Non-local Nonlinear Schrödinger Equation

Yu.B. Gaididei[2], K.Ø. Rasmussen[1],

P.L. Christiansen[1], and S.F. Mingaleev[2]

[1] Institute of Mathematical Modelling
Technical University of Denmark
2800 Lyngby, Denmark

[2] Bogolyubov Institute for Theoretical Physics,
Metrologicheskaya Street 14 B, 252 143 Kiev 143,
Ukraine

September 19, 1995

Abstract

A nonlocal Schrödinger equation applicable for molecular systems with long-range interactions and for media with saturating dispersion curves is proposed. Two types of stationary solutions are found. One of them becomes a crest soliton at the maximum of the spectral parameter. The dynamics of the standing solitons is investigated and collapse-like behavior is observed.

1 Introduction

Molecular aggregates, such as Scheibe aggregates, serve as energy funnels for sunlight in biological systems. In cyanine Scheibe aggregates , Möbius and Kuhn [1, 2] have observed highly efficient energy transfer over unusually large distances between donor and acceptor molecules. A recent survey of the various models of the Scheibe aggregate is presented in Ref. [3]. Temperature effects were considered in Refs. [4, 5]. In [6] a continuum version of the two-dimensional Davydov system is used to study the interplay between nonlinear localization and thermal incoherence. It is concluded that for sufficiently large values of the ratio nonlinearity to dispersion collapse may occur up to a certain critical temperature. The collapse time increases with temperature. It is noted that Möbius and Kuhn [2] deduce from experimental observations that the life time of the coherent excitation increases proportionally with the temperature. A connection between the lifetime and the collapse time resulting from the nonlinear [7] model is thus a possibility. In an ongoing investigation [8] a nonlinear damping term , establishing a balance between energy input and output of the system, is included in the model. The presence of a acceptor molecule in the Scheibe aggregate is modelled by an impurity term in the nonlinear Schrödinger equation. In this inhomogeneous two-dimensional system complex dipole-like nonlinear excitations have been found [9, 10]. In the present work a nonlocal nonlinear Schödinger equation is proposed and investigated. This model is applicable for molecular systems in which long range interactions between the molecules, such as dipole interactions, are taken into account. Also for media where there is a resonant interaction between an excitation with a narrow bandwidth ($\omega(k) \simeq \omega_0 = \text{const.}$) and an excitation with a broad bandwidth the approach applies. In this case our model describes nonlinear properties of the system for $\omega < \omega_0$ where the dispersion curve of the combined excitation approaches an asymptote $\omega = \omega_0$ corresponding to saturation.

The present paper is devoted to the non-local nonlinear Schrödinger equation (NL-NLS)

$$i\psi_t + \int_{\infty}^{\infty} dy K(x-y)(\psi(y) - \psi(x)) + V|\psi|^2\psi = 0, \tag{1}$$

in which the kernel $K(x-y)$ is the Kac-Baker function

$$K(x-y) = J \cdot \exp(-\alpha|x-y|). \tag{2}$$

The model given by Eq.(1) can be derived from the Hamiltonian

$$H = -\int_{-\infty}^{\infty} dx dy K(x-y)(\psi(x)^*\psi(y) - |\psi(x)|^2) - \frac{1}{2}V\int_{-\infty}^{\infty} |\psi|^4, \tag{3}$$

with the Possion brackets

$$\begin{aligned} \{\psi(x), \psi^*(y)\} &= i\delta(x-y), \\ \{\psi(x), \psi(y)\} &= \{\psi^*(x), \psi^*(y)\} = 0, \end{aligned} \tag{4}$$

and the equation of motion

$$\psi_t(x,t) = \{H, \psi(x,t)^*\}. \tag{5}$$

The Hamiltonian Eq.(3) models self-localization, self-trapping phenomena when the interaction with all neighbors in the lattice is taken into account. In the case of

$\psi(x,t)$ being a wave function the kernel $K(x-y)$ describes an excitation transfer (α^{-1} is the radius of the interaction, J is its intensity) and V is a self-interaction which can be caused by interaction with phonons or by anharmonicity effects. The kernel Eq.(2) is the Green function of the operator $(\frac{\partial^2}{\partial x^2}-\alpha^2)$

$$(\frac{\partial^2}{\partial x^2}-\alpha^2)\exp(-\alpha|x-y|) = -2\alpha\delta(x-y). \tag{6}$$

