^{-1} - iBA^{-1}\dot{A}A^{-1} - BA^{-1}BA^{-1} + Q_V + 2iR_\Omega BA^{-1}\right) y = 0.$$

In a first step, this implies

$$i\dot{A}A^{-1} + BA^{-1} + \Lambda = 0, \tag{2.16}$$

where Λ is any matrix such that $\mathrm{Tr}(\Lambda) = 0$. By choosing $\Lambda = i[R_\Omega, A]A^{-1}$ this fact is guaranteed and we directly obtain the first equation of (2.15). Using the right hand side of this equation as the new expression for $\dot{A}$, we find, in a second step, the following condition for B:

$$y^\top\Big(\dot{B} - iQ_V A + [R_\Omega, B]\Big)A^{-1}y + y^\top\Big(BA^{-1}R_\Omega + R_\Omega BA^{-1}\Big)y = 0. \tag{2.17}$$

In fact, since

$$y^\top R_\Omega BA^{-1}y = -(BA^{-1}R_\Omega y)^\top y = -y^\top BA^{-1}R_\Omega y,$$

we have $y^\top\big(BA^{-1}R_\Omega + R_\Omega BA^{-1}\big)y = 0$, which means that (2.17) simplifies to

$$y^\top\Big(\dot{B} - iQ_V A + [R_\Omega, B]\Big)A^{-1}y = 0,$$

which is guaranteed to hold, provided B satisfies the second equation of (2.15).

To prove that $A(t)$ and $B(t)$ satisfy (2.13), we employ the same argument as in [10, Lemma 2.1]: We first define two functions

$$F(t) := A^*(t)B(t) + B^*(t)A(t), \quad G(t) := A^\top(t)B(t) - B^\top(t)A(t).$$

and note that

$$\dot{F}(t) = (iB - [R_\Omega, A])^*B + A^*(iQA - [R_\Omega, B])$$
$$+ (iQA - [R_\Omega, B])^*A + B^*(iB - [R_\Omega, A]) = 0,$$

as R_Ω is skewed-symmetric and $Q_V(t)$ is symmetric. Hence,

$$F(t) = F(0) = A_0^*B_0 + B_0^*A_0 = A_0^*\Big(B_0 A_0^{-1} + (A_0^*)^{-1}B_0^*\Big)A_0$$
$$= A_0^*\Big(2\mathrm{Re}(B_0 A_0^{-1})\Big)A_0 = 2A_0^*\Big((A_0 A_0^*)^{-1}\Big)A_0 = 2\mathbb{I}.$$

For any $z \in \mathbb{C}$, we thus have

$$\langle z,\, z\rangle = \frac{1}{2}\langle z,\, F(t)z\rangle = \frac{1}{2}\langle A(t)z,\, B(t)z\rangle + \frac{1}{2}\langle B(t)z,\, A(t)z\rangle,$$

which equals zero only if $z = 0$. Thus, $\ker A(t) = \ker B(t) = \{0\}$, i.e., $A(t)$ and $B(t)$ are invertible.

Similarly, we infer that $\dot{G}(t) = 0$, and thus $G(t) = G(0)$, where

$$G(0) = A_0^\top\Big(B_0 A_0^{-1} - (A_0^\top)^{-1}B_0^\top\Big)A_0$$
$$= A_0^\top\Big(B_0 A_0^{-1} - (B_0 A_0^{-1})^\top\Big)A_0 = 0,$$

since $B_0 A_0^{-1}$ is symmetric. Hence, $A^\top(t)B(t) = B^\top(t)A(t)$, which shows that $B(t)A(t)^{-1}$ is symmetric. Finally, since $F(t) = 2\mathbb{I}$, we have

$$2\mathbb{I} = A^*\Big(BA^{-1} + (A^*)^{-1}B^*\Big)A = A^*\Big(BA^{-1} + \big(BA^{-1}\big)^*\Big)A = 2A^*\mathrm{Re}\big(BA^{-1}\big)A,$$

and thus $\mathrm{Re}\big(BA^{-1}\big) = (AA^*)^{-1}$. This also proves that $\mathrm{Re}(BA^{-1})$ is strictly positive definite. $\square$

