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Finite-Time Singularities of Solutions of a Class of Nonlinear Schrödinger Equations

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Solutions to the initial-boundary value problem for a class of nonlinear Schrödinger equations are considered. Sufficient conditions are found so that the solutions do not exist for all times $t > 0$. An explicit upper bound of the t interval of existence of the solutions is obtained. The time evolution of a singularity is demonstrated numerically in the case of the one-dimensional Schrödinger equation.

1. INTRODUCTION

The nonlinear Schrödinger equation occurs in many applications of physical sciences; for a review see Kivshar and Malomed (1989). For recent mathematical studies see Gridnev *et al.* (1996), Kamvissis (1996), Mahmood (1996), and Pelinovsky and Grimshaw (1996).

In the present paper we investigate finite-time singularities of solutions for the initial-boundary value problem of Schrödinger equations with potential term $U(x)\Psi$, nonlinear term $f(|\Psi|^2)\ \Psi$, and antidamping $i\alpha\Psi$ with $\alpha \geq 0$. Finite upper bounds are worked out for the time where a singularity evolves. This is done for bounded space domains in R^n, $n = 1, 2, \ldots$ In particular, we are interested in what type of singularity appears.

For other types of Schrödinger equations similar studies are carried out in Bainov and Minchev (1996), De Bouard (1991), Domarkas (1991), Glassey (1977), Nawa and Tsutsumi (1989), and Zakharov (1972).

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2. PRELIMINARY NOTES

Let $\Omega \subset R^n$ be a bounded domain containing the origin, with boundary $\partial\Omega$ and $\overline{\Omega} = \Omega \cup \partial\Omega$. The smoothness of $\partial\Omega$ must allow the application of the divergence theorem, that is, $\partial\Omega$ is a C^1-smooth or piecewise smooth boundary. We assume that $x \cdot \nu \geq 0$ for any fixed $x = (x_1, \ldots, x_n) \in \partial\Omega$, where ν is the unit outward normal vector at the same point.

Consider the initial-boundary value problem (IBVP) for the following nonlinear Schrödinger equation:

$$i\Psi_t = -\Delta\Psi + U(x)\Psi - f(|\Psi|^2)\,\Psi + i\alpha\Psi, \quad t > 0, \quad x \in \Omega \tag{1}$$

$$\Psi(0, x) = \Psi_0(x), \qquad x \in \overline{\Omega} \tag{2}$$

$$\Psi(t, x)|_{x \in \partial\Omega} = 0, \qquad t \geq 0 \tag{3}$$

where $U \in C^1(\overline{\Omega}, R)$ and $f \in C(R_+, R)$ are given functions, Ψ_0 is a given complex-valued function, and $\alpha \geq 0$ is a constant. We note that equivalent forms of equation (1) as found in the literature can be obtained by writing the complex conjugate of (1) and substituting $U(x) \to -U(x)$, $f \to -f$, $\overline{\Psi} \to \Psi$, where $\overline{\Psi}$ denotes the complex conjugate of Ψ.

Definition 1. The function Ψ which is defined on $[0, T_\Psi) \times \overline{\Omega}$ $(0 < T_\Psi \leq +\infty)$ is called a solution of the IBVP (1)–(3) if:

(i) Ψ and $\nabla\Psi$ are continuous in $[0, T_\Psi) \times \overline{\Omega}$.

(ii) The derivatives Ψ_t, Ψ_{tx_j}, and $\Psi_{x_i x_j}$ $(i, j = 1, \ldots, n)$ exist and are continuous in $(0, T_\Psi) \times \overline{\Omega}$.

(iii) Ψ satisfies (1)–(3).

Furthermore, let

$$L^q(\Omega) = \left\{\Psi : \|\Psi\|_{q,\Omega} = \left(\int_\Omega |\Psi(x)|^q\,dx\right)^{1/q} < +\infty\right\}$$

Lemma 1. Each solution Ψ of the IBVP (1)–(3) satisfies the relation

$$\|\Psi(t)\|^2_{2,\Omega} = \|\Psi_0\|^2_{2,\Omega} e^{2\alpha t} \qquad \text{for} \quad t \in [0, T_\Psi) \tag{4}$$

Proof. Multiplying both sides of (1) by $\overline{\Psi}$, taking the imaginary part, and integrating, we obtain

