Quantum bound states for a derivative nonlinear Schrödinger model and number theory

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A derivative nonlinear Schrödinger model is shown to support localized N-body bound states for several ranges (called bands) of the coupling constant η. The ranges of η within each band can be completely determined using number theoretic concepts such as Farey sequences and continued fractions. For $N \geq 3$, the N-body bound states can have both positive and negative momentum. For $\eta > 0$, bound states with positive momentum have positive binding energy, while states with negative momentum have negative binding energy.

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Integrable quantum models in 1+1 dimensions which support bound states have been studied extensively for many years [1–8]. For an integrable Hamiltonian, the coordinate Bethe ansatz can yield the exact eigenfunctions. If an eigenfunction decays exponentially fast when any of the interparticle distances tends towards infinity (keeping the center of mass coordinate fixed), we call such a localized square-integrable eigenfunction a bound state. Bound states of quantum integrable models are usually found to have positive binding energy [1–5].

In this paper, we will study the quantum bound states of an integrable derivative nonlinear Schrödinger (DNLS) model [6,7]. Classical and quantum versions of the DNLS model have found applications in many areas of physics like circularly polarized nonlinear Alfven waves in a plasma [9], quantum properties of solitons in optical fibers [10], and some chiral Luttinger liquids [11]. The classical DNLS model is known to have solitons with momenta in only one direction [12,13].

Using the coordinate Bethe ansatz, it had been found earlier that quantum N-body bound states exist for the DNLS model provided that the interaction parameter η (defined in Eq. (1) below) lies in the range $0 < |\eta| < \tan(\pi/N)$. It was also observed that, similar to the classical case, such N-body bound states can have only positive values of P/η, where P is the momentum [6]. However, it was found recently that bound states can exist with $P/\eta < 0$ provided that $\tan(\pi/N) < |\eta| < \tan[\pi/(N-1)]$, and that these states have *negative* binding energy [8]. This naturally leads one to ask: are there other ranges of values of η for which quantum bound states exist, and, if they exist, what are their momenta and binding energies?

In this paper, we will solve the problem of determining the *complete* ranges of values of η for which quantum N-body bound states exist in the DNLS model, for *all* values of N. After presenting the conditions which are required for a quantum N-body bound state to exist, we will use the idea of Farey sequences in number theory to show that there are certain ranges of η, called bands, in which bound states exist. We find that the bound states appearing within each band can have both positive and negative values of P/η; these have positive and negative binding energies respectively. We will then use another concept from number theory, that of continued fractions, to address the inverse problem of finding the values of N for which N-body bound states exist for a given value of η.

For N particles, the Hamiltonian of the DNLS model is given by

$$H_N \;=\; -\hbar^2 \sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} \;+\; i2\hbar^2\eta \sum_{l<m} \delta(x_l - x_m) \left(\frac{\partial}{\partial x_l} + \frac{\partial}{\partial x_m} \right) , \tag{1}$$

where we have set the particle mass $m = 1/2$. H_N commutes with the momentum operator $P_N = -i\hbar \sum_{j=1}^{N} \partial/\partial x_j$. We note that H_N remains invariant while P_N changes sign if we change the sign of η and transform all the $x_i \rightarrow -x_i$

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at the same time; we call this the parity transformation. Hence it is sufficient to study the model for one particular sign of η, say, $\eta > 0$. The eigenfunctions for $\eta < 0$ can then be obtained by changing $x_i \to -x_i$.