It permits us to rewrite Eq.(1) in the form

$$i\psi_t + 2J\alpha^{-1}(\alpha^2-\frac{\partial^2}{\partial x^2})^{-1}\frac{\partial^2}{\partial x^2}\psi + V|\psi|^2\psi = 0. \tag{7}$$

It is seen from Eq.(7) that when the radius of the interaction is small (α large) we can neglect the operator $\frac{\partial^2}{\partial x^2}$ in the inverse operator in the dispersive term and in the limit $\alpha\to\infty$, $J\to\infty$, $\frac{J}{\alpha^3}=$ const. obtain the usual one dimensional NLS equation. However, when the radius of the interaction is not small or the characteristic length of the excitation and the radius of the interaction are of the same order we must take into account the complicated form of the dispersive term in Eq.(7). We also see that Eq.(7) can be written as

$$i\psi_t + \omega(-i\partial_x)\psi + V|\psi|^2\psi = 0 \tag{8}$$

where $\omega(k)\equiv\frac{2J}{\alpha}\frac{k^2}{k^2+\alpha^2}$. Thus as it was mentioned above, Eq.(7) describes also nonlinear properties of excitations whose dispersion curves exhibit saturation. Besides the Hamiltonian the excitation number

$$P = \int_{-\infty}^{\infty} dx|\psi(x,t)|^2, \tag{9}$$

is an integral of the motion.

It is convenient to rescaled the variables in Eq.(7) as follows

$$z=\alpha x,\quad \tau=\frac{2J}{\alpha}t,\quad \psi(x,t)=\sqrt{\frac{2J}{\alpha V}}\phi(z,\tau). \tag{10}$$

In terms of the new variables Eqs. (7),(9) and (3) have the form

$$i\phi_\tau + (1-\frac{\partial^2}{\partial x^2})^{-1}\frac{\partial^2}{\partial x^2}\phi + |\phi|^2\phi = 0 \tag{11}$$

$$\int_{-\infty}^{\infty} dz|\phi(z,\tau)|^2 = \frac{P}{\alpha P_{sh.r}} \equiv N, \tag{12}$$

$$H = \frac{4J^2}{\alpha^3 V}\int_{-\infty}^{\infty} dz\left\{(\frac{\partial\phi}{\partial z}(1-\frac{\partial^2}{\partial z^2})^{-1}(\frac{\partial\phi}{\partial z})^2 - \frac{1}{2}|\phi|^4\right\} \equiv \frac{4J^2}{\alpha^3 V}\mathcal{H} \tag{13}$$

where $P_{sh.r}=\frac{2J}{\alpha^3 V}$ is the number of excitation in the short-range limit.

Lets consider the stationary solution of Eq.(11) in the form

$$\phi(z,\tau) = \exp(i\Lambda\tau)F(\xi)\sqrt{\Lambda+1}, \tag{14}$$

where Λ is the spectral parameter and $\xi = B^{-1/2}z$ with $B = 1 + \Lambda^{-1}$. Introducing Eq.(14) into Eq.(11) and multiplying Eq.(11) by the operator $(1 - \frac{\partial^2}{\partial x^2})$ we get

$$\frac{\partial^2}{\partial \xi^2}(F - F^3) - F + BF^3 = 0 \tag{15}$$

It is interesting to note here that Eq.(15) can be obtained from minimizing the action

$$S = \int_{-\infty}^{\infty} d\xi (T - U) \tag{16}$$

of an equivalent mechanical particle with the kinetic energy

$$T = \frac{1}{2}(1 - 3F^2)(\frac{\partial F}{\partial \xi})^2 \tag{17}$$

and the potential energy

$$U = -\frac{B}{2}F^2(F^2 - F_1^2)(F^2 - F_2^2) \tag{18}$$

where

$$F^2_{\frac{1}{2}} = \frac{1}{B}\left(\frac{B+3}{4} \mp \sqrt{\left(\frac{B+3}{4}\right)^2 - B}\right) \tag{19}$$

We see from Eqs.(16)-(19) that Eq.(15) describes the motion of a particle with a variable mass in a potential with one minimum and two maxima (Fig 1).