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |\Psi|^2\,dx = \alpha\int_\Omega |\Psi|^2 dx \tag{5}$$

which gives (4). ∎

Now we define

$$F(s) = \int_0^s f(u)\, du \qquad (0 \le s < +\infty) \tag{6}$$

Lemma 2. Suppose that $\alpha \ge 0$, and

$$F(s) \le sf(s), \qquad \forall s \ge 0 \tag{7}$$

Then each solution Ψ of the IBVP (1)–(3) satisfies the inequality

$$\|\nabla\Psi\|_{2,\Omega}^2 + \int_\Omega U(x)|\Psi|^2\, dx - \int_\Omega F(|\Psi|^2)\, dx \le E_0 e^{2\alpha t}, \qquad t \in [0, T_\Psi) \tag{8}$$

where

$$E_0 = \|\nabla\Psi_0\|_{2,\Omega}^2 + \int_\Omega U(x)|\Psi_0|^2\, dx - \int_\Omega F(|\Psi_0|^2)\, dx \tag{9}$$

Proof. We multiply both sides of equation (1) by $\overline{\Psi}_t$. Then, taking the real part and integrating, we obtain

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}\int_\Omega |\nabla\Psi|^2\, dx + \frac{1}{2}\frac{d}{dt}\int_\Omega U(x)|\Psi|^2\, dx - \frac{1}{2}\frac{d}{dt}\int_\Omega F(|\Psi|^2)\, dx \\ &\quad = -\alpha\, \mathrm{Im} \int_\Omega \overline{\Psi}\Psi_t\, dx \\ &\quad = \alpha\, \mathrm{Re} \int_\Omega \overline{\Psi}\, [-\Delta\Psi + U(x)\Psi - f(|\Psi|^2)\, \Psi + i\alpha\Psi]\, dx \end{aligned} \tag{10}$$

Making use of (7), we can write

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}\left\{\|\nabla\Psi\|_{2,\Omega}^2 + \int_\Omega U(x)|\Psi|^2 dx - \int_\Omega F(|\Psi|^2)\, dx\right\} \\ &\quad = \alpha\left\{\|\nabla\Psi\|_{2,\Omega}^2 + \int_\Omega U(x)|\Psi|^2 dx - \int_\Omega F(|\Psi|^2)\, dx\right\} \\ &\qquad + \alpha\int_\Omega [F(|\Psi|^2) - f(|\Psi|^2)|\Psi|^2]\, dx \\ &\quad \le \alpha\left\{\|\nabla\Psi\|_{2,\Omega}^2 + \int_\Omega U(x)|\Psi|^2\, dx - \int_\Omega F(|\Psi|^2)\, dx\right\} \end{aligned} \tag{11}$$

Integration of the last inequality yields (8). ■

3. MAIN RESULTS

We introduce the following assumptions:

H1. $E_0 < 0$,
H2. $E_0 = 0$, $S(0) < 0$,
H3. $E_0 > 0$, $S(0) < 0$, $S^2(0) > 16E_0W(0)$.

Here

$$S(t) = 4\,\mathrm{Im}\int_\Omega (x\cdot\nabla\Psi)\overline{\Psi}\,dx \qquad (0 \le t < T_\psi) \tag{12}$$

and

$$W(t) = \int_\Omega |x|^2|\Psi|^2\,dx \qquad (0 \le t < T_\psi) \tag{13}$$

Theorem 1. Let the following conditions hold:
(*i*) One of the assumptions H1–H3 is satisfied, and $\alpha \ge 0$.
(*ii*) We have

$$\max\left\{F(s), \left(1 + \frac{2}{n}\right)F(s)\right\} \le sf(s), \qquad \forall s \ge 0 \tag{14}$$

(*iii*) We have

$$2U(x) + x\cdot\nabla U(x) \ge 0, \qquad \forall x \in \overline{\Omega} \tag{15}$$

Then the solution Ψ of the IBVP (1)–(3) does not globally exist and the time interval is bounded by

$$T_\psi \le T_{\psi_0} = 2W(0)\{[S^2(0) - 16E_0W(0)]^{1/2} - S(0)\}^{-1} \tag{16}$$

Proof. Multiply both sides of (1) by $|x|^2\overline{\Psi}$. Then, taking the imaginary part and integrating, we obtain

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |x|^2|\Psi|^2\,dx = -\mathrm{Im}\int_\Omega \mathrm{div}(\overline{\Psi}\nabla\Psi)\,|x|^2\,dx + \alpha\int_\Omega |x|^2|\Psi|^2\,dx \tag{17}$$

The first term on the right-hand side of (17) can be rewritten as

$$-\mathrm{Im} \int_\Omega \operatorname{div}(\overline{\Psi}\nabla\Psi)|x|^2\, dx = 2\ \mathrm{Im} \int_\Omega (x \cdot \nabla\Psi)\overline{\Psi}\, dx \tag{18}$$

