

INSTABILITY FOR THE SEMICLASSICAL NON-LINEAR SCHRÖDINGER EQUATION

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1. INTRODUCTION

In this note we adapt recent results of Burq-Gérard-Tzvetkov [2] and Christ-Colliander-Tao [3] on instability for non-linear Schrödinger equations to the semi-classical setting. Rather than work with Sobolev spaces we estimate the sizes of solutions and their differences in terms of the small constant, \hbar , coming from the equation. The ideas remain exactly the same but we gain in the simplicity of the arguments and, we hope, in physical relevance.

Our motivation comes from the Gross-Pitaevski equations used in the study of Bose-Einstein condensation [6]:

$$(1.1) \quad i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) = \left(-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}) + g|\Phi(\mathbf{r}, t)|^2 \right) \Phi(\mathbf{r}, t),$$

where the coupling constant g is given in terms of the Planck constant \hbar and the scattering length a :

$$(1.2) \quad g = \frac{4\pi\hbar^2 a}{m} (N - 1).$$

Here N is the number of particles in the condensate, typically a very large number. In this equation we normalize the wave function so that it gives a probability distribution:

$$\|\Phi(\bullet, t)\|_{L^2}^2 \stackrel{\text{def}}{=} \int_{\mathbb{R}^3} |\Phi(\mathbf{r}, t)|^2 d\mathbf{r} = 1.$$

The energy functional associated to (1.1) is given by the usual expression which we divide into *kinetic*, *exterior*, and *interaction* energies:

$$(1.3) \quad E[\Phi] = \int_{\mathbb{R}^n} \left(\frac{\hbar^2}{2m} |\nabla \Phi(\mathbf{r}, t)|^2 + V_{\text{ext}}(\mathbf{r}) |\Phi(\mathbf{r}, t)|^2 + \frac{g}{2} |\Phi(\mathbf{r}, t)|^4 \right) d\mathbf{r},$$

$$E[\Phi] = E_{\text{kin}}(t) + E_{\text{pot}}(t) + E_{\text{int}}(t).$$

The total energy $E[\Phi]$ is conserved and (1.1) is rewritten from the variational point of view as $i\hbar \partial_t \hbar \Phi = \delta E / \delta \Phi^*$ where \bullet^* denotes the complex conjugate.

The scattering length a appearing in the constant g is a physical parameter of the system and it is defined using two body particle interaction: it is positive for repulsive interactions and negative for attractive ones. Classically it is determined using the far field approximation in scattering theory: it is the radius of an attractive or repulsive sphere with the leading far field behaviour same as the two molecule subsystem of the condensate.

In principle, using the method based on the existence of Feshbach resonances [6], the scattering length can be tuned to any value, including values close to zero, or values of different signs. This can lead to very interesting instability phenomena as investigated recently in [5],[7].

The mathematical instability results we are using are of considerably weaker nature – see the table below. The main problem with the results of [3] is the non-physical nature of the initial conditions. The more geometric and physical results of [2] suffer from the requirement of small $a(N - 1)$ – see Fig.1. Clearly

the case of large $a(N - 1)$ is more interesting but then the mechanism must be completely different than in [2].

As the first mathematical approximation to (1.1) we will consider the non-linear Schrödinger equation with two parameters, a small *pseudo*-Planck constant h , and $a > 0$ a *pseudo*-scattering length:

$$(1.4) \quad ih\partial_t u = -h^2\Delta u + V(x)u + h^2a|u|^2u, \quad u = u_h(t, x), \quad x \in \mathbb{R}^3, \quad \Delta := \sum_{j=1}^3 \partial_{x_j}^2.$$

In quantum mechanics instability should be considered with respect to *complex projective distance*:

$$(1.5) \quad v_j \in L^2(\mathbb{R}^3), \quad d_{\text{pr}}(v_1, v_2) \stackrel{\text{def}}{=} \cos^{-1} \left(\frac{|\langle v_1, v_2 \rangle|}{\|v_1\| \|v_2\|} \right).$$

We will consider two different types of instability:

- **High energy:** $u^j = u_h^j(t)$, $j = 1, 2$, bounded in L^2 , but with unbounded (as $h \rightarrow 0$) energies solve (1.4), and

$$(1.6) \quad \frac{d_{\text{pr}}(u_h^1(t_h), u_h^2(t_h))}{d_{\text{pr}}(u_h^1(0), u_h^2(0))} \rightarrow \infty, \quad \frac{E_{\text{kin}}(t_h)}{E_{\text{kin}}(0)} \rightarrow \infty, \quad t_h \rightarrow 0, \quad h \rightarrow 0.$$

- **Geometric:** $u^j = u_h^j(t)$, $j = 1, 2$, with $\|u_h^j(t)\|_{L^2} \sim E(0) \gg E_{\text{int}}(0)$, solve (1.4), $a = o_{h \rightarrow 0}(1)$, and for h -dependent times t_h ,

$$(1.7) \quad \frac{\|u_h^1(t_h) - u_h^2(t_h)\|_{L^2}}{\|u_h^1(0) - u_h^2(0)\|_{L^2}} \geq t_h a \rightarrow \infty, \quad h \rightarrow 0.$$

For some potentials we can also show that we have projective instability along a sequence of values of h :

$$(1.8) \quad \frac{d_{\text{pr}}(u_h^1(t_h), u_h^2(t_h))}{d_{\text{pr}}(u_h^1(0), u_h^2(0))} \rightarrow \infty, \quad t_h \rightarrow \infty, \quad h = h_k \rightarrow 0, \quad k \rightarrow \infty.$$

The instability in (1.7) is extremely weak and all we can say at this stage is that we have a phenomenon which is impossible in linear unitary propagation. In fact, the semiclassical adaptation of the result of [2] can be considered as a stability result: some eigenstates of the Schrödinger operator $-h^2\Delta + |x|^2$ (see (3.3) below) persist in non-linear propagation long enough to develop a global change phase which implies (1.7) but not (1.6). However for a class of potentials with cylindrical symmetry we can obtain (1.8).