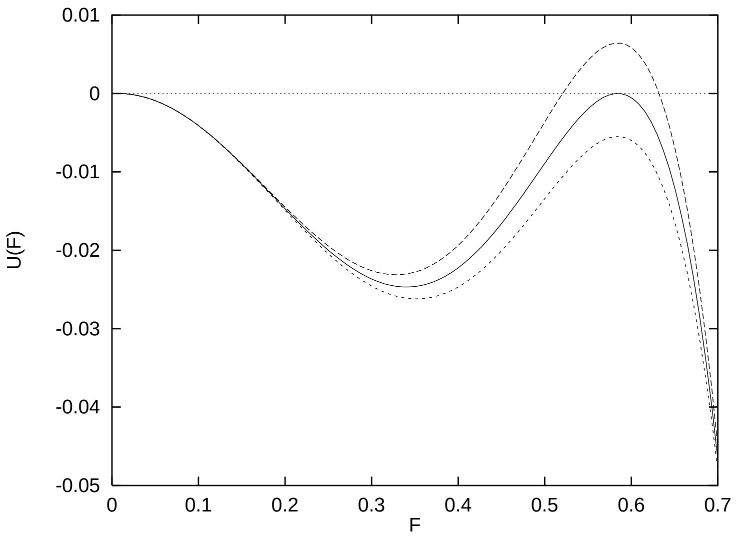

Figure 1: The potential U versus F for 3 values of the spectral parameter Λ. Λ=0.1249 (long dashed line), $\Lambda = 0.125$ (solid line) and $\Lambda = 0.1251$ (short dashed line). For all curves $N = 1$.

Under the boundary conditions $F(\pm\infty) = 0$ Eq.(15) has a solution

$$\exp(2\xi) = \frac{F_1 + F_2\mu}{F_1 - F_2\mu}\left(\frac{1-\mu}{1+\mu}\right)^{3B^{-1/2}} \tag{20}$$

with

$$\mu = \left(\frac{F_1^2 - F^2}{F_2^2 - F^2} \right)^{1/2} \tag{21}$$

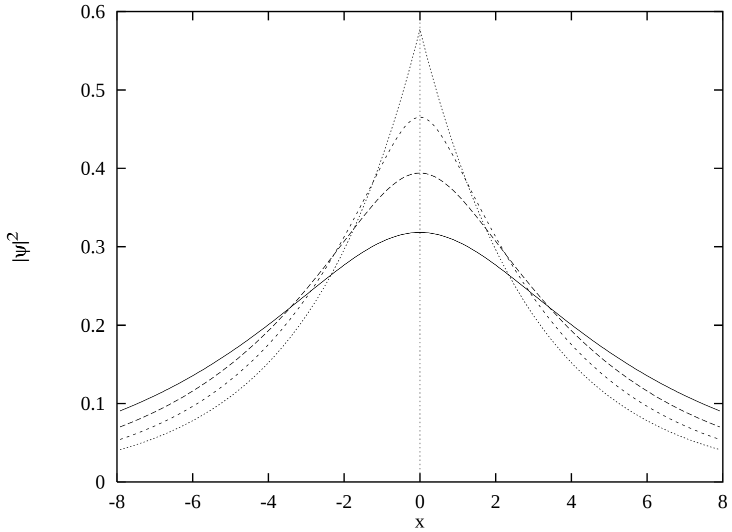

Figure 2: The stationary solution given by Eqs.(20) and (21) for several values of the spectral parameter Λ. $\Lambda = 0.05$ (solid line), $\Lambda = 0.075$ (long dashed line), $\Lambda = 0.01$ (short dashed line) and $\Lambda = 0.125$ (dotted line). For $\Lambda = 0.125$ the crest soliton appears.

This solution is plotted in Fig. 2 for different values of the spectral parameter Λ (B). It exists when $B \geq 9$ ($\Lambda \leq 0.125$). In this case the right maximum of the potential function Eq.(18) is higher than the left one (Fig. 1). But if $B < 9$ the right maximum is lower and a pulse-like solution cannot exist.

