NORTH-HOLLAND
PHYSICS
PUBLISHING

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Reprinted from PHYSICA B&C

Physica B 151 (1988) 193–198
North-Holland, Amsterdam

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We report numerical solution of a Schrödinger equation modified by the nonlinear term $b \ln|\psi|^2$ as proposed by Bialynicki-Birula and Mycielski. Experiments on the diffraction of cold neutrons at an absorbing straight edge performed earlier had set a very low upper limit on b, the strength of the nonlinearity, and it was the purpose of the present calculations to check the validity of some approximations made in the evaluation of that experiment. The numerical solutions show diffraction both in the usual spatial domain and in the time domain. When compared with the earlier estimates we find agreement within a factor of two.

1. Introduction

The linearity of the Schrödinger equation is crucial for such fundamental properties of quantum mechanics as the spreading of wave packets during their temporal evolution or the unlimited validity of the superposition principle. Specifically, it is the understanding of many physicists that the quantum measurement problem could be resolved if the Schrödinger equation were suitably nonlinear [1]. Though we do not share this point of view, we certainly consider the question of the linearity of the Schrödinger equation to be one which has to be subject to experimental test.

Of the various types of nonlinear variants proposed in the literature, the one by Bialynicki-Birula and Mycielski (BBM) [2] has been developed far enough to permit experimental tests. This nonlinear Schrödinger equation (NLSE) is

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r) + F(|\psi|^2)\right)\psi(r,t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\psi(r,t) \qquad (1)$$

in standard notation. The new nonlinear term $F(|\psi|^2)$ can conceptually be understood as a kind of 'self-potential'. It has been shown by BBM that many of the important features of standard wave mechanics can be retained within their nonlinear equation. The specific functional form of $F(|\psi|^2)$ is then a separate question, which can ultimately only be answered by experiment. According to BBM a very interesting variant of eq. (1) follows for the case of a logarithmic nonlinearity

$$F(|\psi|^2) = -b\ln(|\psi|^2). \qquad (2)$$

Here, b measures the strength of the nonlinearity. It has the dimension of energy and has to be positive in order to lead to solutions bounded from below in energy. The most significant feature of an NLSE with logarithmic nonlinearity is the separability of noninteracting subsystems. In view of the excellent agreement of standard linear wave mechanics with experiment, it is evident that b has to be very small. On the basis of Lamb shift measurements BBM arrive at an upper limit of $b < 4 \times 10^{-10}$ eV.

2. The neutron experiments

It was first realized by Shimony [3] that this limit could be further lowered by neutron interferometry. The experiment proposed by him was then performed by Shull et al. [4] leading to an upper limit of the strength b of the nonlinearity of $b < 3.4 \times 10^{-13}$ eV. The crucial step in the evaluation of that experiment was the realization that for small enough b the WKB approximation

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is applicable to the time-independent variant of the NLSE. Then, the nonlinear 'self-potential' term leads to a phase shift analogous to other potentials.

As with nonlinear equations in general, a most sensitive test results if a disturbance as steep as possible is introduced into the amplitude. This is related to the breakdown of the linear equivalence of the evolutions in real space and in Fourier space for such equations. For neutrons, a related experiment was performed by Gähler et al. [5] by introducing an absorbing straight edge into a beam of cold neutrons with a wavelength of $\lambda = 20$ Å. The Fresnel diffraction pattern was then measured precisely and carefully checked for possible deviations from the pattern predicted by standard linear theory. No statistically significant deviation was found. From the known sensitivity of the experiment one could then deduce a new upper limit for the nonlinearity of $b < 3.3 \times 10^{-15}$ eV.