In the two cases the relevant time scales and the localizations of the initial data leading to the instability are different and correspond to the regimes considered in [3] and [2] respectively. In the first case the structure of the exterior potential V is irrelevant and in the second case the semi-classical dynamics of $-h^2\Delta + V(x)$ replaces the compact manifold geometry. This is represented schematically in the following table:

Time scale	Effect of V	Expected instability	Initial data
$t \ll h$	The potential plays no rôle, $ a > c > 0$	Type (1.6) instability	$h^{-3/2}\phi_0(x/h)$
$t \rightarrow \infty$	global Hamiltonian flow in the energy surface of $\xi^2 + V(x)$ relevant, $a = o(1)$.	Type (1.7) instability	Special excited modes of $-h^2\Delta + V(x)$

NOTATION. In this paper C denotes a bounded constant the value of which may change from line to line. We use the notation $a \sim b$ if $a/C \leq b \leq Ca$, and $a \ll b$, if $a \leq Kb$ for some fixed large constant K .

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2. HIGH ENERGY INSTABILITY

In this section we will prove a precise version of (1.6). We assume that $V \in \mathcal{C}^\infty(\mathbb{R}^3)$ and that $V \geq -C$.

Theorem 1. *Suppose that the initial conditions for (1.4) are given by*

$$(2.1) \quad \begin{aligned} u_h^j(x) &= h^{-3/2} \phi \left(\frac{x - x_j}{h} \right), \quad j = 1, 2, \quad \phi \in \mathcal{C}_c^\infty(\mathbb{R}^3), \quad \|\phi\|_{L^2(\mathbb{R}^3)} = 1, \\ |x_1 - x_2| &= C_0 h \left(\log \left(\frac{1}{h} \right) \right)^{-\alpha}, \quad \alpha < 1, \end{aligned}$$

where C_0 is a fixed large constant. Suppose also that ϕ is real valued and has a nondegenerate maximum. Then for $|a| > h^\delta$, $\delta < 1$, we have

$$(2.2) \quad \frac{d_{\text{pr}}(u_h^1(t), u_h^2(t))|_{t=|a|^{-1}h^2(\log(1/h))^\alpha}}{d_{\text{pr}}(u_h^1(0), u_h^2(0))} \sim \left(\log \left(\frac{1}{h} \right) \right)^{\alpha/2},$$

and for the energy of u_h^j 's we have

$$(2.3) \quad \frac{E_{\text{kin}}(|a|^{-1}h^2(\log(1/h))^\alpha)}{E_{\text{kin}}(0)} \sim \left(\log \left(\frac{1}{h} \right) \right)^\alpha.$$

If $a \simeq 1$ this means that at very short times we have logarithmic divergence for the projective distance quotient, and an energy transfer from interaction energy to kinetic energy. The generic condition that ϕ has a nondegenerate maximum is made for technical convenience only – see Lemma 2.1 below.

2.1. The ansatz. In this section the sign the constant a in front of the non linearity does not matter. For clarity we fix it to be equal to + (defocusing) Let u_h^j be as in the statement of Theorem 1:

$$u_h^j(x) = h^{-(3/2)} \phi \left(\frac{x - x_j}{h} \right).$$

Denote

$$(2.4) \quad v_h^j(t, x) = h^{-(3/2)} \phi((x - x_j)/h) e^{-itah^{-2}\phi^2((x-x_j)/h)}$$

solution of

$$ih\partial_t v_h^j = ah^2 |v_h^j|^2 v_h^j$$

We will now check that with the choices of x_j in (2.1) we obtain (2.2) for the two ansätze. We see that

$$(2.5) \quad d_{\text{pr}}(u_h^1, u_h^2) = \cos^{-1}(|\langle u_h^1, u_h^2 \rangle|) = \cos^{-1}(1 - \mathcal{O}(|x_1 - x_2|/h)) = \mathcal{O}(|(x_1 - x_2)/h|^{1/2}) = \left(\log \left(\frac{1}{h} \right) \right)^{-\alpha/2}.$$

We also compute

$$(2.6) \quad d_{\text{pr}}(v_h^1(t), v_h^2(t)) = \cos^{-1} \left(\left| \int_{\mathbb{R}^3} \phi(x - x_1/h) \phi(x - x_2/h) e^{ith^{-2}a(\phi^2(x-x_1/h) - \phi^2(x-x_2/h))} dx \right| \right).$$

We now need

Lemma 2.1. *Suppose that $\phi \in C_c^\infty(\mathbb{R}^3; \mathbb{R})$ has a nondegenerate maximum and that $\|\phi\|_{L^2} = 1$. Then for $\sigma \gg |y|^{-1} \gg 1$,*

$$\left| \int_{\mathbb{R}^3} \phi(x-y)\phi(x)e^{i\sigma(\phi^2(x-y)-\phi^2(x))} dx \right| \leq b + \mathcal{O}(|y| + 1/(\sigma|y|)),$$

where $b < 1$ depends only on ϕ .