Thus (17) takes on the form

$$\frac{dW}{dt} - 2\alpha W = S \tag{19}$$

Next we consider

$$\begin{aligned} \frac{dS}{dt} &= 4\ \mathrm{Im} \int_\Omega (x \cdot \nabla\Psi_t)\overline{\Psi}\, dx + 4\ \mathrm{Im} \int_\Omega (x \cdot \nabla\Psi)\overline{\Psi}_t\, dx \\ &= -4n\ \mathrm{Im} \int_\Omega \Psi_t\overline{\Psi}\, dx - 8\ \mathrm{Im} \int_\Omega (x \cdot \overline{\nabla\Psi})\Psi_t\, dx \end{aligned} \tag{20}$$

The first term on the right-hand side of (20) can be written as

$$\begin{aligned} -4n\ \mathrm{Im} \int_\Omega \Psi_t\overline{\Psi}\, dx &= 4n\|\nabla\Psi\|_{2,\Omega}^2 + 4n \int_\Omega U(x)|\Psi|^2\, dx \\ &\quad - 4n \int_\Omega f(|\Psi|^2)|\Psi|^2\, dx \end{aligned} \tag{21}$$

The second term on the right-hand side of (20) can be written as

$$\begin{aligned} &-8\ \mathrm{Im} \int_\Omega (x \cdot \overline{\nabla\Psi})\Psi_t\, dx \\ &= 8\ \mathrm{Re} \int_\Omega (x \cdot \overline{\nabla\Psi})[-\Delta\Psi + U(x)\Psi - f(|\Psi|^2)\Psi + i\alpha\Psi]\, dx \\ &= I_1 + I_2 + I_3 + 2\alpha S \end{aligned} \tag{22}$$

where

$$I_1 = -8\ \mathrm{Re} \int_\Omega (x \cdot \overline{\nabla\Psi})\Delta\Psi\, dx \tag{23}$$

$$\begin{aligned} &= -4 \sum_{j=1}^n \int_\Omega \left[x_j \frac{\overline{\partial\Psi}}{\partial x_j} \operatorname{div}(\nabla\Psi) + x_j \frac{\partial\Psi}{\partial x_j} \operatorname{div}(\overline{\nabla\Psi}) \right] dx \\ &= -4 \sum_{k,j=1}^n \int_\Omega \left[\frac{\partial}{\partial x_k}\left(x_j \frac{\overline{\partial\Psi}}{\partial x_j}\frac{\partial\Psi}{\partial x_k} \right) + \frac{\partial}{\partial x_k}\left(x_j \frac{\partial\Psi}{\partial x_j}\frac{\overline{\partial\Psi}}{\partial x_k} \right) \right] dx \end{aligned} \tag{24}$$

$$+ 4 \sum_{k,j=1}^{n} \int_{\Omega} \left[\delta_{kj} \overline{\frac{\partial \Psi}{\partial x_j}} \frac{\partial \Psi}{\partial x_k} + \delta_{kj} \frac{\partial \Psi}{\partial x_j} \overline{\frac{\partial \Psi}{\partial x_k}} \right] dx$$

$$+ 4 \sum_{j=1}^{n} \int_{\Omega} x_j \frac{\partial}{\partial x_j} (|\nabla \Psi|^2)\ dx \tag{25}$$

$$= -8 \operatorname{Re} \int_{\partial\Omega} (x \cdot \overline{\nabla \Psi})(v \cdot \nabla \Psi)\ d\sigma + (8 - 4n)\|\nabla \Psi\|^2_{2,\Omega}$$

$$+ 4 \int_{\partial\Omega} (x \cdot v)|\nabla \Psi|^2\ d\sigma \tag{26}$$

We further have

$$I_2 = 8 \operatorname{Re} \int_{\Omega} (x \cdot \overline{\nabla \Psi}) U(x) \Psi\ dx \tag{27}$$

$$= -4n \int_{\Omega} U(x)|\Psi|^2\ dx - 4 \int_{\Omega} (x \cdot \nabla U(x))|\Psi|^2\ dx$$

$$+ 4 \int_{\Omega} \operatorname{div}(xU(x)|\Psi|^2)\ dx \tag{28}$$

$$= -4n \int_{\Omega} U(x)|\Psi|^2\ dx - 4 \int_{\Omega} (x \cdot \nabla U(x))|\Psi|^2\ dx \tag{29}$$

