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A Solution Spectrum of the Nonlinear Schrödinger Equation

W. Ulmer[1]

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The soliton solutions of the form $\Psi = A/\cosh kx$ and $\Psi = B\tanh kx$ of the nonlinear Schrödinger equation have been considered with respect to many problems. In this paper, it is shown that the nonlinear Schrödinger equation also possesses a solution manifold that generalizes the above soliton functions and provides a discrete spectrum of eigenfunctions and eigenvalues. With the help of a slight modification of these eigenfunctions, it is possible to extend them to the relativistic case, where they become solutions of a nonlinear Klein-Gordon equation associated with a discrete mass spectrum.

1. INTRODUCTION

The nonlinear Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} + \frac{\hbar^2}{2m} \Delta \Psi = \lambda |\Psi|^2 \Psi \tag{1}$$

has become of growing interest in many disciplines of modern physics [e.g., the theory of measuring processes and particle physics (Jackiw, 1977; Mielnik, 1974; Barut, 1977; Mielke, 1981), solid state and plasma physics (Kubo *et al.*, 1976; Satsuma and Yajima, 1974; Zakharov and Shabat, 1973; Scott, 1973; Das and Sihi, 1979; Davey and Stewartson, 1974; Bertrand and Felix, 1976; Auer, 1979; Fogel *et al.*, 1976; Flannery, 1982), and molecular and biophysics (Davydov, 1976, 1977, 1979; Ulmer and Hartmann, 1978; Ulmer, 1980, 1983; Gupta, 1979)] because this equation exhibits soliton solutions, which can readily be obtained via consideration of the stationary version of equation (1) in one space coordinate:

$$E\Psi + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi = \lambda |\Psi|^2 \Psi \tag{2}$$

[1]FB Radiologie, St. Marienkrankenhaus, Med. Physik und Biophysik, 5900 Siegen, West Germany.

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Thus, the two solitary-wave solutions

$$\Psi = A(\cosh kx)^{-1} \tag{3}$$

with

$$E = -\hbar^2k^2/2m, \qquad A^2 = -\hbar^2k^2/m\lambda \tag{3a}$$

and

$$\Psi = B \tanh kx \tag{4}$$

with

$$E = \hbar^2k^2/m, \qquad B^2 = \hbar^2k^2/m\lambda \tag{4a}$$

have been carefully studied with respect to various problems in the cited references, but there are also solutions of equation (2) of the form $\Psi = C(\sinh kx)^{-1}$ and $\Psi = D(\tanh kx)^{-1}$, exhibiting singularities at the origin $x=0$. The solution (3) refers to a bound state for $\lambda < 0$. If $\lambda > 0$, then A^2 in equation (3a) must be replaced by $|A|^2$. The solution (4) is related to a scatter state with $E > 0$. With respect to equations (1) and (2), it should be noted that if $\Psi(x)\exp(-iEt)/\hbar)$ is a solution function, then for arbitrary velocity v the Galilei-transformed wave function is

$$\Psi'(x, t) = \exp[imvx/\hbar - i(E + mv^2/2)t/\hbar]\,\Psi(x - vt) \tag{5}$$

obeying solely equation (1), and with reference to the solutions (3) and (4) the Galilei-transformed solutions can be associated with soliton signals propagating with the velocity v. In particular, the solution (3) is L_2-integrable, whereas the solution (4) is not. However, if the additional assumption $\|\Psi\|_2 = A^2 \int_{-\infty}^{+\infty} (\cosh kx)^{-2}\, dx = 1$ is introduced, then the parameter k can only assume the numerical value

$$|k| = m|\lambda|/2\hbar^2 \tag{3b}$$

If k does not satisfy the relation (3b), the norm of the wave function (3) is completely undefined.

It might seem surprising that equation (2) with regard to the relations (3), (3a), (3b), (4), (4a) has been applied to problems of rather different fields, as already indicated. However, one reason is provided by relation (3b), exhibiting a proportionality between k and the coupling constant λ, and therefore λ determines whether k^{-1} is of the order 10^{-7}–10^{-5} cm (characteristic length in solid state and molecular physics) or $k^{-1} \approx 10^{-12}$ cm (plasma physics).

In solid state physics, molecular physics, and biophysics, solitonlike signals are related to collective excitations (or quasiparticles) in sufficiently long (molecular) chains, and, according to Davydov (1977), excitons and solitons may be produced via intramolecular electric dipole vibrations. Thus, excitons are collective excitations induced by light quanta and damped by emission of photons and phonons. Due to the Frank-Condon principle, the traveling of excitons along a chain is not related to lattice deformations, and their group velocity is greater than that of longitudinal sound.

Solitons are similar quasiparticles, which may be induced by a local deformation at a specific molecule site via suitable interactions [e.g., chemical reactions, such as proton transfer or electron transfer in semiconductors (Petrov, 1979)], and the energy released by such interactions is stored in the chain in the form of solitons. The energy of solitons consists of the following three parts:

1. Kinetic energy of the quasiparticle
2. Elastic deformation of the chain
3. Reorganization of the electric charge distribution, when the soliton travels along the chain (potential energy).

The points 2 and 3 are responsible for the nonlinear term of equations (1) and (2), and the propagation velocity is less than that of sound. Thus, solitons can only be produced by external light, when, e.g., via singlet-triplet transitions the Frank-Condon principle is violated, and a change of electric charge distribution may be related to molecular deformations (change of conformation).