Proof. We first note that

$$\int_{\mathbb{R}^3} \phi(x-y)\phi(x)e^{i\sigma(\phi^2(x-y)-\phi^2(x))} dx = \int_{\mathbb{R}^3} \phi^2(x)e^{i\sigma(\phi^2(x-y)-\phi^2(x))} dx + \mathcal{O}(|y|).$$

The phase in the integral can be written as $\sigma\langle y, \psi_y(x) \rangle$ where at the maximum of ϕ , x_0 , $|D\psi_y(x_0)| > c > 0$, uniformly in y . All derivatives of ψ_y are also bounded uniformly in y . Hence when we cut-off to a small neighbourhood of x_0 the phase has no stationary points and the integral decays rapidly as $\sigma|y| \rightarrow \infty$. Since $\|\phi\|_{L^2} = 1$ the contribution away from that neighbourhood is strictly smaller than 1. \square

We apply the lemma with $\sigma = tah^{-2} \log(1/h)^\alpha$ and $y = (x_1 - x_2)/h$, $|y|^{-1} \ll \sigma$ if C_0 (in the condition on $x_1 - x_2$) large enough. Hence (2.6) shows

$$(2.7) \quad d_{\text{pr}}(v_h^1(t), v_h^2(t)) > c > 0,$$

and consequently we have (2.2) with $u_h^j(t)$ replaced by v_h^j . The proof of Theorem 1 amounts to showing that for times of the order $|a|^{-1}h^2 \log(1/h)^\alpha$, and for $|a|$ bounded away from 0, the ansatz dominates the solution of the non-linear equation.

In preparation for the analysis of the solution we record the following simple

Lemma 2.2. *Let*

$$P_h = -h^2\Delta + V(x), \quad V \in C^\infty(\mathbb{R}^3), \quad V \geq -C.$$

If $v = v_h$ is given by (2.4) then

$$\begin{aligned} \|(hD_x)^\alpha v\|_{L^\infty} &\leq C_\alpha h^{-\frac{3}{2}}(1 + (th^{-2}|a|)^{|\alpha|}), \\ \|(hD_x)^\alpha v\|_{L^2} &\leq C_\alpha(1 + (th^{-2}|a|)^{|\alpha|}), \quad \|P_h v\|_{L^2} \leq (1 + (th^{-2}|a|)^2). \end{aligned}$$

2.2. Non linear analysis. We start with a remark about the existence of solutions to the non-linear equation (1.4). The norm involved in the standard fixed point argument is the H_h^2 semi-classical norm: in dimension 3, the H_h^2 norm controls the L^∞ norm with a large constant, and consequently the equation (1.4) is easily shown to be locally well posed in $H_h^2(\mathbb{R}^3)$. Using this local existence result, the well posedness for the time $t \sim |a|h^2(\log(1/h))^\alpha$ given in Theorem 1 follows from a priori bounds on the solution which we prove in this subsection.

We recall that the semi-classical Sobolev norms are defined as follows

$$\|u\|_{H_h^k} = \sum_{|\alpha| \leq k} \|(hD)^\alpha u\|_{L^2}.$$

The following lemma provides a translation of the standard Sobolev embeddings:

Lemma 2.3. *For $2 \leq p \leq \infty$ satisfying*

$$\frac{1}{2} - \frac{m}{n} \leq \frac{1}{p}, \quad p < \infty, \quad \frac{1}{2} - \frac{m}{n} < 0, \quad p = \infty,$$

we have

$$\|u\|_{L^p(\mathbb{R}^n)} \leq Ch^{n(\frac{1}{p}-\frac{1}{2})} \|u\|_{H_h^m(\mathbb{R}^n)}.$$

Proof. With $h = 1$ this is one of the standard Sobolev inequalities. Applying it to $v_h(x) = u(hx)$ gives the lemma: $(hD_x)^\alpha u = D_x^\alpha v_h$,

$$\|v_h\|_{H^m(\mathbb{R}^n)} = h^{-\frac{n}{2}} \|u\|_{H_h^m(\mathbb{R}^n)}, \quad \|v_h\|_{L^p(\mathbb{R}^n)} = h^{-\frac{n}{p}} \|u\|_{L^p(\mathbb{R}^n)}.$$

□

We now consider u the solution of (1.4) with initial data u_h^1 given in Theorem 1. Write $u = v + w$ where v is the ansatz above. We obtain the following equations for w :

$$(2.8) \quad (ih\partial_t + P_h)w = h^2|a| (\mathcal{O}(|v|^2|w|) + \mathcal{O}(|v||w|^2) + \mathcal{O}(|w|^3)) - P_h v$$

We are going to show that the above equation can be solved by energy methods and that the solution satisfies

$$(2.9) \quad \sup_{t \in [0, h^2|a|^{-1}(-\log(h))^\alpha]} (\|w\|_{L^2}^2 + \|P_h w\|_{L^2}^2) \leq Ch^\epsilon / |a|.$$

As a startup and to make the main ideas clear, we consider a simpler problem for which the fixed point argument can be performed in L^2 . Consider \tilde{w} solution of the *linear* equation

$$(2.10) \quad (ih\partial_t + P_h)\tilde{w} = |a|h^2\mathcal{O}(|v|^2)\tilde{w} - P_h v.$$

Denote $I_0(t) = \|\tilde{w}\|_{L^2}^2$. Then

$$(2.11) \quad \frac{dI_0(t)}{dt} = -\frac{2}{h} \text{Im}\langle \tilde{w}(t), ih\partial_t \tilde{w}(t) \rangle = -\frac{2}{h} \text{Im}\langle \tilde{w}(t), h^2|a|v(t)|^2 \tilde{w}(t) - P_h v \rangle,$$

since the term involving $P_h w$ disappears due to the self adjointness of P_h .