Remark 2.8. One might wonder, why we chose a commutator in equation (2.16), when any other Λ with trace equal to zero would also be a possibility. However, the commutators are a natural choice in view of the following fact: Let

$$A_\Omega(t) = e^{tR_\Omega}A(t)e^{-tR_\Omega}, \quad B_\Omega(t) = e^{tR_\Omega}B(t)e^{-tR_\Omega},$$

be two new matrices obtained by conjugating A and B with time-dependent rotation matrices. Then, one checks that A_Ω, B_Ω solve

$$\begin{cases} \dot{A}_\Omega(t) = iB_\Omega(t) \\ \dot{B}_\Omega(t) = iQ_{V,\Omega}(t)A_\Omega(t), \end{cases} \tag{2.18}$$

which implies that A_Ω, B_Ω also have all the properties (2.13). The system (2.18) is identical to the one originally derived by Hagedorn, provided $Q_{V,\Omega} = Q_V$. The latter is true for potentials V which are symmetric with respect to the rotation axis Ω, since in this case $[R_\Omega, V] = 0$. This reflects the well-known fact that solutions v to (nonlinear) Schrödinger equations with angular momentum term are related to solutions $\tilde{v}$ of the same equation but without angular momentum term, via the following time-dependent unitary transformation

$$v_\Omega(t,y) = e^{it\Omega \cdot L}v(t,y) = v\big(t, e^{tR_\Omega}y\big), \tag{2.19}$$

see [1,2] for more details. Acting with change of variables onto the Gaussian ansatz (2.14), one can see that the latter remains Gaussian, provided A and B are replaced by A_Ω and B_Ω, respectively.

3. Extension to the weakly nonlinear case

In this section, we shall show how to extend the construction of semi-classical wave packets to the case of weakly nonlinear Schrödinger equations with rotation. We thereby follow the ideas of [7] and only consider the critical case, where $\alpha = 1 + \frac{d}{2}$. We consequently are interested in

$$i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V(x)\psi^\varepsilon + \lambda\varepsilon^{1+d/2}|\psi^\varepsilon|^2\psi^\varepsilon + \varepsilon(\Omega \cdot L)\psi^\varepsilon, \quad \psi^\varepsilon_{|t=0} = \psi^\varepsilon_0, \tag{3.1}$$

for $d = 2$ or 3, and initial data ψ^ε_0 given in the form (1.3). Rewriting the unknown ψ^ε in terms of u^ε as given by (2.5), we notice that $|\psi^\varepsilon|^2 \sim \varepsilon^{-d/2}$ and thus, by following the same steps as in the linear case, we (formally) arrive at the corresponding amplitude equation with cubic nonlinearity, i.e.,

$$i\partial_t v = -\frac{1}{2}\Delta v + \frac{1}{2}\big(y \cdot Q_V(t)y\big)v + \lambda|v|^2v + (\Omega \cdot L)v, \quad v_{|t=0} = v_0. \tag{3.2}$$

Remark 3.1. If we had chosen a subcritical $\alpha > 1 + \frac{d}{2}$, the nonlinearity would not appear in (3.2), and thus the situation is very similar to the one in our previous section. The supercritical case $\alpha < 1 + \frac{d}{2}$, however, is much more involved and the only rigorous results available to date are for the case of (nonlocal) Hartree nonlinearities, cf. [3].

Equation (3.2) falls within the class of models studied in [1], and local existence of solutions is guaranteed for smooth initial data. More precisely, we have:

Lemma 3.2. (Local Existence) *Let* $v_0 \in \Sigma^k$ *with* $k > d/2$. *There exists* $T_{\mathrm{crit}} \in (0, +\infty]$ *and a unique maximal solution* $v \in C([0, T_{\mathrm{crit}}); \Sigma^k)$ *to (3.2), such that* $\|v(t, \cdot)\|_{L^2} = \|v_0\|_{L^2}$. *The solution is maximal in the sense that if* $T_{\mathrm{crit}} < \infty$, *then*

$$\lim_{t \to T_{\mathrm{crit}}} \|v(t, \cdot)\|_{\Sigma^k} = +\infty.$$

Remark 3.3. In general, $T_{\mathrm{crit}} < +\infty$, in particular in the focusing case $\lambda < 0$ where the appearance of finite-time blow-up is a possibility, see [1]. The change of variable (2.19) allows one to map solutions to (3.2) onto solutions of NLS without rotation term, but with time-dependent, sub-quadratic potentials, for which the long time behavior is studied in [4].