Finally,

$$I_3 = -8 \operatorname{Re} \int_{\Omega} (x \cdot \overline{\nabla \Psi}) f(|\Psi|^2) \Psi\ dx \tag{30}$$

$$= 4n \int_{\Omega} F(|\Psi|^2)\ dx - 4 \int_{\Omega} \operatorname{div}(xF(|\Psi|^2))\ dx \tag{31}$$

$$= 4n \int_{\Omega} F(|\Psi|^2)\ dx \tag{32}$$

Therefore,

$$I_1 + I_2 + I_3$$

$$= 4(2 - n)\|\nabla \Psi\|^2_{2,\Omega} - 4n \int_{\Omega} U(x)|\Psi|^2\, dx \tag{33}$$

$$-4\int_{\Omega}(x\cdot\nabla U(x))|\Psi|^2\,dx+4n\int_{\Omega}F(|\Psi|^2)\,dx+4\int_{\partial\Omega}(x\cdot v)|\nabla\Psi|^2\,d\sigma$$
$$-8\,\mathrm{Re}\int_{\partial\Omega}(x\cdot\overline{\nabla\Psi})(v\cdot\nabla\Psi)\,d\sigma$$

Noting (3), we have Re $\nabla\Psi \parallel v$ and Im$\nabla\Psi \parallel v$ on $\partial\Omega$ and

$$\mathrm{Re}\int_{\partial\Omega}(x\cdot\overline{\nabla\Psi})(v\cdot\nabla\Psi)\,d\sigma=\int_{\partial\Omega}(x\cdot v)\,|\nabla\Psi|^2\,d\sigma \tag{34}$$

Thus, since $x\cdot v\geq 0$ for any $x\in\partial\Omega$, we get

$$-8\,\mathrm{Im}\int_{\Omega}(x\cdot\overline{\nabla\Psi})\Psi_t\,dx\leq 4(2-n)\|\nabla\Psi\|_{2,\Omega}^2+4n\int_{\Omega}F(|\Psi|^2)\,dx$$
$$-4n\int_{\Omega}U(x)|\Psi|^2\,dx-4\int_{\Omega}(x\cdot\nabla U(x))|\Psi|^2\,dx+2\alpha S \tag{35}$$

Therefore, by virtue of (21) and (8) and noting conditions (ii) and (iii) of Theorem 1, we obtain

$$\frac{dS}{dt}-2\alpha S\leq 8E_0e^{2\alpha t}-4\int_{\Omega}(2U(x)+x\cdot\nabla U(x))|\Psi|^2dx \tag{36}$$
$$+4(2+n)\int_{\Omega}F(|\Psi|^2)\,dx-4n\int_{\Omega}f(|\Psi|^2)|\Psi|^2\,dx\leq 8E_0e^{2\alpha t}$$

Consequently,

$$S(t)\leq(S(0)+8E_0t)e^{2\alpha t} \tag{37}$$

and in view of (19)

$$W(t)\leq(W(0)+S(0)t+4E_0t^2)e^{2\alpha t} \tag{38}$$

Clearly, the right-hand side of the last inequality becomes negative for $t>T_{\Psi_0}$ provided one of assumptions H1–H3 holds. This leads to a contradiction. ■

Remark 1. Let $f(|\Psi|^2)=\beta|\Psi|^{p-1}$ with $\beta>0$. Then condition (ii) of Theorem 1 is satisfied if $p\geq 1+4/n$.

Theorem 2. Let the conditions of Theorem 1 hold.

If

$$\lim_{t\to T_{\Psi*}} \int_{\Omega} |x|^2|\Psi|^2\, dx = 0 \tag{39}$$

where $T_{\Psi*}$ is the smallest positive zero of $W(t)$, then

$$\lim_{t\to T_{\Psi*}} \|\Psi(t)\|_{q,\Omega} = 0 \qquad \text{if} \quad 1 \le q < 2 \tag{40}$$

and

$$\lim_{t\to T_{\Psi*}} \|\Psi(t)\|_{q,\Omega} = +\infty \qquad \text{if} \quad 2 < q \le +\infty \tag{41}$$