Using Lemma 2.2 we see that for $t \in [0, h^2|a|^{-1}(-\log(h))^\alpha]$

$$\begin{aligned} \frac{d}{dt} I_0(t) &\leq C|a|h\|v(t)\|_{L^\infty}^2 I_0(t) + h^{-1} \|P_h v(t)\| I_0(t)^{\frac{1}{2}} \\ &\leq C|a|h^{-2} I_0(t) + Ch^{-1}(1 + (th^{-2}|a|)^2) I_0(t)^{\frac{1}{2}} \\ &\leq C'|a|h^{-2} I_0(t) + C'(1 + (-\log h)^{2\alpha})^2 / |a| \end{aligned}$$

As a consequence, through an application of the Gronwall lemma, we get for $t \in [0, |a|h^2(-\log(h))^\alpha]$.

$$\begin{aligned} I_0(t) &\leq C e^{Ct|a|h^{-2}} \int_0^t e^{-Cs|a|h^{-2}} (1 + (-\log h)^{4\alpha}) ds \\ &\leq C e^{Cth^{-2}|a|} (h^2/|a|) (1 + (-\log h)^{4\alpha}) \\ &\leq C e^{C(-\log h)^\alpha} h^{2-\epsilon} / |a|^2 \leq (h^{1-\epsilon'} / |a|)^2. \end{aligned}$$

Hence the solution of (2.10) is negligible as long as $|a| \geq h^\delta$, $\delta < 1$.

We come back to the estimation of the true nonlinear correction term w . We proceed as in the model case (2.10) and use the energy method as in (2.11), now with

$$I(t) \stackrel{\text{def}}{=} \|w(t)\|_{L^2}^2 + \|P_h w(t)\|_{L^2}^2.$$

We recall (2.8):

$$(ih\partial_t + P_h)w = h^2|a| (\mathcal{O}(|v|^2|w|) + \mathcal{O}(|v||w|^2) + \mathcal{O}(|w|^3)) - P_h v,$$

which using (2.11) gives,

$$(2.12) \quad \frac{d}{dt} \|w(t)\|_{L^2} = \mathcal{O}(1/h) (h^2|a| (\langle |v||w|^2, |w| \rangle + \langle |w|, |w||v|^2 \rangle + \langle |w|^3, |w| \rangle) + \langle |P_h w|, |v| \rangle).$$

The operator applied to w , $P_h w$, satisfies the equation

$$\begin{aligned} (ih\partial_t + P_h)P_h w &= h^2 a (\mathcal{O}(vP_h v)w + \mathcal{O}(v^2)P_h w + \mathcal{O}(P_h v)w^2 + \mathcal{O}(v)wP_h w \\ &\quad + \mathcal{O}(w^2)P_h w + \mathcal{O}(|h\nabla v|^2)w + \mathcal{O}(v|h\nabla v||h\nabla w|) \\ &\quad + \mathcal{O}(v|h\nabla w|^2) + \mathcal{O}(|h\nabla w|^2 w)) - P_h^2 v, \end{aligned}$$

and the same method as in (2.11) gives

$$\begin{aligned} (2.13) \quad \frac{d}{dt} \|P_h w(t)\|_{L^2} &= \mathcal{O}(1/h) \left(|a|h^2 (\langle |vP_h v| |w|, |P_h w| \rangle + \langle |v|^2 |P_h w|, |w| \rangle + \langle |P_h v| |w|^2, |P_h w| \rangle \right. \\ &\quad + \langle |v| |w| |P_h w|, |P_h w| \rangle + \langle |w|^2, |P_h w|^2 \rangle + \langle |h\nabla v|^2 |w|, |P_h w| \rangle + \langle |v| |h\nabla v| |h\nabla w|, |P_h w| \rangle \\ &\quad \left. + \langle |v| |h\nabla w|^2, |P_h w| \rangle + \langle |h\nabla w|^2 |w|, |P_h w| \rangle + \langle |P_h^2 v|, |P_h w| \rangle \right), \end{aligned}$$

By putting (2.12) and (2.13) we obtain

$$\begin{aligned} (2.14) \quad \frac{dI}{dt} &\leq C|a|h(\|v\|_{L^\infty}^2 I(t) + \|w\|_{L^4}^4 + \|v\|_{L^2} \|w\|_{L^6}^3 + \|v\|_{L^\infty} \|P_h v\|_{L^\infty} I(t) \\ &\quad + \|P_h v\|_{L^\infty} \|w\|_{L^4}^2 I(t)^{\frac{1}{2}} + \|v\|_{L^\infty} \|w\|_{L^\infty} I(t) \\ &\quad + \|w\|_{L^\infty}^2 I(t) + \|h\nabla v\|_{L^\infty}^2 I(t) + \|v\|_{L^\infty} \|h\nabla w\|_{L^4}^2 I(t)^{\frac{1}{2}} \\ &\quad + \|w\|_{L^\infty} \|h\nabla w\|_{L^4}^2 I(t)^{\frac{1}{2}} + \|v\|_{L^2} I(t)^{\frac{1}{2}} + \|P_h v\|_{L^2}^2 I(t)^{\frac{1}{2}}, \end{aligned}$$

where all the norms are taken in $L^p(\mathbb{R}^3)$ at time t .