Our main result in this section is as follows:

Theorem 3.4. (Weakly nonlinear wave packets) *Let $d = 2$ or 3, $v_0 \in \Sigma^3$ and V satisfy Assumption 1.1. Let S be the classical action* (2.3) *and*

$$\varphi^\varepsilon(t, x) = \varepsilon^{-d/4} v\Big(t, \frac{x - q(t)}{\sqrt{\varepsilon}}\Big) e^{i(S(t) + p(t) \cdot (x - q(t)))/\varepsilon}$$

be a semiclassical wave packet concentrated, as before, along the trajectories (2.2), *but with an amplitude $v \in C([0, T_{\mathrm{crit}}); \Sigma^3)$ given by the maximal solution to the nonlinear equation* (3.2). *Then, for any $T < T_{\mathrm{crit}}$, we have*

$$\sup_{0 \leqslant t \leqslant T} \|\psi^\varepsilon(t, \cdot) - \varphi^\varepsilon(t, \cdot)\|_{L^2(\mathbb{R}^d)} \lesssim \sqrt{\varepsilon}.$$

Even in cases where the maximal life-span of solutions to (3.2) is $T_{\mathrm{crit}} = +\infty$, it is not clear whether this nonlinear approximation result extends up to Ehrenfest times $t \sim \mathcal{O}(\log \frac{1}{\varepsilon})$. With considerably more effort, however, it was shown in [7] that time-scales of order $t \sim \mathcal{O}(\log \log \frac{1}{\varepsilon})$ can be reached in the critical case. Here, we only treat the case of finite, macroscopic times $t \sim \mathcal{O}(1)$, in the interest of giving a short and not too technical proof which relates to the linear case in a transparent way.

Proof. As in the linear case, we denote the remainder by $r^\varepsilon(t, y) = u^\varepsilon(t, y) - v(t, y)$, and first note that the unknown u^ε defined via (2.5) solves

$$i\partial_t u^\varepsilon = -\frac{1}{2}\Delta u^\varepsilon + \mathcal{V}^\varepsilon(t, y)u^\varepsilon + (\Omega \cdot L)u^\varepsilon + \lambda|u^\varepsilon|^2 u^\varepsilon, \quad u^\varepsilon_{|t=0} = v_0, \tag{3.3}$$

where $\mathcal{V}^\varepsilon$ is given by (2.7). We recall the definition of $\Delta_V^\varepsilon(t, y)$ given by (2.10) and consequently infer that r^ε is the solution to

$$i\partial_t r^\varepsilon = -\frac{1}{2}\Delta r^\varepsilon + \mathcal{V}^\varepsilon(t, y)r^\varepsilon + (\Omega \cdot L)r^\varepsilon + \Delta_V^\varepsilon(t, y)v + \lambda\Big(|u^\varepsilon|^2 u^\varepsilon - |v|^2 v\Big), \tag{3.4}$$

subject to initial data $r^\varepsilon(0, y) = 0$.

Next, we denote by $U_\Omega^\varepsilon(t, s)$ the L^2-unitary operator furnishing the Schrödinger dynamics associated with the time-dependent Hamiltonian

$$H_\Omega^\varepsilon(t) = -\frac{1}{2}\Delta + \mathcal{V}^\varepsilon(t, x) + (\Omega \cdot L). \tag{3.5}$$

By applying Duhamel's formula to (3.4), we obtain

$$r^\varepsilon(t + \tau) = U_\Omega^\varepsilon(\tau, t)r^\varepsilon(t) - i \int_t^{t+\tau} U_\Omega^\varepsilon(t + \tau, s)\Delta_V^\varepsilon v(s)\, ds$$

$$- i\lambda \int_t^{t+\tau} U_\Omega^\varepsilon(t + \tau, s)\Big(|u^\varepsilon|^2 u^\varepsilon - |v|^2 v\Big)(s)\, ds.$$