Next, the coordinate space $R^N \equiv \{x_1, x_2, \cdots x_N\}$ is divided into various N-dimensional sectors defined through inequalities like $x_{\omega(1)} < x_{\omega(2)} < \cdots < x_{\omega(N)}$, where $\omega(1), \omega(2), \cdots, \omega(N)$ represents a permutation of the integers $1, 2, \cdots, N$. Given the wave function in the fundamental sector, defined as $x_1 < x_2 < \cdots < x_N$, the wave functions in all the other sectors can be found by Bose symmetry. In the fundamental sector, the Bethe ansatz wave function takes the form

$$\psi = \sum_{\omega} C_\omega \ \exp \ \{i(k_{\omega(1)} x_1 + \cdots + k_{\omega(N)} x_N)\}, \tag{2}$$

where k_n's are all distinct wave numbers, the sum is over all permutations ω of the integers $1, 2, \cdots, N$, and C_ω are appropriate coefficients. The momentum and energy of this eigenfunction are given by

$$P \ = \ \hbar \sum_{j=1}^{N} k_j \ , \quad \text{and} \quad E \ = \ \hbar^2 \sum_{j=1}^{N} k_j^2 \ . \tag{3}$$

In Ref. [6], it was shown that a localized bound state has a wave function consisting of only one plane wave in each sector. Namely, in the fundamental sector, the coefficients C_ω in (2) vanish for all ω's except for the identity permutation. Further, the momenta k_n's satisfy the following conditions:

$$k_n - k_{n+1} \ + \ i \ \eta \ (k_n + k_{n+1}) \ = \ 0 \ , \tag{4}$$

for $n = 1, 2, \cdots, N-1$,

$$\sum_{j=1}^{N} q_j \ = \ 0 \ , \tag{5}$$

where q_j denotes the imaginary part of k_j, and

$$q_1 < 0 \ , \quad q_1 + q_2 < 0 \ , \quad \cdots \quad , \quad \sum_{j=1}^{N-1} \ q_j < 0 \ . \tag{6}$$

Eqs. (5-6) imply that the wave function ψ is square-integrable if one holds the center of mass coordinate $X = \sum_i x_i / N$ fixed, and integrates over the relative coordinates $y_r = x_{r+1} - x_r$, where $r = 1, 2, \cdots, N-1$. In the fundamental sector, the integrals over the y_r's all run from 0 to ∞, and they are independent of each other. Using Eq. (5-6), one can express the probability density as

$$|\psi|^2 \ \sim \ \exp[\ \sum_{r=1}^{N-1} \ (\sum_{j=1}^{r} q_j) \ y_r \ ] \, , \tag{7}$$

which is independent of X. Due to the conditions in (6), integration of this probability density over the y_r's gives a finite result.

The conditions (4) and (5) imply that the k_n's must be complex numbers of the form

$$k_n \ = \ \chi \ e^{-i(N+1-2n)\phi} \ , \tag{8}$$

where χ is a real parameter, and $\phi \equiv \tan^{-1} \eta$. Since $0 < |\eta| < \infty$, we assume that $0 < |\phi| < \pi/2$. Using Eqs. (3) and (8), the momentum and energy of this state are found to be

$$P \ = \ \hbar \chi \ \frac{\sin(N\phi)}{\sin \phi} \ , \quad \text{and} \quad E \ = \ \frac{\hbar^2 \chi^2 \sin(2N\phi)}{\sin(2\phi)} \ . \tag{9}$$

If we define the mass of this state by the relation $E = P^2/(2M)$, we find that

$$M \ = \ \frac{\tan(N\phi)}{2 \tan(\phi)} \ . \tag{10}$$

We now impose the conditions (6) on the k_n's. We find that all the following inequalities must be satisfied,

$$\chi \, \frac{\sin(l\phi)}{\sin\phi} \; \sin[(N-l)\phi] \; > \; 0 \tag{11}$$

for $l = 1, 2, \cdots, N-1$. For $N = 2$, (11) is satisfied when ϕ lies in the range $0 < \phi < \pi/2$ ($-\pi/2 < \phi < 0$) if $\chi > 0$ ($\chi < 0$). Thus any nonzero value of ϕ allows a 2-body bound state. From (9), we see that the ratio $P/\phi > 0$.