We need the following cases of Lemma 2.3:

$$\begin{aligned} (2.15) \quad \|h\nabla f\|_{L^4(\mathbb{R}^3)} + \|f\|_{L^4(\mathbb{R}^3)} &\leq Ch^{-3/4}(\|P_h f\|_{L^2} + \|f\|_{L^2}), \\ \|f\|_{L^6(\mathbb{R}^3)} &\leq Ch^{-1}(\|P_h f\|_{L^2} + \|f\|_{L^2}), \\ \|f\|_{L^\infty(\mathbb{R}^3)} &\leq Ch^{-3/2}(\|P_h f\|_{L^2} + \|f\|_{L^2}). \end{aligned}$$

Using (2.15) to estimate the terms involving w in (2.13) and in (2.8), and using Lemma 2.2 to estimate the terms involving v , we see that (2.14) implies

$$(2.16) \quad \frac{dI(t)}{dt} \leq C|a|h^{-2} \left((1 + |ath^{-2}|^2)(I(t) + I(t)^{\frac{3}{2}}) + I(t)^{\frac{5}{2}} \right) + Ch^{-1} I(t)^{\frac{1}{2}} (1 + |ath^{-2}|^2).$$

Since $I(0) = 0$, we can use a bootstrap argument to show that for $0 < t < h^2|a|\log(1/h)^\alpha$,

$$I(t) \leq (h^{1-\epsilon'} / |a|)^2 \leq h^\epsilon,$$

if $|a| > h^\delta$, $\delta < 1$. For the reader's convenience we briefly recall the standard argument.

Consider the set

$$J = \{t : I(s) \leq h^\beta, 0 \leq s \leq t\} \cap [0, |a|h^2 \log(1/h)^\alpha].$$

Then $J \neq \emptyset$ as $I(0) = 0$, J is clearly closed as $I(t)$ is continuous, and the same Gronwall inequality applied to (2.11) shows that J is open. Hence $J = [0, |a|h^2 \log(1/h)^\alpha]$.

To summarize, we conclude that for $|a| \geq h^\delta$ for some $\delta < 1$ the ansatz v dominates the solutions for times of the order $|a|^{-1}h^2 \log(1/h)^\alpha$.

Remark. It is an interesting question which other initial conditions can produce similar effects, in particular what level of localization is necessary. A natural localization from the point of view of quantum mechanics is given by initial data of the form

$$u_h^j(x) = h^{-\frac{3}{4}} \phi \left(\frac{x - x_j}{h^{\frac{1}{2}}} \right).$$

To see the instability in this case let us consider an example discussed in §3: $V(x) = |x|^2$. Then the unitary transformation $\tilde{u}(\tilde{x}) = h^{\frac{3}{4}}u(h^{\frac{1}{2}}\tilde{x})$ changes the equation (1.4) to

$$i\partial_t\tilde{u} = -\Delta\tilde{u} + |\tilde{x}|^2u + ah^{-\frac{1}{2}}|\tilde{u}|^2\tilde{u}.$$

An argument similar to that above shows that for $a \geq h^{\frac{1}{2}+\epsilon}$, $\epsilon > 0$ and $|x_1 - x_2| \sim h^{\frac{1}{2}}(\log(1/h))^\alpha$ we have (1.6).

3. GEOMETRIC INSTABILITY

In this section we will consider a class of cylindrically symmetric potentials with the principal example given by the harmonic oscillator $V(x) = |x|^2$:

$$(3.1) \quad \begin{aligned} ih\partial_t u &= -h^2\Delta u + V(x) + ah^2|u|^2u, \quad u = u_h(t, x), \quad x \in \mathbb{R}^3, \\ V(R_\theta x) &= V(x), \quad \theta \in [0, 2\pi), \quad \partial^\alpha V(x) = \mathcal{O}(\langle x \rangle^m), \quad V(x) \geq \langle x \rangle^m/C - 1, \end{aligned}$$

where R_θ is the angle θ -rotation with respect to the x_3 axis. The equation (3.1) is ‘‘gauge invariant’’ and consequently, if the initial data satisfies $u_{t=0}(R_\theta x) = e^{in\theta}u_{t=0}(x)$, then the solution satisfies the same invariance for any t . Let us write

$$(3.2) \quad V_n = \{u \in L^2(\mathbb{R}^3) : R_\theta^*u = e^{in\theta}u\}.$$

The operator $P_h|_{V_n}$ can be considered as an operator on $\mathbb{R} \times \mathbb{R}_+$:

$$P_h|_{V_n} = (hD_y)^2 + (hD_r)^2 - i\frac{h}{r}hD_r + V(r, y) + \frac{(nh)^2}{r^2}.$$

We choose $n = n(h)$ so that

$$nh = 1 + \mathcal{O}(h).$$

Suppose that the potential $V(r, y) + r^{-2}$ has a non-degenerate absolute minimum at (y_0, r_0) with the value V_0 . The standard analysis (see for instance [4]) shows that

$$P_h|_{V_n} = \sum_{j=0}^{\infty} \lambda_j e_j \otimes e_j^*,$$

where \bullet^* denotes complex conjugation and,

$$\begin{aligned} e_0(x) &\sim e^{in\theta}\tilde{e}_0(r, y), \quad \frac{1}{C\sqrt{h}}e^{((y-y_0)^2+(r-r_0)^2)/(Ch)} \leq \tilde{e}_0(r, y) \leq \frac{C}{\sqrt{h}}e^{C((y-y_0)^2+(r-r_0)^2)/h}, \\ \lambda_0 &\sim V_0, \quad \lambda_1 - \lambda_0 > h/C, \end{aligned}$$

and from the point of view of counting functions $\lambda_j \sim hj^{1/2}$. Much more precise estimates for e_0 and the counting function are available but this is sufficient for us.