In view of the results described in the Appendix, the propagator $U_\Omega^\varepsilon(t, s)$ allows for ε-independent local in-time dispersive estimates. Recall from [12] that (q, r) is an admissible Strichartz pair associated with the space-time norm $L_t^q L_x^r$, if $2 \leqslant r \leqslant \frac{2d}{d-2}$ (resp. $2 \leqslant r < \infty$ if $d = 2$), and

$$\frac{2}{q} = d\Big(\frac{1}{2} - \frac{1}{r}\Big).$$

Define $I = [t, t + \tau]$, with $t \geq 0$, $\tau > 0$, and let

$$q = \frac{8}{d}, \quad r = 4,$$

such that (q, r) is admissible. In addition, we put

$$q' = \frac{8}{8 - d}, \quad r' = \frac{4}{3}$$

being the Hölder conjugates of (q, r). The Strichartz estimates derived in [12] then imply

$$\|r^\varepsilon\|_{L^{8/d}(I;L^4)} \lesssim \|r^\varepsilon\|_{L^2} + \|\Delta_V^\varepsilon v\|_{L^1(I;L^2)} + \big\||u^\varepsilon|^2 u^\varepsilon - |v|^2 v\big\|_{L^{8/(8-d)}(I;L^{4/3})}.$$

For the last term, we have the following pointwise estimate

$$\Big||u^\varepsilon|^2 u^\varepsilon - |v|^2 v\Big| \lesssim |r^\varepsilon|\Big(|r^\varepsilon|^2 + |v|^2\Big). \tag{3.6}$$

By Hölder's inequality,

$$\begin{aligned}
\|r^\varepsilon\|_{L^{8/d}(I;L^4)} \lesssim{}& \|r^\varepsilon\|_{L^2} + \|\Delta_V^\varepsilon v\|_{L^1(I;L^2)} \\
&+ \Big(\|r^\varepsilon\|_{L^{8/(4-d)}(I;L^4)}^2 + \|v\|_{L^{8/(4-d)}(I;L^4)}^2 \Big)\|r^\varepsilon\|_{L^{8/d}(I;L^4)}.
\end{aligned} \tag{3.7}$$

Since amplitude functions u^ε and v solve evolutionary equations within the same class of nonlinear Schrödinger type models with smooth and sub-quadratic potentials, Lemma 3.2 yields that both $u^\varepsilon, v \in C([0,T]; \Sigma^k)$. Hence, we have

$$\|Pu^\varepsilon\|_{L^\infty([0,T];L^2)} + \|Pv\|_{L^\infty([0,T];L^2)} \leqslant C(T),$$

for any operator $P \in \{\mathrm{Id}, \nabla, x\}$.

Next, we recall the Gagliardo–Nirenberg inequality, i.e.,

$$\|f\|_{L^4(\mathbb{R}^d)} \lesssim \|f\|_{L^2(\mathbb{R}^d)}^{1-d/4} \|\nabla f\|_{L^2(\mathbb{R}^d)}^{d/4}, \quad \forall f \in H^1(\mathbb{R}^d).$$

Applying this to v yields

$$\|v\|_{L^4} \lesssim \|v\|_{L^2}^{2-d/2} + \|\nabla v\|_{L^2}^{d/2} \leqslant C(T),$$

and same is true for u^ε. Hence,

$$\|r^\varepsilon\|_{L^{8/(4-d)}(I;L^4)}^2 + \|v\|_{L^{8/(4-d)}(I;L^4)}^2 \lesssim C(T)\left(\int_t^{t+\tau} ds\right)^{\frac{4-d}{4}} \lesssim \tau^{(4-d)/4}. \tag{3.8}$$

Thus, (3.7) can be reduced to

$$\|r^\varepsilon\|_{L^{8/d}(I;L^4)} \lesssim \|r^\varepsilon\|_{L^2} + \|\Delta_V^\varepsilon v\|_{L^1(I;L^2)} + \tau^{(4-d)/4}\|r^\varepsilon\|_{L^{8/d}(I;L^4)}. \tag{3.9}$$

Now, fix $\tau < 1$ to be sufficiently small, and repeat this estimate a finite number of times to cover $[0,T]$. This yields

$$\|r^\varepsilon\|_{L^{8/d}([0,T];L^4)} \lesssim \|r^\varepsilon\|_{L^1([0,T];L^2)} + \|\Delta_V^\varepsilon v\|_{L^1([0,T];L^2)}. \tag{3.10}$$