A soliton excitation in biophysics has been studied by Davydov (1976, 1979): Thus, by ATP hydrolysis the released energy is stored in α-helical proteins (ATP is covalently bound to these proteins), and Davydov used soliton excitation mechanism in biological problems, such as the contractions of muscle fiber sarcomers (bundles of parallel-packed myofibrils containing protein filaments, ATP molecules, and Mg^{2+} and Ca^{2+} ions). This example belongs to the rather enormous class of molecular chains where soliton processes have become of increasing importance, among which we mention the so-called bond alternation defects (Walmsley and Pople, 1962) occurring in polyacetylene chains $(CH)_x$, which Su *et al.* (1980) identified as soliton excitations (see also Figure 1). In addition, many soliton excitation processes have been considered in connection with molecular electronics and molecular biology (Carter 1981; Campbell and Peyrar, 1983;

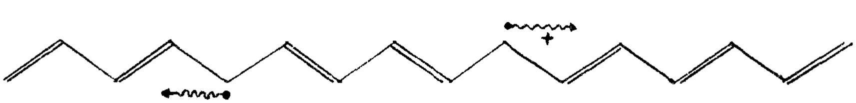

Fig. 1. Walmsley-Pople bond alternation defects in polythylene chains as an example of the excitation of solitons (+) and antisolitons (−).

Su *et al.*, 1980; Beaconsfield and Balanovski, 1983, 1984), and it is mainly the stable form of solitons that may provide interesting concepts in these areas. Solitons appear to exhibit a great similarity to the Cooper pairs of superconductivity, and it is noteworthy that equation (2) is completely equivalent to the Ginzburg-Landau theory of phase transitions (e.g., superconductivity):

$$\mathcal{F} = \int [(\alpha|\nabla\Psi|^2 + \beta|\Psi|^2 + \gamma|\Psi|^4)]\, d\tau \tag{6}$$

$\mathcal{F}$ refers to the free energy, and performing $\delta\mathcal{F} = 0$ with respect to Ψ^* yields equation (2) (α, β, and γ have to be chosen suitably). Although nonlinear Schrödinger equations are, as already indicated, useful in many disciplines, every solution of equations (1) and (2) may be regarded in the light of equation (6) (Ulmer, 1980; Gupta, 1979; Landau and Ginzburg, 1950; Ginzburg, 1955; Feynman, 1976; Klose, 1965). The significantly wide range of possible applications of the nonlinear Schrödinger equation (2) is a motivation to analyze the question of whether there are further solutions of (2) similar to the particular solution (3) which allow us to introduce the L_2-norm $\|\Psi\|_2 = 1$. Although we are interested primarily in a knowledge of a solution spectrum of equation (2) with regard to problems of molecular biology, which will be discussed in a separate communication, the subsequent analysis may also be relevant to other disciplines where nonlinear problems are taken into consideration.

2. A GENERALIZATION OF THE $(\cosh kx)^{-1}$ SOLUTION

We shall verify that the *ansatz*

$$\Psi = \sum_{k'=1}^{\infty} A_{k'}(\cosh kx)^{-k'} \tag{7}$$

incorporates indeed the desired generalization of the solution (3) (L_2-integrable wave function with $E < 0$).

With the help of the expansion (7), equation (2) takes the form

$$\begin{aligned} E \sum_{k'=1}^{\infty} A_{k'}(\cosh kx)^{-k'} &+ \frac{\hbar^2 k^2}{2m} \sum_{k'=1}^{\infty} A_{k'} k'^2 (\cosh kx)^{-k'} \\ &- \frac{\hbar^2 k^2}{2m} \sum_{k'=1}^{\infty} A_{k'} k'(k'+1)(\cosh k)^{-k'-2} \\ &= \lambda \sum_{p,q,r=1}^{\infty} A_p \mathcal{A}_q \mathcal{A}_r (\cosh kx)^{-(p+q+r)} \end{aligned} \tag{7a}$$

Equation (7a) has to be satisfied for arbitrary values of the argument x, and because of the impossibility of representing a power $(\cosh kx)^{-k'}$ by a finite linear combination of other polynomials $\sum_l a_l(\cosh kx)^{-1}$ with $l \neq k'$, all coefficients belonging to each power of cosh kx in equation (7a) have to satisfy this equation; otherwise a polynomial equation of infinite order and with arbitrary $A_{k'}$ with respect to the argument x would have to be solved (similar conclusions hold in the case of hypergeometric series). Therefore equation (7a) is considered by referring to each power of $(\cosh kx)^{-\beta}$ ($\beta = 1, 2, 3, 4, \ldots$):

$\beta = 1$. This condition implies the relation

$$(E + \hbar^2 k^2 k'^2/2m)A_1 = 0 \qquad (k' = 1) \tag{8}$$

For $A_1 \neq 0$ the energy E is equated to $E = E_1 = -\hbar^2 k^2/2m$, and thus the energy agrees with that of equation (3a).

$\beta = 2$. For this case

$$(E + 4\hbar^2 k^2/2m)A_2 = 0 \tag{8a}$$

This equation yields a contradiction to equation (8), where we have already fixed the energy E, and therefore we have to put $A_2 \equiv 0$. However, a consideration of the cases $\beta = 4, 6, 8, \ldots$, shows that each A_n with even n has to vanish identically with reference to condition (8).

$\beta = 3$. This case provides the determination of A_3 as a function of A_1:

$$A_3 = A_1/4 + (m\lambda/4\hbar^2 k^2)A_1^3 \tag{8b}$$

and by considering the powers $\beta = 5, 7, 9, \ldots$, in equation (7a) the following coefficients are fixed recursively (see also Table I): $A_1 \to A_3 \to A_5 \to A_7 \to \cdots A_{2n+1}$. The computation of the higher order contributions $A_5, A_7, \ldots$ is a combinatorial task; they are always defined in terms of A_1 (see also Appendix A). However, A_1 is not determined by equation (7a), and only by the introduction of a norm can this amplitude be fixed. We assume that

Table I. The A_1 Dependence of the Expansion Coefficients A_{2n+1} ($n = 0, 1, \ldots, 6$)[a]

n	A_{2n+1}	u^0A_1	$u^1A_1^3$	$u^2A_1^5$	$u^3A_1^7$	$u^4A_1^9$	$u^5A_1^{11}$	$u^6A_1^{13}$
0	A_1	$1/4^0$	0	0	0	0	0	0
1	A_3	$1/4^1$	$1/4^1$	0	0	0	0	0
2	A_5	$2/4^2$	$3/4^2$	$1/4^2$	0	0	0	0
3	A_7	$5/4^3$	$9/4^3$	$5/4^3$	$1/4^3$	0	0	0
4	A_9	$14/4^4$	$28/4^4$	$20/4^4$	$7/4^4$	$1/4^4$	0	0
5	A_{11}	$42/4^5$	$90/4^5$	$75/4^5$	$35/4^5$	$9/4^5$	$1/4^5$	0
6	A_{13}	$132/4^6$	$297/4^6$	$275/4^6$	$154/4^6$	$54/4^6$	$11/4^6$	$1/4^6$