For the evaluation of the Fresnel diffraction pattern the influence of the nonlinear term on the distance between the point P_1 straight down from the absorbing edge (i.e. with 25% intensity) from the position P_2 of the first maximum was studied. In order to arrive at a theoretical prediction some approximations of the NLSE had to be made. These were most notably (a) the replacement of the time-dependent equation by a time-independent one, (b) the assumption that the spatial variations of the amplitude of ψ are small over distances of the order of the wavelength and (c) the assumption that, because of the smallness of the nonlinearity, any change of the diffraction pattern due to a nonlinear term can be expressed as a small variation of the pattern predicted by the linear theory. This finally results in the following expression for the change Y of the distance between the points P_1 and P_2:

$$Y = \frac{2b}{E\sqrt{\lambda}}\, c_1 Z^{3/2}\,, \tag{3}$$

where Z is the distance between the diffracting edge and the observation plane and c_1 is a geometrical constant of order unity. The experimentally observed value was consistent with $Y = 0$ which, using the known sensitivity of the experiment, lead to the limit on b given above. It is important to realize that the validity of the approximations made, though certainly reasonable within the linear theory, is not at all obvious within a nonlinear theory. To investigate this specific question detailed numerical calculations were performed [6] and are reported here.

3. The numerical method

In the numerical calculations the absorbing straight edge was assumed to be infinitely long and oriented along the x-direction, i.e. for its absorbing potential we have $V(x, y, z) = V(y, z)$. The absorption was taken into account by setting the wave function to zero along the absorbing half-plane. The fact that the nonlinearity studied is logarithmic then permits the separation ansatz

$$\psi(r, t) = \chi(x)\phi(y, z, t) \tag{4}$$

leading to a NLSE which depends on the 3 parameters y, z and t only:

$$\left(-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(y, z) - b\ln(|\phi|^2)\right) \times \phi(y, z, t) = i\hbar\frac{\partial}{\partial t}\phi(y, z, t)\,. \tag{5}$$

This differential equation was transformed into a difference equation which was defined on a discrete lattice. The solution was calculated in time steps Δt from a suitably chosen initial wave function. Due to limitations both in computer storage space and in computer time the calculations had to be restricted to a region close to the diffracting edge. For that reason values of the nonlinearity constant b much larger than the upper limits resulting from existing experiments had to be chosen in order to observe significant differences between the linear and the nonlinear equations.

For the calculation two step sizes had to be chosen, a spatial step size Δ and a time step size Δt. If $\phi_{j,k,l}$ denotes the value of the wave function at the lattice site j in y-direction, k in z-direction (the direction of propagation) and l in time direction, the following difference quotients turned out to be most suitable:

$$\left(\frac{\Delta\phi}{\Delta T}\right)_{j,k,l} = \frac{\phi_{j,k,l+1} - \phi_{j,k,l-1}}{2\,\Delta T} \tag{6}$$

and

$$\left(\frac{\Delta^2\phi}{\Delta y^2} + \frac{\Delta^2\phi}{\Delta z^2}\right)_{j,k,l} = [\phi_{j-1,k,l} + \phi_{j+1,k,l} + \phi_{j,k-1,l} + \phi_{j,k+1,l} - 4\phi_{j,k,l}]/\Delta^2 . \tag{7}$$

Insertion of these expressions into the Schrödinger equation results in an expression for $\phi_{j,k,l+1}$ as a function of the six field values $\phi_{j,k,l-1}$, $\phi_{j,k,l}$, $\phi_{j-1,k,l}$, $\phi_{j+1,k,l}$, $\phi_{j,k-1,l}$ and $\phi_{j,k+1,l}$.

The initial conditions were then chosen as

$$\begin{aligned} \phi_{j,k,0} &= [1 - \theta(l\Delta)] , \\ \phi_{j,k,-1} &= [1 - \theta(k\Delta)] \exp(\mathrm{i}\omega\,\Delta T) , \end{aligned} \tag{8}$$

where θ is the Heavyside step function. Physically, this should describe a situation where an absorbing shutter opens the positive-z half-plane at time zero.

An important question is that of the size of the spatial lattice to be used. The amplitudes at the outermost lattice sites can, in principle, not be calculated within the program but have to be chosen through boundary conditions and the final results should not depend critically on the choice made.