It is seen from Eqs.(20) and (21) that a $B \gg 9$ ($\Lambda \ll 0.125$) the solution reduces to $F(\xi) = \mathrm{sech}(\xi)$ and in such a way it coincides with the stationary solution of the normal NLS equation. This is an obvious result because the inequality $B \gg 9$ means that the width of the soliton is large and non-local effects are insignificant. The asymptotic behavior of Eq.(20) can be represented as follows

1) in the tails ($|\xi| \gg 1$)

$$F(\xi) = F_1 F_2 \frac{2}{\sqrt{F_2^2 - F_1^2}} \left(\frac{F_2 - F_1}{F_2 + F_1} \right)^{3/2\sqrt{B}} \exp(-|\xi|) \tag{22}$$

2) near the maximum ($|\xi| < 1$)

$$F(\xi) = F_1 \mathrm{sech}(\kappa \xi) \tag{23}$$

where

$$\kappa = \left(1 - \frac{3F_1}{\sqrt{B} F_2} \right)^{-1/2} \tag{24}$$

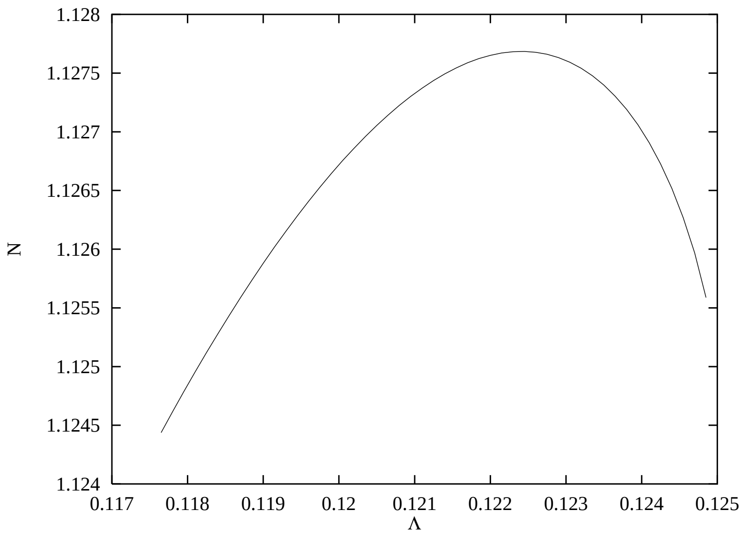

Figure 3: The norm of the stationary solution as function of the spectral parameter Λ

It is seen from Eq.(24) that for $B > B_{cr} \equiv 9$

$$\kappa \simeq 3\sqrt{2}(B - B_{cr})^{-1/2} \tag{25}$$

Thus the peak of the soliton becomes sharp when $B \to B_{cr}$. When $B = B_{cr}$ the roots F_1 and F_2 coincide $F_1 = F_2 = \sqrt{3}$ and the values of the potential function Eq.(18) at the maxima thus become equal. But when the particle described by the action S approaches the right maximum vanishes (see Eq.(17)) and as a result we obtain a crest soliton with the form

$$\phi(z,\tau) = \left(\frac{3}{8}\right)^{1/2} \exp\left(i\frac{\tau}{8} - \frac{1}{3}|z|\right) \tag{26}$$

Introducing Eqs.(20) and (21) into Eqs.(12) and (13) we obtain expressions for the excitation number N and the Hamiltonian $\mathcal{H}$

$$N = \frac{1}{B-1}\left(3\sqrt{B} + \frac{B-9}{8}\ln\frac{B+3+4\sqrt{B}}{B+3-4\sqrt{B}}\right) \tag{27}$$

$$\mathcal{H} = \frac{\mathcal{B}^{\in}}{(\mathcal{B}-\infty)^{\ni}}\left(\frac{\mathcal{B}+\in\imath}{\infty\not{\mathcal{B}}\sqrt{\mathcal{B}}} - \frac{(\mathcal{B}-\exists)^{\in}}{\infty\in\forall\mathcal{B}^{\in}}\ln\frac{\mathcal{B}+\ni+\triangle\sqrt{\mathcal{B}}}{\mathcal{B}+\ni-\triangle\sqrt{\mathcal{B}}}\right) - \frac{\mathcal{N}}{\mathcal{B}-\infty} \tag{28}$$

Figure 3 shows the dependence of the excitation number N on the spectral parameter, Λ. It is seen from Fig. 3 that the stationary solution can exist only at $N \leq N_{max}$ or, coming back to the original variables, at

$$P < \alpha N_{max} P_{sh.r} \tag{29}$$

Thus in contrast with a normal NLS equation for which the stationary state exist at any number of excitations in the non-local case there is a maximum value of excitation number which depends on the radius of the interaction α^{-1}. When the