We now consider the more interesting case with $N \geq 3$. Due to the parity symmetry of (1), we will henceforth assume that $\phi > 0$ (i.e. $\eta > 0$). Eq. (11) can then be rewritten as

$$\chi \; \sin(l\phi) \; \sin[(N-l)\phi] \; > \; 0 \tag{12}$$

for $l = 1, 2, \cdots, N-1$. For $\chi > 0$, Eq. (12) implies

$$\cos[(N-2l)\phi] \; > \; \cos(N\phi) \tag{13}$$

for $l = 1, 2, \cdots, N-1$. Let us now consider a value of ϕ of the form

$$\phi_{N,n} \; \equiv \; \frac{\pi n}{N} \; , \tag{14}$$

where n is an integer satisfying $1 \leq n < N/2$. If n is odd, $\cos(N\phi_{N,n}) = -1$. We then find that all the inequalities in (13) are satisfied provided that N and n are relatively prime, i.e., if the greatest common divisor of N and n is 1. Similarly, for $\chi < 0$, Eq. (12) takes the form

$$\cos[(N-2l)\phi] \; < \; \cos(N\phi) \tag{15}$$

for $l = 1, 2, \cdots, N-1$. We find that all these inequalities are satisfied if n is even, and N and n are relatively prime.

In short, all the inequalities in (12) are satisfied for $\phi = \phi_{N,n}$, if and only if N and n are relatively prime (with n odd for $\chi > 0$, and n even for $\chi < 0$). By continuity, it follows that all the inequalities will hold in a neighborhood of $\phi_{N,n}$ extending from a value $\phi_{N,n,-}$ to a value $\phi_{N,n,+}$. The region $\phi_{N,n,-} < \phi < \phi_{N,n,+}$ will be called the band $B_{N,n}$.

For a given value of N, the number of bands in which bound states exist is equal to the number of integers n which are relatively prime to N and satisfy $1 \leq n < N/2$. This is equal to half the number of integers which are relatively prime to N and satisfy $1 \leq n < N$. The latter number is called Euler's ϕ-function $\Phi(N)$ [14]. The number of bands is therefore equal to $\Phi(N)/2$ for $\eta > 0$.

We now have to determine the end points $\phi_{N,n,-}$ and $\phi_{N,n,+}$ of the band $B_{N,n}$. One or more of the inequalities in (12) will be violated at the end points $\phi_{N,n,\pm}$ if

$$\phi_{N,n,\pm} \; = \; \frac{\pi j_\pm}{l_\pm} \; , \tag{16}$$

where $j_\pm$ and $l_\pm$ are integers satisfying

$$1 \; \leq \; l_\pm \; < \; N \; , \quad \text{and} \quad j_\pm \; < \; \frac{l_\pm}{2} \tag{17}$$

(since $\phi < \pi/2$). Thus the end points of the band $B_{N,n}$ are given by two rational numbers of the form $j_\pm/l_\pm$ which lie *closest* to (and on either side of) the point $\phi_{N,n}/\pi = n/N$. These can be found using the idea of Farey sequences [14].

For a positive integer N, the Farey sequence F_N is defined to be the set of all the fractions a/b in increasing order such that (i) $0 \leq a \leq b \leq N$, and (ii) a and b are relatively prime. For $N \geq 2$, if n/N is a fraction appearing somewhere in the sequence F_N, then it is known that the fractions a_1/b_1 and a_2/b_2 appearing immediately to the left and to the right respectively of n/N satisfy

$$\begin{aligned} a_1 \; , \; a_2 \; \leq \; n \; , \quad & \text{and} \quad a_1 \; + \; a_2 \; = \; n \; , \\ b_1 \; , \; b_2 \; < \; N \; , \quad & \text{and} \quad b_1 \; + \; b_2 \; = \; N \; , \\ nb_1 \; - \; Na_1 = 1 \; , \quad & \text{and} \quad nb_2 \; - \; Na_2 = -\,1 \; , \end{aligned} \tag{18}$$

and $n, \; b_1, \; b_2$ are relatively prime to N.