Concerning the boundary condition we can discriminate four different ranges (fig. 1). Range 1 ($k=0$) contains the absorbing edge. At the absorbing edge itself the amplitude was set identically equal to zero at all times. At the other points of range 1 we have the incident wave which we assume not yet to be influenced by the absorbing edge and therefore of constant amplitude. From time step to time step the amplitude is multiplied by the phase factor $\exp(-\mathrm{i}\omega\,\Delta T)$. Laterally, the lattice was chosen large enough such that the influence of the absorbing edge on the amplitude at range 2 of the

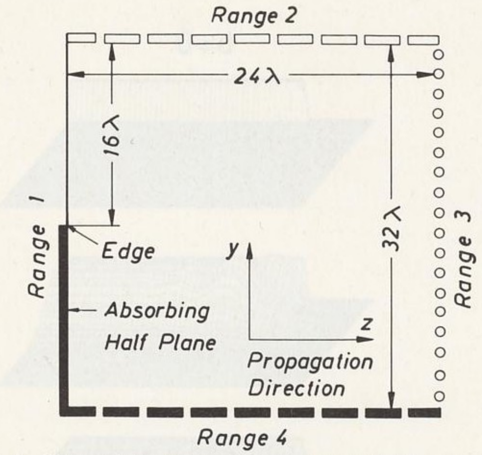

Fig. 1. Size and boundaries of the spatial lattice chosen for the numerical calculations.

boundary ($j_{max} = J$) could be neglected, therefore there we set $\phi_{J,k,l} = \phi_{J-1,k,l}$. The most problematic boundary region was range 3 ($k_{max} = K$) which was downstream from the absorbing edge. It is the region where the diffraction pattern arises finally. This problem was handled such that the lattice was chosen to be large enough in z-direction so that the amplitude at the range 3 lattice points was very small up to the last few time steps. Additionally, the amplitude at $k = K$ was set such that $\phi_{j,K,l} = \phi_{j,K-1,l} \exp(\mathrm{i}k\Delta)$ where $k = 2\pi/\lambda$ is the wave number of the neutrons. Part 4 of the boundary which is the part with $j = j_{min}$ was well inside the geometric shadow and therefore the wave amplitude there could be set equal to zero at all times.

The boundary conditions mentioned above were checked by varying the size of the lattice used and by trying alternative choices. It was found that with the parameters and the lattice size chosen (fig. 1) the results were very stable upon variation of these parameters. The same holds for the step sizes finally used which were $\Delta = \lambda/7$ and $\Delta T = 0.09\Delta/v_{ph}$ with $v_{ph} = \omega/k$.

4. Numerical results

The calculations were made for a neutron wavelength of $\lambda = 20$ Å which was the wavelength of the earlier experiments. Fig. 2 shows the calculated intensity distribution at dif-