[a] $u = m\lambda\hbar^{-2}k^{-2}$. According to this table, A_{13} is determined by $A_{13} = 132A_1/4^6 + 297uA_1^3/4^6 + 275u^2A_1^5/4^6 + 154u^3A_1^7/4^6 + 54u^4A_1^9/4^6 + 11u^5A_1^{11}/4^6 + u^6A_1^{13}/4^6$.

the L_2-norm is appropriate, because this norm usually provides the mathematical frame of (linear) quantum theory, implying the following expressions:

$$\int_{-\infty}^{+\infty} |\Psi|^2 \, dx = \|\Psi\|_2 = 1 \to \sum_{i,j=0}^{\infty} S_{2i+1,2j+1} A_{2i+1} A_{2j+1} = 1 \tag{9}$$

where S_{ij} is given by

$$S_{ij} = \int_{-\infty}^{+\infty} (\cosh kx)^{-(i+j)} \, dx = \frac{2}{k} \prod_{m=2}^{p/2-1} \frac{p-2m}{p-2m+1}, \qquad p = i+j \tag{9a}$$

Using the A_1 dependence of the coefficients $A_{k'}(k'>1)$ and with the help of the substitution $u = A_1^2$, one obtains from (9) a polynomial equation of infinite order:

$$\sum_{n=1}^{\infty} a_n u^n = 1 \tag{9b}$$

and this equation would have to be solved to determine $A_1^{\pm} = \pm\sqrt{u}$ and the forthcoming coefficients. However, equation (9b) makes apparent an essential problem. A very low-order (and probably rather insufficient) approximation of Ψ would be

$$\Psi \approx A_1(\cosh kx)^{-1} + A_3(\cosh kx)^{-3} \tag{9c}$$

implying a polynomial equation of degree 3 to be solved by the Cardan formula and yielding $A^{1,2,3+} = +(u_{1,2,3})^{1/2}$ and $A_1^{1,2,3-} = -(u_{1,2,3})^{1/2}$, but already by taking account of the term A_5 the corresponding polynomial equation can only be solved by numerical methods. Therefore the convergence problems cannot be solved on the basis of equation (9b) and will have to be regarded separately in Section 4. Equation (9b) provides an infinite set of coefficients $A_1^{M\pm}, A_3^{M\pm}, \ldots, A_{2k'+1}^{M\pm}$ $(M = 1, 2, 3 \ldots)$, and the first eigenfunction of (2) is given by

$$\Psi_1^{M\pm} = \sum_{k'=0}^{\infty} A_{2k'+1}^{1,M\pm} (\cosh kx)^{-2k'+1} \qquad (M = 1, 2, 3 \ldots) \tag{10}$$

The energy eigenvalue is $E_1 = -\hbar^2 k^2/2m$ and the degree of degeneracy is infinite (Ψ_1^{M+} stands for soliton solution and Ψ_1^{M-} for antisoliton solution). Because we consider convergence problems in Appendix A, here we give a sketch of the results:

The energy eigenvalue E_1 is only defined in a particular valence band with the smallest and highest k values.

The subsequent eigenvalues and eigenfunctions are also related to specific valence bands.

If these results are taken into consideration with regard to the Ginzburg-Landau theory of superconductivity [equation 6)], then it can be seen that equation (6) already describes the effect of energy lowering when a material becomes superconducting (energy gap).

3. FURTHER SOLUTIONS OF EQUATION (2)

The solution function (10) is not the only possible solution of equation (2) with respect to the expansion (7). By putting $A_1 \equiv 0$, we obtain, according to equation (7a),

$$(E_2 + 4\hbar^2 k^2/2m)A_2 = 0, \qquad E_2 = -4\hbar^2 k^2/2m \tag{12}$$

where A_2 is a free parameter defined by the norm. Regarding equation (7a) with respect to the powers $\beta = 3, 4, 5, \ldots$, we find that now all coefficients of odd order A_3, A_5, $A_7, \ldots$ have to vanish, and only the coefficients of even order are of relevance. The A_2 dependence of A_4 and A_6 is given by (see also Table II)

$$\begin{aligned} A_4 &= A_2/2 \\ A_6 &= 5A_2/16 + (m\lambda/16\hbar^2 k^2)A_2^3 \end{aligned} \tag{12a}$$

The subsequent coefficients will be determined by considering the powers $\beta = 8, 10, 12, \ldots$ With the help of the L_2-norm and the substitution $A_2^2 = u$, the polynomial equation (9b) furnishes $A_2^{M\pm}(M = 1, 2, 3, 4, \ldots)$ and hence $A_4^{M\pm}$, $A_6^{M\pm}(M = 1, 2, 3, 4, \ldots)$.

Table II. The A_2 Dependence of the Expansion Coefficients A_{2n} $(n = 1, 2, \ldots, 8)^a$

n	A_{2n}	u^0A_2	$u^1A_2^3$	$u^2A_2^5$	$u^3A_2^7$
1	A_2	$1/4^0$	0	0	0
2	A_4	$2/4^1$	0	0	0
3	A_6	$5/4^2$	$1/4^2$	0	0
4	A_8	$14/4^3$	$6/4^3$	0	0
5	A_{10}	$42/4^4$	$27/4^4$	$1/4^4$	0
6	A_{12}	$132/4^5$	$110/4^5$	$10/4^5$	0
7	A_{14}	$429/4^6$	$429/4^6$	$65/4^6$	$1/4^6$
8	A_{16}	$1430/4^7$	$1456/4^7$	$350/4^7$	$14/4^7$

$^a u = m\lambda\hbar^{-2}k^{-2}$. Here A_{16} is determined by the expression $A_{16} = 1430A_2/4^7 + 1456uA_2^3/4^7 + 350u^2A_2^5/4^7 + 14u^3A_2^7/4^7$.