Next, applying Strichartz estimates again, with a second admissible pair $(q_1, r_1) = (\infty, 2)$ on $J = [0,t]$ for $0 \leqslant t \leqslant T$,

$$\|r^\varepsilon\|_{L^\infty(J;L^2)} \lesssim \|\Delta_V^\varepsilon v\|_{L^1(J;L^2)} + \big\||u^\varepsilon|^2 u^\varepsilon - |v|^2 v\big\|_{L^{8/(8-d)}(J;L^{4/3})}. \tag{3.11}$$

Using the pointwise estimate (3.6) and repeating the steps (3.7)–(3.9), we obtain

$$\begin{aligned}
\|r^\varepsilon\|_{L^\infty(J;L^2)} &\lesssim \|\Delta_V^\varepsilon v\|_{L^1(J;L^2)} + \|r^\varepsilon\|_{L^{8/d}(J;L^4)} \\
&\lesssim \|r^\varepsilon\|_{L^1(J;L^2)} + \|\Delta_V^\varepsilon v\|_{L^1(J;L^2)} \\
&\lesssim \|r^\varepsilon\|_{L^1(J;L^2)} + \sqrt{\varepsilon}\,\big\||y|^3 v(t,y)\big\|_{L^1(J;L^2)},
\end{aligned}$$

where the last inequality follows by Taylor expansion, just like in the linear case. The above estimate is readily observed to be of Gronwall type, which consequently yields

$$\|r^\varepsilon(t)\|_{L^2} \lesssim \sqrt{\varepsilon}e^t, \quad t \in [0,T],$$

and thus

$$\sup_{0 \leqslant t \leqslant T} \|u^\varepsilon(t,\cdot) - v(t,\cdot)\|_{L^2} \equiv \sup_{0 \leqslant t \leqslant T} \|r^\varepsilon(t,\cdot)\|_{L^2} \lesssim \sqrt{\varepsilon}.$$

By recalling the fact that the wave-packet rescaling (2.5) leaves the L^2-norm invariant, the proof is complete. $\qquad\square$

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Appendix A. On the existence of Strichartz estimates

We briefly discuss the existence of ε-independent Strichartz estimates for the propagator $U_\Omega^\varepsilon(t,s)$ associated with the Hamiltonian $H_\Omega^\varepsilon(t)$ as given by (3.5). To this end, we first consider the case without rotation $\Omega = 0$, i.e., we study solutions

$$u^\varepsilon(t,x) = U^\varepsilon(t,s)u_0(x),$$

to the non-autonomous Schrödinger equation

$$i\partial_t u^\varepsilon + \frac{1}{2}\Delta u^\varepsilon = \mathcal{V}^\varepsilon(t,x)u^\varepsilon, \quad u^\varepsilon(s,x) = u_0(x), \tag{A.1}$$

where we recall from (2.7) that

$$\mathcal{V}^\varepsilon(t,y) = \frac{1}{\varepsilon}\big(V(q(t) + \sqrt{\varepsilon}y) - V(q(t)) - \sqrt{\varepsilon}y \cdot \nabla V(q(t))\big).$$

One seeks to construct a strongly continuous map $(t,s) \mapsto U^\varepsilon(t,s)$ which is unitary on $L^2(\mathbb{R}^d)$, and which satisfies $U^\varepsilon(t,t) = \mathrm{Id}$,

$$U^\varepsilon(t,\tau)U^\varepsilon(\tau,s) = U^\varepsilon(t,s), \quad U^\varepsilon(t,s)^* = U^\varepsilon(t,s)^{-1}.$$