Using Eqs. (16) and (17), we now see that the end points of the band $B_{N,n}$ are given by

$$\phi_{N,n,-} \; = \; \frac{\pi a_1}{b_1} \; , \quad \text{and} \quad \phi_{N,n,+} \; = \; \frac{\pi a_2}{b_2} \; , \tag{19}$$

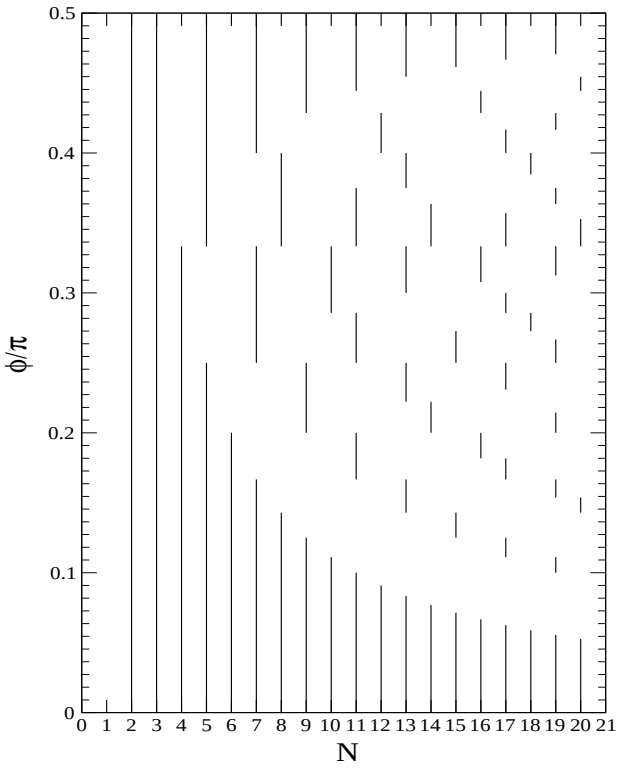

FIG. 1. The values of ϕ/π for which N-body bound states exist for various values of N.

where a_1/b_1 and a_2/b_2 are the fractions lying to the left and right of n/N in the Farey sequence F_N.

For $N \geq 3$, the lowest band is given by $n = 1$; by using Eq. (18), the range of this band is obtained as $0 < \phi/\pi < 1/(N-1)$. For higher values of n, the end points of the band $B_{N,n}$ (i.e., the integers a_i and b_i) can be determined numerically by using the properties given in Eq. (18). Fig. 1 shows the ranges of values of ϕ for which bound states exist for $N = 2$ to 20.

Eq. (18) implies that the width of the right side of the band $B_{N,n}$ from $\phi_{N,n}$ to $\phi_{N,n,+}$ is $\pi/(Nb_2)$, while the width of the left side from $\phi_{N,n,-}$ to $\phi_{N,n}$ is $\pi/(Nb_1)$. For later use, we note that each of these widths is larger than π/N^2, since $b_1,\ b_2 < N$.

We now calculate the momentum and binding energy for the N-body bound states in a particular band $B_{N,n}$ using Eq. (9). The form of the end points given in Eq. (19) shows that $\sin(N\phi) = 0$ at only one point in the band $B_{N,n}$, namely, at $\phi = \phi_{N,n}$. In the right part of the band (i.e., from $\phi_{N,n}$ to $\phi_{N,n,+}$), the sign of $\sin(N\phi)$ is $(-1)^n$. In the left part of the band (i.e., from $\phi_{N,n,-}$ to $\phi_{N,n}$), the sign of $\sin(N\phi)$ is $(-1)^{n+1}$. Since χ has the same sign as $(-1)^{n+1}$, the momentum given in Eq. (9) is positive in the left part of the band, negative in the right part of the band, and zero at $\phi = \phi_{N,n}$.