Proof. Let $q \in [1, 2)$ be a fixed number. We choose a constant γ such that

$$0 < \gamma < \min\left\{q, \frac{n}{2}(2-q)\right\} \tag{42}$$

Then applying the Hölder inequality two times, we get with regard to (4)

$$\int_{\Omega} |\Psi|^q dx = \int_{\Omega} |x|^{-\gamma}|x|^{\gamma}|\Psi|^q\, dx \tag{43}$$

$$\le \left(\int_{\Omega} |x|^{-2\gamma/(2-q)}\, dx\right)^{(2-q)/2} \left(\int_{\Omega} |x|^{2\gamma/q}|\Psi|^2\, dx\right)^{q/2} \tag{44}$$

$$= A_0 \left(\int_{\Omega} |x|^{2\gamma/q}|\Psi|^{2\gamma/q}|\Psi|^{2(1-\gamma/q)}\, dx\right)^{q/2} \tag{45}$$

$$\le A_0 \left(\int_{\Omega} |x|^2|\Psi|^2\, dx\right)^{\gamma/2} \left(\int_{\Omega} |\Psi|^2\, dx\right)^{(q-\gamma)/2} \tag{46}$$

$$= A_0 \left(\int_{\Omega} |x|^2|\Psi|^2\, dx\right)^{\gamma/2} \|\Psi_0\|_{2,\Omega}^{q-\gamma}\, e^{\alpha(q-\gamma)t} \to 0 \tag{47}$$

as $t \to T_{\Psi*}$, $t < T_{\Psi*}$, where A_0 is a positive constant. Therefore,

$$\lim_{t\to T_{\Psi*}} \|\Psi(t)\|_{q,\Omega} = 0 \qquad \text{if} \quad 1 \le q < 2 \tag{48}$$

If $q > 2$, then we use the Hölder inequality once more to obtain

$$0 < \|\Psi_0\|_{2,\Omega}^2\, e^{2\alpha t} = \|\Psi(t)\|_{2,\Omega}^2 \le \|\Psi(t)\|_{q,\Omega}\, \|\Psi(t)\|_{s,\Omega} \tag{49}$$

where $s \in [1, 2)$ and $1/q + 1/s = 1$. Noting (40) and the assumption that

$$\int_{\Omega} |x|^2 |\Psi|^2 \, dx \to 0 \qquad \text{as} \quad t \to T_{\Psi^*}, \quad t < T_{\Psi^*} \tag{50}$$

we conclude

$$\lim_{t \to T_{\Psi^*}} \|\Psi(t)\|_{q,\Omega} = +\infty \qquad \text{if} \quad 2 < q \leq +\infty. \quad \blacksquare \tag{51}$$

Remark 2. Let the conditions of Theorem 2 hold. The inequality

$$\|\nabla\Psi\|_{2,\Omega} \geq \frac{n}{2} \frac{\|\Psi\|_{2,\Omega}^2}{\|x\Psi\|_{2,\Omega}} \tag{52}$$

implies that

$$\lim_{t \to T_{\Psi^*}} \|\nabla\Psi(t)\|_{2,\Omega} = +\infty \tag{53}$$

if $\int_{\Omega} |x|^2 |\Psi|^2 \, dx \to 0$ as $t \to T_{\Psi^*}$, $t < T_{\Psi^*}$.

Remark 3. Let us consider the IBVP for the following nonlinear Schrödinger equation with damping term ($\alpha < 0$):

$$i\Psi_t = -\Delta\Psi + U(x)\Psi - e^{\beta t} |\Psi|^{p-1} \Psi + i\alpha\Psi, \qquad t > 0, \quad x \in \Omega \tag{54}$$

$$\Psi(0, x) = \Psi_0(x), \qquad x \in \overline{\Omega} \tag{55}$$

$$\Psi(t, x)|_{x \in \partial\Omega} = 0, \qquad t \geq 0 \tag{56}$$

where β, p, α are given constants such that $p > 1$, $\alpha < 0$. Using the transformation $\Psi(t, x) = \exp[-\beta t/(p-1)] \, \phi(t, x)$, the IBVP (54)–(56) takes the form

$$i\phi_t = -\Delta\phi + U(x)\phi - |\phi|^{p-1} \phi + i\gamma\phi, \qquad t > 0, \quad x \in \Omega \tag{57}$$

$$\phi(0, x) = \Psi_0(x), \qquad x \in \overline{\Omega} \tag{58}$$

$$\phi(t, x)|_{x \in \partial\Omega} = 0, \qquad t \geq 0 \tag{59}$$

where $\gamma = \alpha + \beta/(p-1)$.

If we assume that $\beta \geq -\alpha(p-1)$, then $\gamma \geq 0$ and we obtain the IBVP with antidamping term, to which Theorems 1 and 2 can be applied.