Under our hypothesis on the potential V, this can be done using the approach developed in [9] (see also [8] for a detailed revisit of this technique). Indeed, Assumption 1.1 implies that $\mathcal{V}^\varepsilon$ is a real-valued C^∞-function, such that $\mathcal{V}^\varepsilon \in L_t^2 L_{\mathrm{loc},x}^\infty$ and, for any fixed $t \in \mathbb{R}$, $\mathcal{V}^\varepsilon(t,\cdot)$ is sub-quadratic in space. A short computation also shows that

$$\forall\, |\alpha| = 2\,:\, \partial_y^\alpha \mathcal{V}^\varepsilon(t,y) = \partial_x^\alpha V(q(t) + \sqrt{\varepsilon}y),$$

which in view of Lemma 2.1 and Assumption 1.1 implies that for $t \in [0,T]$:

$$M := \|\nabla_y^2 \mathcal{V}^\varepsilon\|_{L_t^2 L_x^\infty} = \|\nabla_y^2 V\|_{L_t^2 L_x^\infty} \leqslant c(T). \tag{A.2}$$

In particular, $M > 0$ is ε-independent.

The propagator $U^\varepsilon(t,s)$ can thus be constructed, using Fujiwara's time-slicing approach, from an associated family of parametrices given by

$$E^\varepsilon(t,s)\varphi(y) = \left(\frac{1}{2\pi i(t-s)}\right)^{d/2} \int_{\mathbb{R}^d} e^{iS^\varepsilon(t,s,y,z)}\varphi(z)\,dz, \quad \varphi \in \mathcal{S}(\mathbb{R}^d),$$

where S^ε is the associated classical action, cf. [8, Chapter 1.5]. For small enough $\delta > 0$ and $0 < |t-s| < \delta$, this oscillatory integral defines a bounded operator

$$\|E^\varepsilon(t,s)\varphi\|_{L^2} \leqslant \gamma\|\varphi\|_{L^2},$$

where the constant $\gamma > 0$ only depends on δ and M defined in (A.2) above. Thus, also $\gamma > 0$ is seen to be ε-independent. Taking a partition of the time-interval $[s,t]$ and an associated iterated integral operator induced by $E^\varepsilon(t,s)$, one obtains the propagator $\{U^\varepsilon(t,s) \ : \ t,s \in [-T,T]\}$ by taking the size of the partition step to zero (in an appropriate sense), cf. [8, Chapter 1.6] for full details. In particular, $U^\varepsilon(t,s)$ inherits the dispersive properties of $E^\varepsilon(t,s)$ in the sense that

$$\|U^\varepsilon(t,s)\varphi\|_{L^\infty(\mathbb{R}^d)} \leqslant \frac{C}{|t-s|^{d/2}}\|\varphi\|_{L^1(\mathbb{R}^d)},$$

where $C = C(\delta, M) > 0$. The general theory developed in [12] shows that this short-time dispersive estimate is sufficient to imply the existence of local in-time Strichartz estimates for the propagator $U^\varepsilon(t,s)$, and thus for the solution u^ε to (A.1).

Finally, we note that by applying the time-dependent change of variables (2.19) to u^ε, i.e., by defining

$$u^\varepsilon_\Omega(t,y) = e^{it\Omega\cdot L}u^\varepsilon(t,y) = u^\varepsilon\big(t, e^{tR_\Omega}y\big),$$

we obtain the solution u^ε_Ω to a Schrödinger equation with rotation

$$i\partial_t u^\varepsilon_\Omega + \frac{1}{2}u^\varepsilon_\Omega = \mathcal{V}^\varepsilon_\Omega(t,y)u^\varepsilon_\Omega + \Omega\cdot Lu^\varepsilon_\Omega, \quad u^\varepsilon_\Omega(s,x) = u_0(x), \tag{A.3}$$

where $\mathcal{V}^\varepsilon_\Omega(t,y) = \mathcal{V}^\varepsilon\big(t, e^{tR_\Omega}y\big)$. Since R_Ω is the generator of an orthogonal time-dependent rotation, this change of variables leaves every $L^p(\mathbb{R}^d)$-norm of u^ε invariant and guarantees that $\mathcal{V}^\varepsilon_\Omega$ is of the same class as $\mathcal{V}^\varepsilon$ itself. In particular, it holds

$$M = \|\nabla^2_y\mathcal{V}^\varepsilon\|_{L^2_t L^\infty_x} = \|\nabla^2_y\mathcal{V}^\varepsilon_\Omega\|_{L^2_t L^\infty_x}.$$

The short-time Strichartz estimates available for solutions u^ε without rotation therefore directly transfer to u^ε_Ω, a fact which has already been recognized in [6, Remark 2.2].

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