To calculate the binding energy, we consider a reference state in which the momentum P of the N-body bound state is equally distributed among N single-particle scattering states. From Eqs. (3) and (9), the wave number associated with each of these single-particle states is found to be $k_0 = \chi \sin(N\phi)/(N \sin\phi)$. The total energy for the N single-particle scattering state is therefore given by

$$E_s \ = \ \hbar^2 N k_0^2 \ = \ \frac{\hbar^2 \chi^2 \sin^2(N\phi)}{N \sin^2\phi} \ . \tag{20}$$

Subtracting E in (9) from E_s in (20), we obtain the binding energy of the N-body bound state as

$$E_B(\phi, N) \ = \ \frac{\hbar^2 \chi^2 \sin(N\phi)}{\sin\phi} \Big\{ \frac{\sin(N\phi)}{N \sin\phi} - \frac{\cos(N\phi)}{\cos\phi} \Big\}. \tag{21}$$

Substituting $N = 2$ in Eq. (21), we obtain $E_B(\phi, 2) = 2\hbar^2 \chi^2 \sin^2\phi$. Thus $E_B(\phi, 2) > 0$ for any nonzero value of ϕ. Let us now consider the case $N \geq 3$. We can rewrite Eq. (21) in the form

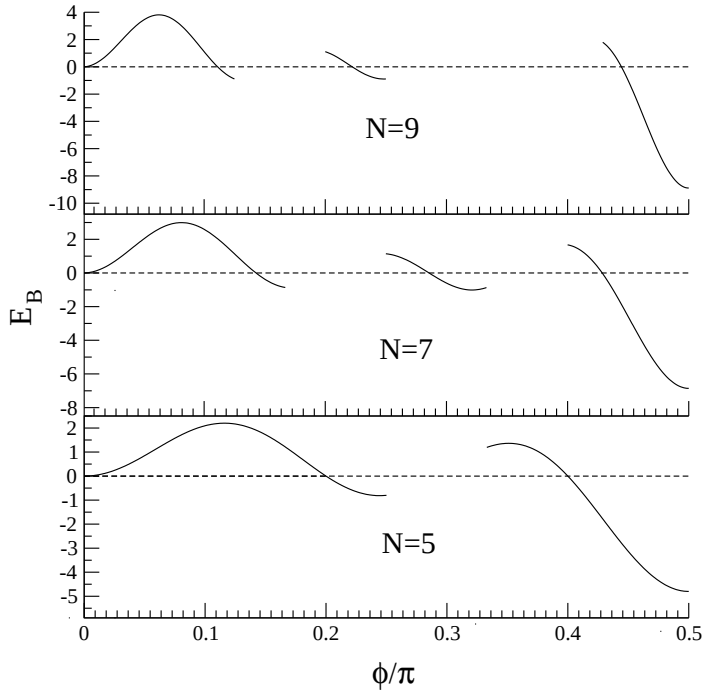

FIG. 2. The binding energy E_B of the N-body bound state as a function of ϕ/π for three different values of N.

$$E_B(\phi,N) = \frac{\hbar^2\chi\sin(N\phi)}{N\sin^2\phi\cos\phi}\ f(\phi,N)\ ,$$
$$f(\phi,N) = \chi\ [\sin(N\phi)\cos\phi\ -\ N\cos(N\phi)\sin\phi]. \tag{22}$$

On adding up all the inequalities given in (13) or (15), and using the identity $\sum_{l=1}^{N-1}\cos[(N-2l)\phi] = \sin[(N-1)\phi]/\sin\phi$, we find that $f(\phi,N)$ is positive in all the bands $B_{N,n}$ for all values of N and n. Hence, E_B given in (22) has the same sign as $\chi\sin(N\phi)$. Following arguments similar to that of the momentum, we find that the binding energy is positive in the left part of each band, negative in the right part, and zero at the point $\phi = \phi_{N,n}$.

We thus see that for $\phi > 0$, the momentum and the binding energy are both positive in the left part of each band, and they are both negative in the right part. [If $\phi < 0$, we can similarly show that bound states with positive (negative) values of P/ϕ have positive (negative) binding energy]. In Fig. 2, we show the binding energy E_B as a function of ϕ/π for three different values of N. (We have set $\hbar^2\chi^2 = 1$ in the figure). We see that E_B is indeed positive (negative) in the left (right) part of each band.