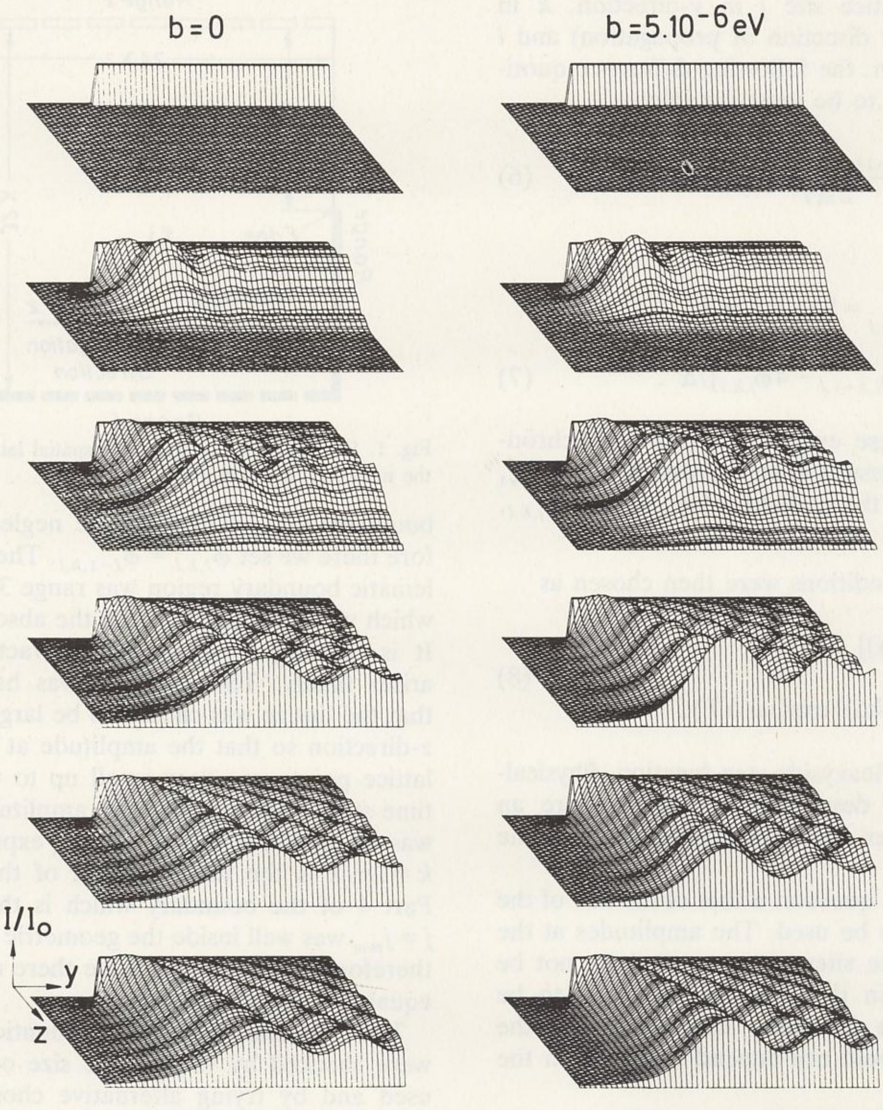

Fig. 2. Intensity distributions behind the diffracting edge at different times after the start of the evolution both for the linear (left column) and the nonlinear case (right column). The times are $t = 0$, 39, 78, 117, 156, and 195 ps, respectively, from top to bottom.

ferent times after the start of the evolution. As mentioned above, at $T = 0$ a shutter was opened and at that time the intensity distributions are identical by definition for both the linear case $(b = 0)$ and the nonlinear case, i.e. the initial conditions were identical. The part of the line $z = 0$ with zero intensity is the position of the absorbing edge in all graphs. We should also mention that only a part of the calculated intensity patterns is shown, the lattice used was larger than the one displayed.

Various features of the patterns of fig. 2 deserve comment. Firstly, one can clearly see the emergence of the Fresnel diffraction pattern not only in y-direction, which is the conventional direction along which diffraction patterns are scanned in experiment, but also in z-direction (the propagation direction), a feature to our knowledge never observed in a matter–wave experiment until present. Another feature also not observed in experiment yet is the emergence of a Fresnel diffraction pattern at a given position as a function of time as can be seen by comparing the graphs for different times in fig. 2. These last features need ultrafast chopping and detection procedures in experiment. An important step in this direction is being made presently by the introduction of the quantum chopping technique [7, 8].

When comparing in fig. 2 the evolution patterns of the nonlinear case with the linear one, one notices that the maxima are more pronounced in the nonlinear solutions. This is to be expected because one of the motivations for introducing nonlinear terms in the Schrödinger equation is to provide a mechanism preventing the unlimited spreading of wave packets. Qualitatively, this may be understood as a mechanism compressing the wave maxima spatially.

In the quantitative comparison of the linear and the nonlinear cases (fig. 3), this enhancement of the maxima and minima can be seen very clearly. For the relation to the experiment one notices that both the position of the 25% intensity point P_1 and the position of the first maximum P_2 are shifted. Their relative shift is then the sum of both these shifts ($Y = Y_1 + Y_2$).