We can now state the precise version of (1.7):

Theorem 2. *Let V be a cylindrically symmetric potential satisfying the assumptions above. Suppose that e_0 is the ground state of $P_h|_{V_n}$, where V_n is given by (3.2) with $nh \sim 1$, and that two initial conditions for (3.1) are given by*

$$(3.3) \quad u_j^h(x) = \kappa_j e_0(x), \quad j = 1, 2, \quad \kappa_1 = \kappa, \quad \kappa_2 = \kappa + \epsilon, \quad \kappa^4 a \ll 1,$$

Then for $t(a\kappa^4)^{3/2} \ll \epsilon\kappa at \ll 1$,

$$(3.4) \quad \frac{\|u_h^1(t) - u_h^2(t)\|_{L^2}}{\|u_h^1(0) - u_h^2(0)\|_{L^2}} \geq (t\kappa a + 1)/C,$$

uniformly in h , $a \ll 1$, $a\kappa^4 \ll 1$, and $\kappa \geq 1$.

3.1. The instability. We first discuss the consequences of the theorem. Since we can take $\kappa \sim 1$, $a \sim h^\delta$, $t \sim h^{-\gamma}$, $\epsilon \sim h^\rho$,

$$\delta < \gamma < \frac{3}{2}\delta, \gamma - \delta < \rho < \frac{3}{2}\delta - \gamma,$$

we obtain,

$$\frac{\|u_h^1(t) - u_h^2(t)\|_{L^2}}{\|u_h^1(0) - u_h^2(0)\|_{L^2}} \geq h^{\delta-\gamma}/C \longrightarrow \infty, \quad h \longrightarrow 0,$$

and (1.7) follows. That choice of parameters might be interesting since a is the (renormalized) scattering length: that is the essential ‘‘interaction’’ size of the molecules forming the condensate.

As we will see, for $a\kappa^4 \ll 1$, the phase of the solution of (3.1) with the initial data $\kappa e_0(x)$ is essentially $t\lambda_0/h + \kappa^2 at$. The ‘‘non-linear’’ phase shift produces instability (3.4) but since it is global in x we do not have instability using the projective norms (1.5).

3.2. Structure of the solution. Denote by u the solution of (3.1) with initial data $\kappa e_0(x)$. We recall the two standard conservation laws:

$$(3.5) \quad \|u\|_{L^2}^2(t) = \|u\|_{L^2}^2(0) = \kappa^2,$$

and

$$(3.6) \quad E(u)(t) = \int |h\nabla u|^2 + |x|^2|u|^2 + \frac{1}{2}h^2a|u|^4 = E(u)(0)$$

We write $E = E_{\text{lin}} + E_{\text{int}}$, grouping kinetic and exterior energies together in E_{lin} .

We have $E(u)(0) = \kappa^2\lambda_0 + \kappa^4F_h$ where $\lambda_0 \sim 1$ is the ground energy of $P_h \upharpoonright_{V_n}$ and

$$F_h = h^2a\|e_0\|_{L^4}^4 \sim ah.$$

To obtain estimates in the nonlinear propagation, we slightly modify the argument of [2]. For that we decompose u on the L^2 basis of eigenfunctions of the operator $P_h \upharpoonright_{V_n}$:

$$(3.7) \quad \begin{aligned} u(t, x) &= \kappa e^{-\frac{it}{h}(\lambda_0 + \kappa^2 F_h)} \gamma(t) e_0(x) + \sum_{j=1}^{\infty} u_j(t) e_j(x) \\ &= \kappa e^{-\frac{it}{h}(\lambda_0 + \kappa^2 F_h)} \gamma(t) e_0(x) + q(t, x). \end{aligned}$$

To estimate the norm of $q(t, \bullet)$ we write

$$\begin{aligned} E_{\text{int}}(0) &= E(0) - E_{\text{lin}}(0) \\ &= E(0) - \lambda_0 \|u(0)\|_{L^2}^2 \\ &= E(t) - \lambda_0 \|u(t)\|_{L^2}^2, \end{aligned}$$

with the last equality following from the conservation laws (3.5) and (3.6). Since $E_{\text{int}}(0) = \kappa^4 F_h \sim ah\kappa^4$ and

$$E(t) = E_{\text{lin}}(t) + E_{\text{int}}(t) = \kappa\lambda_0|\gamma(t)|^2 + \sum_{j=1}^{\infty} \lambda_j |u_j(t)|^2 + \frac{ah^2}{2} \|u\|_{L^4}^4(t),$$

we conclude that

$$(3.8) \quad C\kappa^4 ah \geq \sum_{j=1}^{\infty} (\lambda_j - \lambda_0) |u_j(t)|^2 + \frac{ah^2}{2} \|u\|_{L^4}^4(t) \geq h \|q(t)\|_{L^2}^2 + \frac{ah^2}{2} \|u\|_{L^4}^4(t),$$

as $\lambda_j - \lambda_0 \geq h$ for $j \geq 1$. Thus

$$(3.9) \quad \|q(t)\|_{L^2}^2 + ah \|u\|_{L^4}^4(t) \leq C a \kappa^4.$$

On the other hand

$$\|q(t)\|_{L^2}^2 = \|u\|_{L^2}^2(t) - \kappa^2 |\gamma(t)|^2 = \kappa^2 (1 - |\gamma(t)|^2)$$

Combined with (3.9) we obtain $\kappa^2(1 - |\gamma(t)|^2) \leq Ca\kappa^4$, that is,

$$(3.10) \quad |1 - |\gamma(t)|| \leq Ca\kappa^2.$$

and consequently, according to (3.9)

$$(3.11) \quad \begin{aligned} \|q\|_{L^4}^4(t) &\leq Ch^{-1} (\kappa^4 + h\|\kappa\gamma(t)e_0\|_{L^4}^4) \\ &\leq Ch^{-1}\kappa^4 (1 + Ca\kappa^2hh^{-1}) \leq Ch^{-1}\kappa^4(1 + a\kappa^2). \end{aligned}$$

Since $\gamma(0) = 1$ the estimates (3.9) and (3.10) show that for $a\kappa^2 \leq a\kappa^4 \ll 1$ the term corresponding to first eigenfunction dominates in the non-linear propagation.