The second eigenfunction of equation (2) is also of infinite degree of degeneracy and is given by

$$\Psi_2^{M\pm} = \sum_{n=1}^{\infty} A_{2n}^{2,M\pm}(\cosh kx)^{-2n} \tag{12b}$$

where the corresponding eigenvalue is $E_2 = -4\hbar^2k^2/2m$.

The same procedure can readily be performed for all eigenvalues E_β, and according to equation (7a) we have to put $A_{k'} \equiv 0$ for all $k' < \beta$, whereas the subsequent coefficients $A_{\beta+2}, A_{\beta+4}, A_{\beta+6}, \ldots$ have to be determined by their A_β dependence and A_β is itself defined by the norm. We thus obtain an energy spectrum of equation (2):

$$E_\beta = -\beta^2\hbar^2/2m \qquad (\beta = 1, 2, 3, \ldots) \tag{13}$$

and to each eigenvalue E_β an infinite set of degenerate eigenfunctions may be associated:

$$\Psi_\beta^{M\pm} = \sum_{k'=\beta}^{\infty} A_{2k'-\beta}^{\beta,M\pm}(\cosh kx)^{-2k'+\beta} \tag{13a}$$

The convergence problems of the expansion (13a) are completely identical to those of the eigenfunction Ψ_1^M (see Appendix A).

A general property of the eigenfunctions (13a) is that they are all symmetric. However, equation (2) may also be solved by an antisymmetric set of L_2-integrable functions showing the general form

$$\Psi = \sum_{k'=2}^{\infty} B_{k'}(\cosh kx)^{-k'} \sinh kx \tag{14}$$

Higher order powers of sinh kx are not required, since the relation $\cosh^2 x - \sinh^2 x = 1$ can always be used to obtain the expansion (14), and with the help of this *ansatz*, equation (2) reads

$$\sum_{k'=2}^{\infty} \left\{ B_{k'} \left[E + \frac{\hbar^2k^2}{2m}(1-k')^2 \right] (\cosh kx)^{-k'} \sinh kx \right\}$$
$$- \frac{\hbar^2k^2}{2m} \sum_{k'=2}^{\infty} B_{k'} k'(k'+1)(\cosh kx)^{-k'-2} \sinh kx$$
$$= \lambda \sum_{\beta_1,\beta_2,\beta_3=2}^{\infty} B_{\beta_1} B_{\beta_2} B_{\beta_3} (\cosh kx)^{-\beta_1-\beta_2-\beta_3} \sinh kx (\cosh^2 kx - 1) \tag{15}$$

This equation has to be treated using the same principles discussed above. Thus, by considering $\beta = 2$, we obtain $E = -\hbar^2k^2/2m$ and the corresponding first eigenfunction

$$\Psi_1^{M\pm} = \sum_{k'=1}^{\infty} B_{2k'}^{1,M\pm}(\cosh kx)^{-2k'} \sinh kx \tag{16}$$

and with respect to the determination of the coefficients B_2, $B_4, \ldots$ the same remarks are valid as for the coefficients $A_2, A_4, \ldots$ Thus, the B_2 dependence of B_4 and B_6 is given by

$$B_4 = 0.75 B_2 + (\lambda m/4\hbar^2 k^2) B_2^3$$
$$B_6 = \tfrac{5}{6} B_4 + (\lambda m/4\hbar^2 k^2) B_2^2 B_4 - (m\lambda/12\hbar^2 k^2) B_2^3 \tag{17}$$

and the determination of B_2 via the L_2-norm again involves the relations (9a), (9b) and the substitution $u = B_2^2$. The energy spectrum related to the *ansatz* (14) is

$$E_{\beta-1} = -\hbar^2 k^2 (1-\beta)^2/2m \qquad (\beta = 2, 3, 4, \ldots) \tag{18}$$

and the associated set of eigenfunctions (the degree of degeneracy is infinite) reads

$$\Psi_{\beta-1}^{M\pm} = \sum_{k'=\beta}^{\infty} B_{2k'-\beta}^{\beta-1, M\pm} (\cosh kx)^{-(2k'-\beta)} \sinh kx$$
$$(\beta = 2, 3, 4, \ldots; \quad M = 1, 2, 3, 4, \ldots) \tag{18a}$$

The special case $\beta = 1$ has been excluded in the expansion (18a) [or (14)] because $B_1 \neq 0$ cannot be determined by the L_2-norm. If the case $B_1 \neq 0$ is taken into account, then B_1 is not a free parameter defined by the norm, but is given by (15) providing $E = \hbar^2 k^2/m$ and $B_{k'} \equiv 0 (k' > 1)$. A similar situation occurs when, according to equation (6), we assume $A_1 \neq 0$, $A_{k'} \equiv 0 (k' > 1)$; then equation (7a) would provide $E = -\hbar^2 k^2/2m$ and A_1 corresponding to equation (3a).