Remark 4. The existence of the L^q—norms of Ψ in the interval $0 \leq t < T_{\Psi^*}$ ($T_{\Psi^*} \leq T_{\Psi_0}$) does not prevent the occurrence of a singularity of $\nabla\Psi$. If the solution of the IBVP (1)–(3) exists for $0 \leq t < T_{\Psi^*}$, then Theorem 2 would imply that the wave function Ψ concentrates at the origin

$x = 0$. Since this is not plausible in view of the arbitrary possible choice of the origin, Theorem 2 strongly suggests that a singularity of Ψ_{x_i} or $\Psi_{x_i x_j}$ occurs before the time $T_{\Psi*}$; $T_{\Psi*}$ is the smallest positive zero of $W(t)$.

4. NUMERICAL EXAMPLES

We give some numerical examples which confirm the predictions of Theorem 1 and also discuss the nature of the evolving singularity. For simplicity we choose the one-dimensional case of equation (1) with damping factor $\alpha = 0$. Furthermore, we adopt the potential and nonlinear term as $U(x) = x^2$ and $f(|\Psi|^2) = C|\Psi|^4$, respectively. Here C is a positive constant. Both choices are consistent with the conditions of Theorem 1, namely (14) and (15). Equation (1) then reads

$$i\Psi_t = H\Psi; \qquad H = -\frac{\partial}{\partial x^2} + x^2 - C|\Psi|^4; \qquad x \in (-1, 1); \tag{60}$$

$$\Psi(t, x = \pm 1) = 0$$

The formal solution for small time steps Δt is written, in terms of a unitary operator (Press *et al.*, 1992, pp. 851–853), as follows:

$$\Psi(t + \Delta t, x) = \left[\frac{1 - iH\,\Delta t/2}{1 + iH\,\Delta t/2}\right]\Psi(t, x) + O(\Delta t^2) \tag{61}$$

When the operator H is discretized by means of second-order differences, the formula

$$\left(1 - iH\frac{\Delta t}{2}\right)\Psi(t + \Delta t, x) = \left(1 + iH\frac{\Delta t}{2}\right)\Psi(t, x) \tag{62}$$

amounts to the Crank–Nicholson scheme.

Using $N + 1$ grid points along the x axis, we arrive at an $(N - 1) \times (N - 1)$ complex, nonlinear, algebraic system of the form

$$A^{(n+1)}\,\Psi^{(n+1)} = B^{(n)} \tag{63}$$

where

$$\begin{aligned} \Psi^{(n+1)} &= [\Psi_2^n, \ldots, \Psi_N^n]^t; \\ \Psi_j^n &= \Psi(n\Delta t, -1 + (j - 1)\Delta x) \\ j &= 1, \ldots, N + 1; \\ n &= 0, 1, 2, \ldots \end{aligned} \tag{64}$$

with space step Δx such that $N \cdot \Delta x = 2$.

Moreover, $A^{(n)}$ is a tridiagonal matrix with a_j, b_j^n, and c_j as subdiagonal, diagonal, and superdiagonal entries, respectively. They read

$$a_j = -\frac{1}{2} i \frac{\Delta t}{\Delta x^2}; \qquad j = 3, \ldots, N \tag{65}$$

$$b_j^n = 1 + i \frac{\Delta t}{2} \left[\frac{2}{\Delta x^2} + x_j^2 - C|\Psi_j^n|^4 \right];$$

$$j = 2, \ldots, N;$$

$$x_j = -1 + (j - 1)\Delta x \tag{66}$$

$$c_j = -\frac{1}{2} i \frac{\Delta t}{\Delta x^2};$$

$$j = 2, \ldots, N - 1 \tag{67}$$

Note that the diagonal entries depend on time due to the nonlinear term. In our case, because of the boundary conditions, $\Psi_1^n = \Psi_{N+1}^n = 0$, we have

$$B^{(n)} = \overline{A^{(n)}}\Psi^{(n)} \tag{68}$$

Equation (63) is solved for the vector $\Psi^{(n+1)}$ as follows:

$$\Psi^{(n+1)} = [A^{(n+1)}]^{-1} \overline{A^{(n)}}\Psi^{(n)} \tag{69}$$

Since $A^{(n+1)}$ depends on $\Psi^{(n+1)}$, we proceed iteratively starting with $A^{(n+1)} = A^{(n)}$. The inversion of $A^{(n+1)}$ is effectively computed by means of the Thomas algorithm (Press *et al.*, 1992, pp. 50–51).