3.3. Non-linear propagation of leading term. From the formula for $\gamma(t)$:

$$\gamma(t) = e^{it(\lambda_0 + \kappa^2 F_h)/h} \langle u, e_0 \rangle,$$

we derive the equation satisfied by γ :

$$(3.12) \quad ih\dot{\gamma} - \kappa^2 F_h(1 - |\gamma|^2)\gamma = -\kappa^2 ah^2 (2\zeta|\gamma|^2 + \bar{\zeta}\gamma^2 + 2\epsilon\gamma + \eta\bar{\gamma} + \sigma)$$

where

$$\begin{aligned} \zeta &= (q, |e_0|^2 e_0)_{L^2} \implies |\zeta| \leq \|q\|_{L^2} \|e_0\|_{L^6}^3 \leq Ca^{1/2}\kappa^2 h^{-1} \\ \epsilon &= \int |e_0|^2 |q|^2, \quad \eta = \int q^2 \bar{e}_0^2 \implies |\eta| \leq \epsilon \leq \|e_0\|_{L^\infty}^2 \|q\|_{L^2}^2 \leq Ch^{-1} a\kappa^4 \\ \sigma &= \int |q|^2 q e_0 \implies |\sigma| \leq \|e_0\|_{L^\infty} \|q\|_{L^3}^3 \leq \|e_0\|_{L^\infty} \|q\|_{L^4}^2 \|q\|_{L^2} \leq Ch^{-1} \kappa^4 a^{1/2} \end{aligned}$$

If $a\kappa^4 \ll 1$, with κ large, we obtain

$$(3.13) \quad |\dot{\gamma}| \leq Ca\kappa^2 (a^{1/2}\kappa^2(1 + Ca\kappa^4) + a\kappa^4 + a^{1/2}\kappa^4) \leq C'(a\kappa^4)^{3/2}.$$

Thus

$$\gamma(t) = 1 + \mathcal{O}(t(a\kappa^4)^{3/2}),$$

and for $t \ll (a\kappa^4)^{-3/2}$, $\gamma(t) \simeq 1$.

Proof of Theorem 2: Due to our estimates we need to consider the leading term

$$\kappa\gamma(t)e^{-it(\lambda_0 + F_h\kappa^2)/h}, \quad F_h \sim ah.$$

We now note that, in the notation of (3.3),

$$\left| e^{it\kappa_1^2 F_h/h} - e^{it\kappa_2^2 F_h/h} \right| \simeq 2\epsilon\kappa t F_h/h,$$

for $\kappa\epsilon t F_h/h \sim \epsilon t a\kappa \ll 1$. Since that difference gives a lower bound for $\|u_h^1(t) - u_h^2(t)\|/\kappa$ with an error $\mathcal{O}(t(a\kappa^4)^{3/2})$. Since

$$\|u_h^1(0) - u_h^2(0)\| = \epsilon,$$

we obtain (3.4). □

3.4. Projective instability. Following a suggestion of Mike Christ we modify the above construction to obtain a stronger projective instability (1.8) along a sequence of h_k 's. For that we assume that, in the notation of Theorem 2,

The function $(r, y) \mapsto V(r, y) + r^{-2}$ has two distinct absolute non-degenerate minima (r_j, y_j) , $j = 1, 2$, and its Hessians at (r_j, y_j) are equal.

In this case, with $V_0 = V(r_j, y_j)$,

$$P_h \upharpoonright_{V_n} = \sum_{k,j=1}^2 a_{kj} e_0^k \otimes e_0^j + \sum_{j=1}^{\infty} \lambda_j e_j \otimes e_j^*,$$

$$(3.14) \quad e_0^j(x) \sim e^{in\theta} \tilde{e}_0^j(r, y), \quad \frac{1}{C\sqrt{h}} e^{-((y-y_j)^2+(r-r_j)^2)/(Ch)} \leq \tilde{e}_0^j(r, y) \leq \frac{C}{\sqrt{h}} e^{-C((y-y_j)^2+(r-r_j)^2)/h},$$

$$(3.15) \quad \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} \lambda_0^1 & \mathcal{O}(h^\infty) \\ \mathcal{O}(h^\infty) & \lambda_0^2 \end{pmatrix}, \quad \lambda_0^1 - \lambda_0^2 = \mathcal{O}(|nh - 1| + h^2),$$

see [4, Theorem 6.10]. The functions e_0^j , $j = 1, 2$, are very close to linear combinations of the eigenfunctions corresponding to the lowest eigenvalues of $P \upharpoonright_{V_n}$. They are almost orthogonal to e_k with $k > 0$:

$$\langle e_k, e_0^j \rangle = \mathcal{O}(h^\infty).$$

If we choose a sequence of h 's for which $|nh - 1| = \mathcal{O}(h^2)$ then

$$\lambda_j - \lambda_0^k > h/C, \quad j > 0.$$

Suppose now that we solve (3.1) with

$$u_h(0, x) = \kappa_1 e_0^1(x) + \kappa_2 e_0^2(x),$$

where $0 \leq \kappa_j \sim \kappa$. Let a, t and κ satisfy the assumptions of Theorem 2:

$$(3.16) \quad a\kappa^4 \ll 1, \quad t \ll (a\kappa^4)^{-3/2}, \quad \kappa \gg 1,$$

and in addition assume that these parameters are h -tempered, by requiring that

$$a > h^N.$$

Then

$$u_h(t, x) = \kappa_1 e^{i(\lambda_0^1 + F_h \kappa_1^2)/h} \gamma_1(t) e_0^1(x) + \kappa_2 \gamma_2(t) e^{i(\lambda_0^2 + F_h \kappa_2^2)/h} e_0^2(x) + q(t, x),$$

where, using the same argument as before, we can show that $\gamma_j(t)$ is bounded and $q(t, x)$ satisfies estimates (3.8), (3.9). On the other hand the modes e_0^1 and e_0^2 do not interact (see (3.14)), and hence the estimates on q give

$$\left| \frac{d}{dt} |\gamma_j|^2 \right| \leq C_M \left(h^M + (a\kappa^4)^{3/2} \right)$$