4. AN EXTENSION TO THE RELATIVISTIC CASE

The Lorentz-invariant analog to the nonlinear Schrödinger equation (1) is a scalar nonlinear field equation of the type of a generalized Klein-Gordon equation

$$\Box \Psi = \frac{m^2 c^2}{\hbar^2} \Psi + \lambda |\Psi|^2 \Psi \tag{19}$$

This equation has been taken as a starting point in nonlinear field theory (see, e.g., Jackiw, 1977; Mielnik, 1974; Mielke, 1981; and references cited therein) because the soliton functions of (19) have been related to problems of particle physics. These soliton functions are readily obtained via the solutions (3) and (4) of equation (2) because they have only to be slightly modified to yield

$$\Psi = A \cosh(k\gamma x + k\gamma vt)^{-1} \tag{20}$$

where

$$k^2 = m^2c^2/\hbar^2; \qquad A^2 = -2k^2/\lambda \tag{20a}$$

and

$$\Psi = B\tanh(k\gamma x - k\gamma vt) \tag{21}$$

where

$$2k^2 = -m^2c^2/\hbar^2; \qquad B^2 = -2k^2/\lambda \tag{21a}$$

γ is given by $\gamma = 1/(1 - v^2/c^2)^{1/2}$. Thus, the solution (20) requires either $\lambda < 0$ to yield $k^2 > 0$ or $\lambda > 0$; then A^2 has to be replaced by $|A|^2$. The solution (21) is not convenient in the relativistic case, as can be verified from the relation (21a), because the condition $m^2 > 0$ must always hold. However, our main interest is a discussion of the symmetric solutions (7) and antisymmetric solutions (14) of equation (2) in the relativistic case (19). Thus, the relativistic analog of the solution manifold (13a) is

$$\Psi_{\beta}^{M\pm} = \sum_{k'=\beta}^{\infty} A_{2k'-\beta}^{\beta,M\pm}[\cosh(k\gamma x - k\gamma vt)]^{-2k'+\beta} \tag{22}$$

$$(\beta = 1, 2, 3, \ldots; \quad M = 1, 2, 3)$$

and of the solution manifold (18a)

$$\Psi_{\beta-1}^{M\pm} = \sum_{k'=\beta}^{\infty} B_{2k'-\beta}^{\beta-1,M\pm}[\cosh(k\gamma x - k\gamma vt)]^{-2k'+\beta} \times \sinh(k\gamma x - k\gamma vt) \qquad (\beta = 2, 3, \ldots; \quad M = 1, 2, 3) \tag{23}$$

With respect to the procedure for determining the expansion coefficients $A_1, A_2, A_3, \ldots$ and $B_1, B_2, B_3, \ldots$, we refer to the remarks of the preceding sections, and we note that even the numerical effort has not increased in the relativistic case (19). Since the expression $m^2c^2/\hbar^2$ plays the same role as the energy E in equation (2), the eigenvalue spectrum of equation (19) with respect to the solution manifold (22), (23) yields

$$\text{equation (22):} \qquad m^2 = \beta^2\hbar^2k^2/c^2, \qquad \beta = 1, 2, 3, \ldots \tag{24}$$

$$\text{equation (23):} \qquad m^2 = (1-\beta)^2\hbar^2k^2/c^2, \qquad \beta = 2, 3, 4, \ldots \tag{25}$$

We mention again that each eigenvalue of equations (24) and (25) is related to an infinite set of degenerate eigenfunctions characterized by the parameter M with $M = 1, 2, 3, \ldots$, and the only reason that we can consider in practical computations a finite subset is the polynomial equation (9b), which has to be solved numerically.

Because for each β the allowed k values are only defined in the corresponding valence band (see Appendix A), equidistant levels of the mass spectrum according to equations (22) and (23) are not obtained.

The eigenfunctions (22) and (23) may be considered as an indication that it is not satisfactory to treat nonlinear terms as perturbations of linear field equations, since these solutions do not exhibit convergence (and therefore they do not exist) in the case of the linear Klein–Gordon equation $\Box\Psi=(m^2c^2/\hbar^2)\Psi$ because this transition ($\lambda\Rightarrow 0$) may produce a singularity (see also Appendix A with respect to the behavior of the linear Schrödinger equation).

APPENDIX A. CONVERGENCE PROBLEMS AND SOME PHYSICAL CONSIDERATIONS

In the preceding sections we assumed that the basis expansion (7) and its slight modification (14) represent convergent series providing the solution spectra of the nonlinear Schrödinger (and, if appropriately modified, Klein–Gordon) equation. However, some essential properties referring to the convergence of the expansion (7) can be provided by applying (7) to the linear Schrödinger equation of free particles ($\lambda\equiv 0$):

$$E\Psi+(\hbar^2/2m)\,\partial^2\Psi/\partial x^2=0 \tag{A1}$$

implying the relations

$$E\sum_{k'=1}^{\infty}A_{k'}(\cosh kx)^{-k'}+\frac{\hbar^2k^2}{2m}\sum_{k'=1}^{\infty}A_{k'}k'^2(\cosh kx)^{-k'} =\frac{\hbar^2k^2}{2m}\sum_{k'=1}^{\infty}A_{k'}k'(k'+1)(\cosh kx)^{-k'-2} \tag{A1a}$$

and

$$\begin{aligned} E&=-\hbar^2k^2/2m \qquad (k'=1)\\ A_{k'}(k'+1)&=A_{k'-2}(k'-2) \qquad (k'=3,5,\ldots)\end{aligned} \tag{A1b}$$

Thus, in the linear case the recursive determination of the coefficients $A_{2k'+1}$ would be considerably simplified, but the expansion (7) does not converge with respect to (A1), and by putting $\varepsilon=1/\cosh kx$, where $\varepsilon=1$ for $x=0$ and $\varepsilon<1$ for $|kx|>0$, it is readily seen that it is the *zero point* ($\varepsilon=1$) that causes the principal difficulty:

$$\lim_{k'\to\infty}\{\varepsilon^{k'}A_{k'}/A_{k'-2}\,\varepsilon^{k'-2}=[(k'+1)/(k'-1)]\varepsilon^2\} \tag{A1c}$$

Thus, a necessary and sufficient criterion of absolutely convergent series is that (besides $\lim_{k'\to\infty}A_{k'}\to 0$) the limit of the ratio (A1c) is always <1, but this condition is readily satisfied for $\varepsilon < 1$ (outside the zero point), whereas for $\varepsilon = 1$ ($x = 0$) the relation (A1c) provides 1, and therefore the zero point of the (free) particle causes the divergent behavior. The result (A1b) is related to a serious contradiction: If the expansion (7) is L_2-integrable with respect to (A1) and (A1a), then for a free particle the total energy (= kinetic energy) has to be >0, and because of the relation (A1b) and the singularity at the zero point, equation (A1a) does not provide L_2-integrable wave functions. Therefore, the case $\lambda \equiv 0$ yielding (A1) has to be excluded, as this case leads to a singularity at the zero point with respect to the expansion (7). One might be surprised by this condition, but it should be noted that there are similar situations in other problems. The harmonic oscillator eigenfunctions $\Psi_n = H_n(\alpha x) \exp(-\alpha^2 x^2)$ with $\alpha^2 = m^2\omega_0^2/2\hbar^2$ become singular and non-L_2-integrable by taking $\omega_0 \to 0$. So the wave function of free particles is not obtained by this limit.