We checked numericaly three cases corresponding to the three main assumptions (H1–H3) of Theorem 1. As first case we considered equation (60) with $C = 15$ and initial condition $\Psi(0, x) = 1 - x^2$. With this, all conditions of Theorem 1 are fulfilled including the assumption H1. According to Theorem 1, the upper bound of the time interval in which a singularity will occur is $T_{\psi_0} \simeq 0.25$. Using the numerical method discribed above with $\Delta x = 10^{-3}$ and $\Delta t = 10^{-6}$ we find evidence for a singularity at time $T_\Psi \simeq 0.081$ (see Fig. 1).

As a second case we considered equation (60) with $C = 15.08203125$ and initial condition $\Psi(0, x) = (1 - x^2) \exp[-ix^2]$, and as a third case $C = 45$ with initial condition $\Psi(0, x) = (1 - x^2)\exp[-i3x^2/2]$. Again, all conditions of Theorem 1 are fulfilled including the assumptions H2 and H3 for the second and the third cases, respectively. With the same time and space steps ($\Delta x = 10^{-3}$, $\Delta t = 10^{-6}$) we find evidence for a singularity at time $T_\Psi \simeq 0.06$ for the second and $T_\Psi \simeq 0.031$ for the third case. The predictions for the corresponding upper bound of Theorem 1, are $T_{\Psi_0} \simeq 0.125$ and $T_{\Psi_0} \simeq 0.1$ respectively.

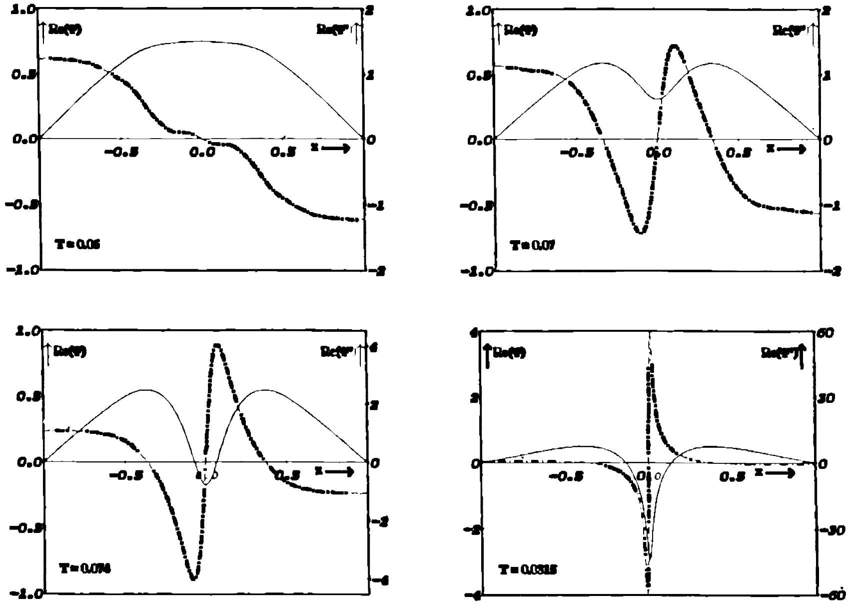

Fig. 1 Real part of the wave function Ψ (solid line) and its space derivative (dot-dashed line) at times $t = 0.06$, 0.07, 0.074, and 0.0815. The initial function is $\Psi(0, x) = 1 - x^2$.

The results are stable with respect to different discretization steps. In a range starting from 10^{-2} up to 10^{-4} for Δx and from 10^{-4} up to 10^{-6} for Δt we confirm qualitatively the same results and the same critical time T_Ψ.

5. FINAL COMMENTS

In the proof of Theorem 1 we obtained an inequality for the variance function $W(t)$ rather than a conservation law as found in Ablowitz and Segur (1979) because (a) the derivatives of the field Ψ are not necessarily zero at the boundary $\partial\Omega$ and (b) the nonlinearity is not restricted to cubic terms.

According to Theorem 2, if the singularity appears at time $T_{\Psi*}$ ($T_{\Psi*} \leq T_{\Psi_0}$) which is the smallest positive zero of $W(t)$, then the wave function completely focuses at the origin $x = 0$. This is not observed in the numerical example considered. Rather we have evidence that a significant part of the norm $\|\Psi\|_{2,\,\Omega}$ has support in the interval $0 < |x| < 1$. This implies that in the examples of the last section singularities emerge at a time $T < T_{\Psi*}$.