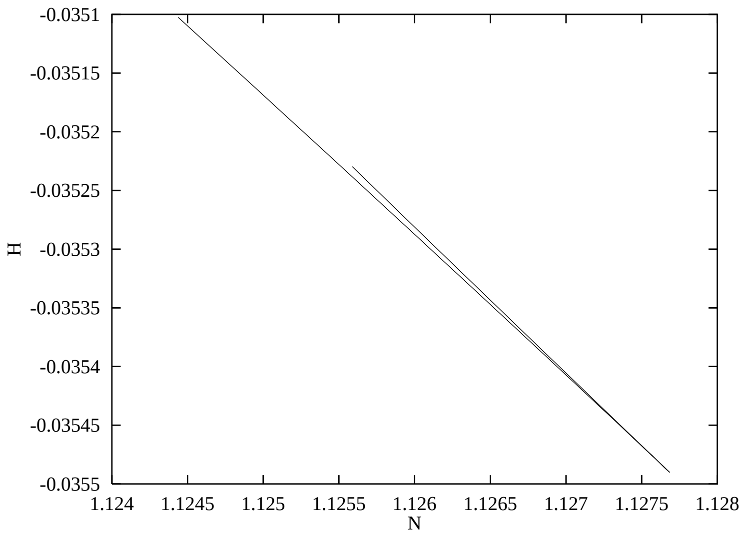

Figure 4: The Hamiltonian of the stationary solution versus the norm.

excitation number N varies in the interval $[N_{crest}, N_{max}]$ there are two values of the spectral parameter, Λ which correspond to a given N. To put it in another way in the interval two branches of soliton solutions exist. The first branch corresponds to the part of the curve $N(\Lambda)$ for which $\frac{dN}{d\Lambda} > 0$ and it exists for any $N \leq N_{max}$. The second branch exists only in the interval $N_{crest} \leq N \leq N_{max}$. $\frac{dN}{d\Lambda} < 0$ and at $\Lambda = 0.125$ $(N = N_{crest})$ the crest soliton appears. In Fig. 4 the dependence of the Hamiltonian on the excitation number N is shown. It is seen that the function $\mathcal{H}(\mathcal{N})$ has a characteristic behavior which is called a "cusp" in the catastrophe theory. A cusp is a singularity of the bifurcation diagram of the catastrophe manifold and it characterizes the surface Φ in the space defined by $\mathcal{H}$, N and Λ which is called a "Whithney gather". The extremal points of this surface correspond to the soliton solutions we have found.

The surface Φ has two extrema (minimum and maximum) for $N_{crest} < N < N_{max}$ and there is only one minimum at $N \leq N_{crest}$. For $N < N_{max}$ the surface does not have any extrema. It was proved for the case of the normal NLS equation that the branch that corresponds to $\frac{dN}{d\Lambda} > 0$ is stable. But in our case application of this theorem is not obvious and it should be investigated.

We investigate also the dynamical properties of the excitations. In Fig. 5 we show the behavior of the second moment

$$W(t) = \int_{-\infty}^{\infty} x^2 |\phi|^2 dx \tag{30}$$

calculated numerically using initial conditions which are slightly perturbed versions of the exact solutions on the branch with $\frac{dN}{d\Lambda} > 0$. The quantity is seen to oscillate and thereby suggest that the exact solution is stable. Using solutions on the branch with $\frac{dN}{d\Lambda} < 0$, W behaves quite differently. On this branch W tends monotonically towards zero. The behavior of the excitation is shown in Fig.6 in such a case. This behavior seems similar to the blow-up phenomenon of the two-dimensional NLS.