As a consequence we obtain

$$|1 - |\gamma_j|^2| \leq Ct(a\kappa^4)^{3/2},$$

and coming back to the equation satisfied by γ_j ,

$$\gamma_j(t) = 1 + \mathcal{O}(t(a\kappa^4)^{3/2}) + \mathcal{O}(t^2 a^{5/2} \kappa^8) = 1 + \mathcal{O}(t(a\kappa^4)^{3/2}).$$

The last equality came from noticing that (3.16) implies that

$$t^2 a^{5/2} \kappa^8 = (t(a\kappa^4)^{3/2})^2 (a\kappa^4)^{-1/2} \kappa^{-2} \leq t(a\kappa^4)^{3/2}.$$

Now suppose that we take another initial condition,

$$\tilde{u}_h(x, 0) = (\kappa_1 + \epsilon) e_0^1(x) + (\kappa_2 + \epsilon) e_0^2(x), \quad \epsilon > h^N.$$

We first check that

$$(3.17) \quad d_{\text{pr}}(u_h(0), \tilde{u}_h(0)) \sim \epsilon |\kappa_1 - \kappa_2| / \kappa.$$

In fact, the left hand side is equal to

$$\cos^{-1} \left(\frac{\kappa_1(\kappa_1 + \epsilon) + \kappa_2(\kappa_2 + \epsilon)}{(\kappa_1^2 + \kappa_2^2)^{1/2} ((\kappa_1 + \epsilon)^2 + (\kappa_2 + \epsilon)^2)^{1/2}} + \mathcal{O}(h^\infty) \right).$$

Putting $\vec{\kappa} = (\kappa_1, \kappa_2)$ and $\vec{a} = (1, 1)$ the main term inside \cos^{-1} is

$$\begin{aligned} \frac{\|\vec{\kappa}\|^2 + \epsilon \langle \vec{a}, \vec{\kappa} \rangle}{\|\vec{\kappa}\|^2 (1 + 2\epsilon \langle \vec{\kappa}, \vec{a} \rangle / \|\vec{\kappa}\|^2 + \epsilon^2 \|\vec{a}\|^2 / \|\vec{\kappa}\|^2)^{\frac{1}{2}}} &= 1 - \epsilon^2 \left(\frac{\|\vec{a}\|^2}{2\|\vec{\kappa}\|^2} - \frac{\langle \vec{a}, \vec{\kappa} \rangle^2}{2\|\vec{\kappa}\|^4} \right) + \mathcal{O} \left(\frac{\epsilon^2}{\|\vec{\kappa}\|^3} \right) \\ &= 1 - \epsilon^2 \frac{(\kappa_1 - \kappa_2)^2}{2(\kappa_1^2 + \kappa_2^2)} + \mathcal{O} \left(\frac{\epsilon^3}{\kappa^3} \right). \end{aligned}$$

We now estimate the projective distance between $u_h(t)$ and $\tilde{u}_h(t)$. For that we assume that

$$(3.18) \quad |\kappa_1 - \kappa_2| \sim \kappa, \quad a\kappa^4 \ll \epsilon \ll 1, \quad t^2 a^3 \kappa^{14} \ll \epsilon, \quad 1 \ll t\kappa a,$$

noting that (3.18) imply previously made assumptions. In particular we have $\epsilon \ll \epsilon a t \kappa$. Then using the previous estimates,

$$\begin{aligned} \langle u_h(t), \tilde{u}_h(t) \rangle &= \sum_{j=1}^2 \kappa_j (\kappa_j + \epsilon) e^{it(\kappa_j^2 - (\kappa_j + \epsilon)^2 F_h)/h} + \mathcal{O}(\kappa^{14} t^2 a^3) + \mathcal{O}(a\kappa^4) + \mathcal{O}(h^\infty) \\ &= \sum_{j=1}^2 \kappa_j^2 e^{it(\kappa_j^2 - (\kappa_j + \epsilon)^2 F_h)/h} + \mathcal{O}(\epsilon). \end{aligned}$$

We then have

$$\frac{|\langle u_h(t), \tilde{u}_h(t) \rangle|^2}{\|u_h(t)\|^2 \|\tilde{u}_h(t)\|^2} = \frac{\kappa_1^4 + \kappa_2^4 + 2\kappa_1^2 \kappa_2^2 \cos(t(\kappa_1 - \kappa_2)\epsilon F_h/h)}{(\kappa_1^2 + \kappa_2^2)^2} + \mathcal{O}(\epsilon),$$

and consequently,

$$d_{\text{pr}}(u_h(t), \tilde{u}_h(t)) \sim \epsilon \kappa a t.$$

This gives the following

Theorem 3. *Suppose that $V(x)$ in (3.1) satisfies the assumption of §3.4 and that the initial conditions are chosen as above with the parameters satisfying (3.18). Then for a sequence of h satisfying*

$$nh = 1 + \mathcal{O}(h^2),$$

we have

$$\frac{d_{\text{pr}}(u_h(t), \tilde{u}_h(t))}{d_{\text{pr}}(u_h(0), \tilde{u}_h(0))} \sim 1 + \kappa a t.$$

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