As also predicted by the closed-form approximation (eq. (3)) the distance Y between P_1 and P_2 was found here too to vary linearily with the magnitude of the nonlinearity constant b (fig. 4). Yet, interestingly, the numerical method predicts an effect about half as large as the closed-form approximation for the same value of b. The cause of this discrepancy is presently unknown to us. Only detailed further studies could reveal whether this discrepancy is due to the approximations made in the derivation of eq. (3) or whether it is caused by the limitations of the numerical calculations. Possible causes for the discrepancy could certainly lie in the fact that for the closed-form calculations the Fresnel approximation was used and in the fact that we only compared solutions very close to the diffracting edge. In view of this we find it remarkable that we still obtain such an excellent qualitative and relatively reasonable quantitative agreement at all between the two methods. An indication of the reasonableness of the agreement between both methods is the fact that in the numerical method we also found the $z^{3/2}$ variation of Y

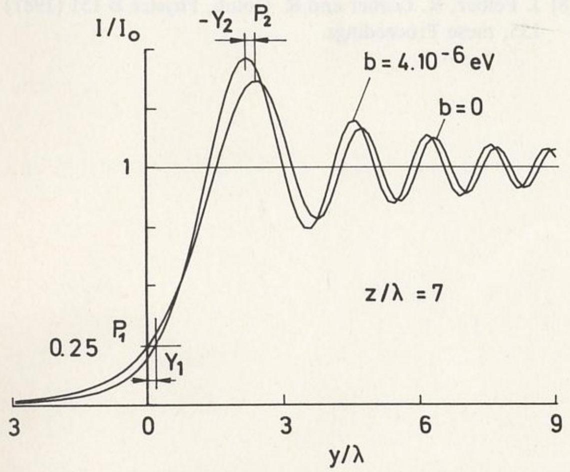

Fig. 3. Comparison of the edge diffraction pattern calculated for a nonlinear case with the one calculated for the linear case.

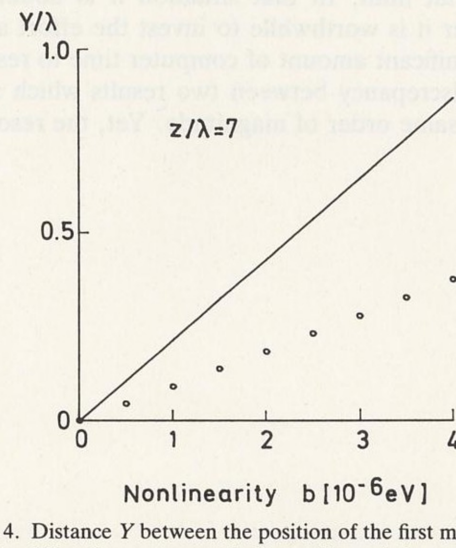

Fig. 4. Distance Y between the position of the first maximum of the diffraction pattern and the position of the point with 25% intensity as a function of the strength b of the nonlinear term. Numerical results (circles) and closed-form approximation (solid line).

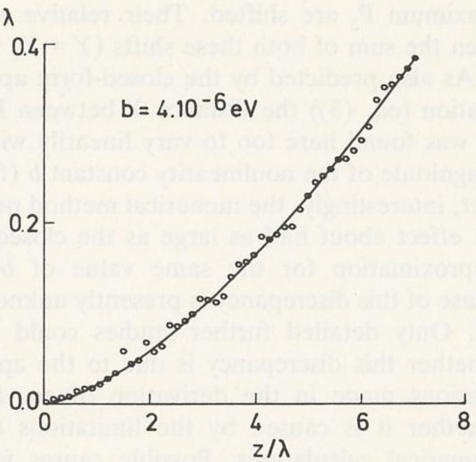

Fig. 5. Distance Y between the maximum intensity point and the 25% intensity point as a function of the propagation distance z from the absorbing edge. In agreement with the closed-form approximation a $z^{3/2}$ dependence is found.

with the distance from the absorbing edge (fig. 5).

The observation of a numerical discrepancy of a factor close to two has to be judged in relation to the experiment. As long as the experiment does not give a definitely nonzero value for b the experimental result provides a limit only, implying that any value of b has to be much smaller than that limit. In that situation it is doubtful whether it is worthwhile to invest the effort and the significant amount of computer time to resolve a discrepancy between two results which are of the same order of magnitude. Yet, the resolution of this discrepancy would be necessary in the unlikely, but certainly extremely important, case of an experimental confirmation of a breakdown of linearity.

Acknowledgements

We wish to thank Professor Bialynicki-Birula and Professor Shimony for suggesting to study the validity of the assumptions made in our earlier study by a numerical investigation. This work was supported by the Austrian Science Foundation, project number S42-01 and P6635T.

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