It might appear that the singularity problem at the zero point ($x = 0$) does not exist when the antisymmetric expansion (14) is applied to the linear Schrödinger equation (A1), because the functions

$$f_\beta = (\sinh kx)(\cosh kx)^{-\beta} \tag{A2}$$

vanish at $X = 0$ and exhibit a maximum for

$$x = k^{-1} \operatorname{arcosh} + [(1 - 1/\beta)^{-1}]^{1/2}\}$$

and a minimum for

$$x = k^{-1} \operatorname{arcosh}\{-[(1 - 1/\beta)^{-1}]^{1/2}\}$$

However, by taking lim $\beta \to \infty$ the maximum and minimum of (A2) are both at the *zero point*, and therefore the same singularity is produced by the expansion (14) with respect to (A1).

By a suitable modification of the expansions (7) and (14) it is possible to pass continuously to the linear limit ($\lambda = 0$) without producing any singularity, but this case will have to be discussed after the present analysis of convergence properties.

The negative-energy eigenvalues referring to bound states are only consistent with an additional attractive potential, and it has been noted (Barut, 1977) that equation (2) may be regarded as a usual Schrödinger equation with a potential proportional to the density of solutions $\varphi\Psi = \lambda|\Psi|^2\Psi$. Because $|\Psi|^2$ has to remain always $\geq 0(-\infty \leq x \leq +\infty)$, an attractive potential or negative-energy eigenvalues must be connected to the condition $\lambda < 0$, and, indeed, we shall verify that convergence of the expansion (7) or (14) is closely related to the condition $\lambda < 0$.

The first problem of convergence of the expansion (7) with respect to equation (2) is the proof of a pointwise convergence; after that, the norm convergence shall be discussed. Even in the nonlinear case [equation (7a)] the pointwise convergence has to be regarded in the zero point ($\varepsilon = 1, x = 0$), since it follows that the expansion

$$\Psi = \sum_{k'} A_{k'} \varepsilon^{k'} \qquad (\varepsilon = 1/\cosh kx) \tag{A3}$$

is convergent for $0 \leq \varepsilon < 1$ (x arbitrary, but nonzero) if it is convergent for $\varepsilon = 1$ (zero point, and therefore the pointwise convergence is established at every arbitrary $x \neq 0$ when the expansion (7) exists at the zero point. We should also point out that our main interest lies in the first eigenfunction Ψ_1^M, representing an infinite set of eigenfunctions related to one energy eigenvalue ($E = -\hbar^2 k^2/2m$). The reasons are:

1. The convergence properties of the other eigenfunctions can be reduced to the standard case to be considered.
2. The eigenfunction Ψ^{M_1} stands in close relationship to the soliton solution (3).
3. Some physical aspects of the eigenfunctions Ψ_β^M and eigenvalues E_β ($\beta > 1$) appear to be somewhat unclear, since the energy E_β becomes lower and lower when β increases (see also the remarks at the end of this Appendix).

Table I shows the dependence of the coefficients A_{2n+1} in terms of the parameters A_1 and the coupling constant λ (from A_1 to A_{13}). Thus, for a bound state ($\lambda < 0$ and being compatible with $E < 0$) the coefficients $A_3, A_5, \ldots$ and higher order are corrected such that a conditionally convergent series can be constructed, whereas for $\lambda > 0$ the expansion (7) with respect to equations (2) and (7a) does not exist. These coefficients exhibit the same linear contributions, being proportional to A_1, as the linear Schrödinger equation, whereas the nonlinearity yields power corrections in terms of λ. For example, the expansion coefficient of A_1 is 1, whereas appropriate conditions lead to $A_3 < 0$, $A_5 > 0$, etc., and therefore the Leibniz criterion for series that do not absolutely converge has to be applied:

$$\sum_{k'} |A_{k'}|(-1)^{k'} < \infty, \qquad |A_1| > A_3| > \cdots > |A_{k'}|, \qquad \lim_{k' \to \infty} |A_{k'}| \to 0 \tag{A4}$$

This is a sufficient (but not necessary) condition for convergence, and, according to a theorem of Riemann, a rearrangement of an infinite partial set is not commutative. In other words, it is impossible first to take the sum of all linear terms (referring to A_1) and thereafter the sum of all contributions $\sim\lambda$, $\sim\lambda^2$, $\sim\lambda^3$, etc., separately. The conditions (A4) can be analyzed by the formation law of A_{2n+1}:

$$A_{2n+1} = A_1 \sum_{j=0}^{n} R_{j,n} \frac{(m\lambda)^{n-j}}{4^n (k^2 \hbar^2)^{n-j}} A_1^{2n-2j} \tag{A5}$$

For even j $(0, 2, 4, \ldots)$, $R_{j,n}$ is given by

$$R_{j,n} = (2^{j/2}/j!)n(n-1)\cdots(n+1-j/2)(2n+1-2j)(2n-1) \times(2n-3)\cdots(2n+3-j) \tag{A6}$$

and for odd j $(1, 3, 5, \ldots)$, $R_{j,n}$ is given by

$$R_{j,n} = (2^{(j-1)/2}/j!)n(n-1)(n-2)\cdots[n-(j-3)/2] \times(2n+1-2j)(2n-1)(2n-3)\cdots(2n-j+2) \tag{A6a}$$