We have no conclusive evidence on the nature of the singularity corresponding to Fig. 1. Most probably we have a cusp with the slope of $\Psi_x|_{x=0}$ jumping from $-\infty$ to $+\infty$. However, we do not know whether or not the cusp is at a finite value of $\Psi(x = 0)$. This question could be examined numerically in principle by an adaptive grid scheme. However, we think that some analytical singularity analysis should be feasible.

Regarding basic hydrodynamic models, numerical evidence for finite-time singularities was found for the Euler equation (Grauer and Sideris, 1995). It is still an open question whether such singularities may arise also in the dissipative case of the Navier–Stokes equations (NSE). This problem is related to the fundamental unsolved problem of global existence and uniqueness of the solutions of the NSE (Doering and Gibbon, 1995; Rauh, n.d.). In view of this we were interested in whether, in the case of the nonlinear Schrödinger equation, Theorem 1 could be extended to the dissipative region with damping parameter $\alpha < 0$. Our attempts have not succeeded so far.

Without effort we found suitable examples which comply with the conditions of Theorem 1. As is immediately seen, the following potentials and nonlinear terms obey conditions (14) and (15):

$$U(x) = \sum_{n=0}^{\infty} a_n x^{2n}; \qquad a_n \geq 0; \qquad \sum_{n=0}^{\infty} a_n < \infty \tag{70}$$

$$f(s) = \sum_{\substack{p \in N \\ p \geq 2/n}}^{\infty} b_p s^p; \qquad b_p \geq 0; \qquad \sum_{p \geq 2/n}^{\infty} b_p < \infty; \qquad s \geq 0 \tag{71}$$

With the choice $U(x) = x^2$ we could write down any initial state $\Psi(t = 0, x) = \Psi_0(x)$ and then adapt the coefficient C of the nonlinear term in order to have a critical case. So we think that Theorem 1 covers more than an exceptional set of models. The finite-time criticality of a nonlinear Schrödinger equation in two space dimensions, as reported in Ablowitz and Segur (1979), is consistent with Theorem 1.

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REFERENCES

Ablowitz, M., and Segur, H. (1979). On the evolution of packets of water waves, *Journal of Fluid Mechanics*, **92**, 691–715.

Bainov, D., and Minchev, E. (1996). Blowing up of solutions to nonlinear Schrödinger equations, *Rendiconti di Matematica VII*, **16**, pp. 109–115.
De Bouard, A. (1991). Nonlinear Schrödinger equations with magnetic fields, *Differential and Integral Equations*, **4**, pp. 73–88.
Doering, C., and Gibbon, J. (1995). *Applied Analysis of the Navier–Stokes Equations*, Cambridge University Press, Cambridge.
Domarkas, A. (1991). Collapse of solutions of a system of nonlinear Schrödinger equations, *Lietuvos Matematikos Rinkinys*, **31**, 598–604.
Glassey, R. (1977). On the blowing up of solutions to the Cauchy problem for nonlinear Schrödinger equations, *Journal of Mathematical Physics*, **18**, 1794–1797.
Grauer, R., and Sideris, T. (1995). Finite time singularities in ideal fluids with swirl, *Physica D*, **88**, 116–132.
Gridnev, K. A., Greiner, W., and Kostavenko, V. G. (1996). Nuclear multifragmentation and soliton theory, *Izvestiya Akademiya Nauk, Seriya Fiziki*, **60**, 11–21.
Kamvissis, S. (1996). Long-time behavior of the focusing nonlinear Schrödinger equation with real spectral singularities, *Communications in Mathematical Physics*, **180**, 325–341.
Kivshar, Y. S., and Malomed, B. A. (1989). Solitons in nearly integrable systems, *Reviews of Modern Physics*, **61**, 764–915.
Mahmood, M. F. (1996). Chirped optical solitons in single mode birefringent fibers, *Applied Optics*, **35**, 6844–6845.
Nawa, H., and Tsutsumi, M. (1989). On blow-up for the pseudo-conformally invariant nonlinear Schrödinger equation, *Funkcialaj Ekvacioj*, **32**, 417–428.
Pelinovsky, D. E., Grimshaw, R. H. J. (1996). An asymptotic approach to solitary wave instability and critical collapse in long wave KdV-type evolution equations, *Physica D*, **98**, 139–155.
Press, W., Teukolsky, S., Vetterling, W., and Flannery, B. (1992). *Numerical Recipes in C*, 2nd ed., Cambridge University Press, Cambridge.
Rauh, A. (n.d.). Remarks on unsolved problems of the Navier–Stokes equations, *Open Systems and Information Dynamics*, to appear.
Zakharov, V. (1972). Collapse of Langmuir waves, *JETP*, **35**, 908–914.