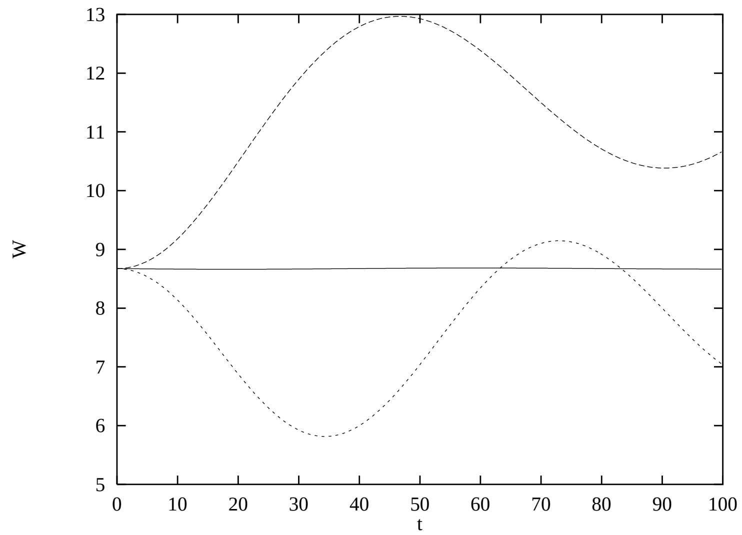

Figure 5: W versus time for initial conditions close to the stationary solution at $N = 1$, $(\Lambda = 0.0778)$ (belongs to the branch in Fig. 3 with $\frac{dN}{d\Lambda} > 0$ and is shown with solid line). The short dashed line is for $N = 0.94$ while the long dashed line is for $N = 1.06$

Conclusion

Solution of the nonlocal nonlinear Schödinger equation are investigated. It is shown that in contrast to the usual NLS equation stationary solutions of the NL-NLS exist only when the number of excitations does not exceed some critical value. This critical value tends to infinity when the radius of the interaction approaches zero. The numerical results indicate that when $\frac{dN}{d\Lambda} < 0$ the stationary solutions are unstable. Blow-up like behavior is observed in these cases. The stability of the standing soliton as well as the properties of the moving soliton are under investigation.

References

[1] D. Möbius and H. Kuhn, Isr. J. Chem. **18** (1979) 375.

[2] D. Möbius and H. Kuhn, J. Appl. Phys. **64** (1988) 5138.

[3] O. Bang, P.L. Christiansen, F. If, K. Ø. Rasmussen and Yu. Gaididei, Phys. Rev. E **49** (1994) 4627.

[4] O. Bang, P.L. Christiansen, F. If, K. Ø. Rasmussen and Yu. Gaididei, Applicable Analysis, **57** (1995) 3.

[5] K.Ø. Rasmussen, Yu. B. Gaididei, O. Bang and P.L. Christiansen, Phys. Lett. A **204** (1995) 121

[6] P.L. Christiansen, K.Ø. Rasmussen, O. Bang and Yu. B. Gaididei, " The temperature dependent collapse regime in a nonlinear dynamical model of Scheibe aggregates", Physica D (*in press*).

[7] M. Johansson, P.L. Christiansen, Yu. B. Gaididei and K.Ø. Rasmussen (*to appear*)

[8] K.Ø. Rasmussen, O. Bang and P.L. Christiansen, Phys. Lett. A **184** (1994) 241.

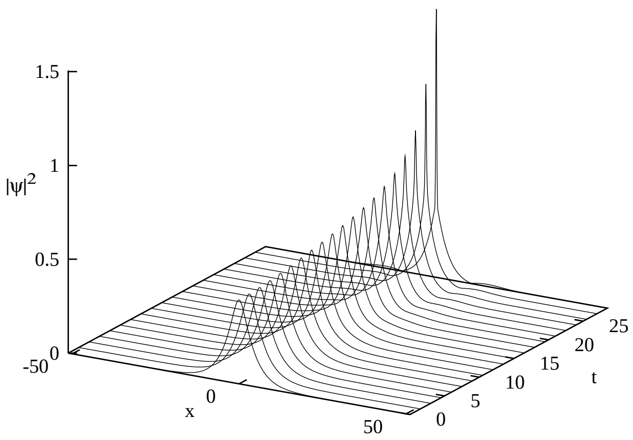

Figure 6: The development of an initial condition close to the stationary solution a $N = 1.126$ ($\Lambda = 0.1247$), belonging to the branch in Fig. 3 with $\frac{dN}{d\Lambda} < 0$.

[9] Yu. B. Gaididei, K.Ø. Rasmussen and P.L. Christiansen, Phys. Lett. A **203** (1995) 175.

[10] Yu. B. Gaididei, K.Ø. Rasmussen and P.L. Christiansen, "Nonlinear excitations in two-dimensional molecular structures with impurities, Phys. Rev. E **52** (1995) 2951.