The recurrence formulas (A6), (A6a) can be constructed by an evaluation of equation (7a), where A_{2n+1} appearing only in the linear part of (2) is determined by the cubic term and therefore the powers of $(\cosh kx)^{-1}$ have to be mutually compared with respect to the coefficients:

$$\lambda \sum_p \sum_q \sum_r A_p A_q A_r (\cosh kx)^{-(p+q+r)}$$
$$= \text{linear contributions} \cdot (\cosh kx)^{-(2n+1)} \qquad (p+q+r=2n+1)$$

There is one combination with $p=q=r=p$, whereas there are three combinations with $p=q\neq r$ (cyclic) and six combinations with $p\neq q\neq r\neq p$ (cyclic). The above recurrence formulas are readily tested by complete induction, and from (A5), (A6), and (A6a) we get the following results:

Result 1:

$$\lim_{n\to\infty} A_{2n+1} \to 0 \tag{A7}$$

A more sophisticated problem is the satisfaction of the remaining conditions sufficient for convergence. Thus, by taking $k=\infty$ $(E_1 \to -\infty)$, all contributions of the powers of A_1 would vanish, whereas the case $k \Rightarrow 0$ would yield infinities. Therefore, there are threshold values for k^2 (and for the energy) to satisfy the remaining conditions of (A4):

Result 2:

$$m|\lambda|A_1^2/5\hbar^2 < k^2 < m|\lambda|A_1^2/2\hbar^2 \tag{A8}$$

Thus, k^2 has to be assumed within these boundaries, but A_1^2 is still completely undefined, and therefore we have to proceed in the following way:

1. A_1^2 is determined by the norm.
2. After fixation of the k dependence of A_1 the allowed values of k can be fixed according to the inequality (A8).

Inequality (A8) states that there is only convergence according to the criterion (A4) when the energy $E_1 = -\hbar^2 k^2/2m$ is restricted to an energy band. It is possible that the modification

$$\frac{m|\lambda|A_1^2}{5\hbar^2} \leq k^2 \leq \frac{m|\lambda|A_1^2}{2\hbar^2} \tag{A8a}$$

also yields convergence, since (A4) is a sufficient condition, but this cannot be proved without explicit calculations.

Assumptions 1 and 2 are plausible, as can be concluded from a comparison with the linear case, where the divergent behavior at the zero point ($\varepsilon = 1$) requires the assumption that $A_1 \equiv 0$ and that A_1^2 should be >0 but finite due to the norm (e.g., <1), and yet the inequality (A8) incorporates a more general validity than the simplification $A_1^2 < 1$.

A further consideration is the proof of the existence of a norm of the wave function. However, this cannot be achieved by the L_2-norm yielding equation (9b). The proof of the existence of the L_2-norm can be given by a stronger condition, namely the existence of a maximum norm M_n and of the L_1-norm ($\int_{-\infty}^{\infty} |\Psi|\, dx < \infty$), whereby the existence of the maximum norm M_n and of the L_1-norm is shown in Appendix B. Let $\Psi = \sum_{\beta=1}^{\infty} A_\beta [\cosh kx]^{-\beta}$ be uniformly convergent on $\mathbb{R}$; then it follows that $\Psi(x)$ is continuous on $\mathbb{R}$, because the following conditions hold:

$$\lim_{|x| \to \infty} \Psi(x) = 0$$
$$\lim A_\beta = 0 \qquad (\beta \to \infty) \tag{A9}$$

Therefore $\Psi(x)$ is also bounded on $\mathbb{R}$. If $M_n = \max|\Psi(x)|$, then the following inequality holds (for all $x \in \mathbb{R}$):

$$[|\Psi(x)|/M_n]^2 \leq |\Psi(x)|/M_n \tag{A10}$$

From this inequality it follows that

$$\int_{-\infty}^{+\infty} |\Psi|^2\, dx = M_n^2 \int_{-\infty}^{+\infty} |\Psi/M_n|^2\, dx \leq M_n^2 \int_{-\infty}^{+\infty} |\Psi/M_n|\, dx \tag{A11}$$

and therefore we obtain the desired result

$$\int_{-\infty}^{+\infty} |\Psi|^2\, dx \leq M_n \int_{-\infty}^{+\infty} |\Psi|\, dx \to \int_{-\infty}^{+\infty} |\Psi|^2\, dx < \infty \tag{A12}$$

In practical problems we can work as follows: A_1 is determined by equation (9b), being related to the L_2-norm with respect to higher order approximations (e.g., $M \gg 20$); then the band of the permitted k values is fixed according to the inequality (A8). In this way a finite approximation of Ψ_1^M with M degenerate functions is obtained.

The same considerations as applied to Ψ_1 can also be taken with regard to the eigenfunctions Ψ_β^M (where $\beta > 1$ and $E_\beta = -\hbar^2 k^2 \beta^2/2m$) and to the antisymmetric eigenfunctions according to the expansion (14). Thus, in the case of Ψ_2^M the inequality (A8) has to be replaced by

$$-13 < \frac{m|\lambda|A_2^2}{\hbar^2 k^2} < -\tfrac{17}{5} \tag{A13}$$

and we note that for each energy eigenvalue $E_\beta(\beta \geq 1)$ an inequality of this kind must be valid in order for the conditions (A4) to be satisfied. We briefly state the consequence: For each negative energy ($E_\beta < 0$) there exists a band of permitted k values with upper and lower limits analogous to the inequality (A4). Since $k^2 \sim |\lambda|$, the bandwidth depends on the coupling constant λ. In analogy to the hole theory, one would assume that all Ψ_β^M states with $\beta > 1$ should be occupied, but this consideration is only consistent with the exclusion principle, and therefore further physical considerations would have to be introduced. However, the solution Ψ_1^M may also be referred to the Ginzburg–Landau theory of superconductivity, and thus we can verify the energy gap of a superconducting state.

We also note that by the modification

$$\Psi_\beta^{M\pm} = \sum_{k'=\beta}^{\infty} (A_{k'} \cosh kx^{-k'} + B_{k'} \cosh kx^{-k'-1} \sinh kx) \exp(ipx) \quad \text{(A14)}$$

where

$$\begin{aligned} B_\beta &= \pm i A_\beta \\ E_\beta &= \hbar^2 p^2/2m - \hbar^2 k^2 \beta^2/2m \end{aligned} \quad \text{(A15)}$$

Equation (2) can also be solved, and, by taking $\lambda = 0$, a singularity at the origin $x = 0$ does not occur, but this *ansatz* has the disadvantage that one cannot obtain real wave functions and there is no possibility to distinguish between symmetric functions (7) and antisymmetric functions (14).

It should further be mentioned that with the help of the *ansatz* (A15) nonlinear spinor equations can be solved exactly, whereas restrictions to the expansions (7) and (14) are not possible, in contrast to the nonlinear Klein–Gordon equation. However, due to the spin–spin coupling there arises a more difficult multiplet structure, and the evaluation of the nonlinear terms according to the expansion (A15) requires more effort than for scalar fields.

Many types of nonlinear field equations have been proposed (Ivanenko, 1979; Heisenberg, 1966),[2] but for brevity we consider a simplified version:

$$\gamma^\nu \frac{\partial \Psi}{\partial x^\nu} = \frac{mc}{\hbar} \Psi + \lambda \Psi(\bar{\Psi} \gamma_5 \Psi) \quad \text{(A16)}$$

[2]The nonlinear spinor equation proposed by Ivanenko (1979) is based on classical field theory (the torsion of $U4$-space is the cause of the nonlinearity), whereas the nonlinear theory according to Heisenberg (1966) is based on quantum field theory with indefinite metric. The group-theoretic assumptions (spin × isospin) are also rather different from the Ivanenko equation, but Heisenberg [see further references in Heisenberg (1966)] has also performed perturbation calculations of the classical version. Therefore the computation method presented here might be interesting for both cases.

A special case is a restriction of the four-component Dirac spinor Ψ to $(\Psi_1, 0, 0, 0)$ and to the two coordinates z, t:

$$-\gamma_z \hbar \frac{\partial \Psi_1}{\partial z} + \frac{\hbar}{c} \gamma_t \frac{\partial \Psi_1}{\partial t} = mc\Psi_1 + \lambda \hbar \Psi_1^3 \tag{A17}$$

Then, by the expansion

$$\Psi_1 = \sum_{k'=\beta}^{\infty} [A_{k'} \cosh(k\gamma z - k\gamma vt)^{-k'} + B_{k'} \sinh(k\gamma z - k\gamma vt) \cosh(k\gamma z - k\gamma vt)^{-k'-t}) \tag{A18}$$

one can solve (A17) using the same principles as above, yielding

$$\begin{aligned} A_\beta &= B_\beta \qquad (\text{for all } \beta = 1, 2, \ldots) \\ k &= mc/\hbar\beta \end{aligned} \tag{A19}$$

With respect to k, note that band structure properties also hold, as obtained in the case of the nonlinear Schrödinger (and Klein–Gordon) equation.

APPENDIX B. EXISTENCE OF THE L_2-NORM

The existence of the L_2-norm of the expansion (7) with respect to equation (2) (and also to the nonlinear Klein–Gordon equation) can be reduced to the existence of a maximum norm and an L_1-norm [see, e.g., relations (A11), (A12)].

Maximum norm (M_n). Let $M_n = \max|\Psi|$; then for all expansions constructed on the basis of equation (7) we have $M_n = \max|\Psi| = |\sum_\beta A_\beta|$, because the set of functions $\{(\cosh kx)^{-\beta}\}$ always exhibits a maximum at the zero point $x = 0$ (for each $\beta \geq 1$). In the nonlinear case, the summation $\sum_\beta A_\beta < \infty$ holds, and therefore $|\sum_\beta A_\beta| < \infty$ is also true, but $\sum_\beta |A_\beta|$ does not exist.

L_1-norm ($\int_{-\infty}^{+\infty} |\Psi| \, dx < \infty$). For convenience, we regard the standard case (the same is true for the other cases):

$$\int_{-\infty}^{+\infty} |\Psi| \, dx = A_1 S_1 + A_3 S_3 + \cdots + \sum_{k'=3}^{\infty} A_{2k'+1} S_{2k'+1}$$

where $S_{2k'+1}$ is given by

$$S_{2k'+1} = \int_{-\infty}^{+\infty} (\cosh kx)^{-(2k'+1)} \, dx$$

The latter integral is readily evaluated to yield

$$S_1 = \frac{\pi}{k}, \qquad S_n = \frac{\pi[1 \cdot 3 \cdot 5 \cdots (n-2)]}{k[2 \cdot 4 \cdot 6 \cdots (n-1)]}, \quad n > 1$$

Defining $S_n = S_1 \cdot S'_n$ ($S'_n < 1$ for $n > 1$ and $S'_n = 1$ for $n = 1$), we obtain

$$\int_{-\infty}^{+\infty} |\Psi|\, dx = S_1 \left| A_1 + A_3 S'_3 + \cdots + \sum_{k'=3}^{\infty} S'_{2k'+1} A_{2k'+1} \right|$$

Because $S'_{n_2} < S'_{n_1}$ (if $n_2 > n_1$) and $S'_n \to 0$ (if $n \to \infty$), we obtain

$$\int_{-\infty}^{+\infty} |\Psi|\, dx \leq S_1 \circ M_n$$

With the help of the relations (A9)-(A12) we have shown that the wave functions are L_2-integrable in the nonlinear case if the maximum norm and L_1-norm exist. With respect to the modified expansion (14), we note that the maximum of these functions ($\sinh kx$) ($\cosh kx)^{-\beta}$ ($\beta \geq 2$) is usually not at the zero point, but at $x_m = k^{-1}$ arcosh$[(1-1/\beta)^{-1}]^{1/2}$. The existence of the maximum norm then requires that the sum

$$M_n = \max|\Psi| = \left| \sum_{\beta=2}^{\infty} B_\beta (1-1/\beta)^{\beta/2} [(1-1/\beta)^{-1} - 1]^{1/2} \right|$$

remains finite.

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