We will now use the technique of continued fractions to study the inverse problem of determining the values of N for which N-body bound states exist for a given value of ϕ. Any positive real number x has a simple continued fraction expansion of the form [14]

$$x\ =\ n_0\ +\ \frac{1}{n_1\ +\ \frac{1}{n_2\ +\ \cdots}}\ , \tag{23}$$

where the n_i's are integers satisfying $n_0 \geq 0$, and $n_i \geq 1$ for $i \geq 1$. The expansion ends at a finite stage with a last integer n_k if x is rational, and does not end if x is irrational. Given a number x, the integers n_i can be found as follows. We define $x_0 = x$. Then $n_0 = [x_0]$, where $[y]$ denotes the integer part of a non-negative number y. We then recursively define $x_{i+1} = 1/(x_i - n_i)$, and obtain $n_{i+1} = [x_{i+1}]$ for $i = 0, 1, 2, \cdots$. If we stop at the $k^{\rm th}$ stage, we obtain a rational number $r_k =< n_0, n_1, n_2, \cdots, n_k >$ which is an approximation to the number x. If we write $r_k = p_k/q_k$, where p_k and q_k are relatively prime, then it is known that

$$|\ x\ -\ \frac{p_k}{q_k}\ |\ <\ \frac{1}{q_k^2}\ , \tag{24}$$

for all values of $k \geq 1$ [14].

Now suppose that we know the expansion

$$\frac{\phi}{\pi} \;=\; < 0, n_1, n_2, \cdots > \;\; . \tag{25}$$

If we stop at the $k^{\rm th}$ stage in this expansion, we obtain $p_k/q_k =< 0, n_1, n_2, \cdots, n_k >$. Eq. (24) then implies that

$$\mid \frac{\phi}{\pi} \;-\; \frac{p_k}{q_k} \mid \;<\; \frac{1}{q_k^2} \; . \tag{26}$$

We now recall the comment that both the right and the left part of the band B_{q_k,p_k} have widths which are larger than $1/q_k^2$. Hence Eq. (26) implies that ϕ/π must lie within the band B_{q_k,p_k}. We have thus found a value of $N = q_k$ for which an N-body bound state exists for the given value of ϕ. We can generate several such values of N by stopping at different stages k in the expansion given in (25). If ϕ/π is rational, the continued fraction expansion stops at a finite stage, so we only obtain a finite number of values of N in this way. This can also be seen directly from Eq. (12). If $\phi/\pi = p/q$ is rational, then at least one of the inequalities in (12) will be violated if $N > q$. We thus conclude that if ϕ/π is rational, there is only a finite number of values of N for which a N-body bound state exists. If ϕ/π is irrational, then the expansion in (25) does not end, and we can use the procedure described above to find an infinite number of possible values of N for which a N-body bound state exists.

To conclude, we have used the ideas of Farey sequences and continued fractions to determine all the allowed ranges (bands) of η for which quantum N-body bound states exist in the DNLS model. For $N \geq 3$, we find that the N-body bound states can have both positive and negative momentum. Bound states with positive (negative) values of P/η have positive (negative) binding energy. Our work brings the analysis of the quantum bound states in the DNLS model to the same level of completion as that of the usual nonlinear Schrödinger model (where bound states are known to exist for all negative values of the coupling constant and all values of $N \geq 2$).

Bound states with negative binding energy are unusual in the field of integrable quantum models. However, such states are known to exist in other areas of quantum physics, such as antibonding states in molecules (see [15] for instance). The negative binding energy states that we have found in the DNLS are stable because the model is integrable. Presumably, these states would decay if one were to add terms to the Hamiltonian which destroy the integrability; any real system would probably have such terms anyway, so it is not clear at the moment if such states can be observed experimentally.

The quantum bound states which exist in the lowest band and have positive binding energy can be related in several ways to the solitons which appear in the classical version of the DNLS model which is integrable. A general method for relating quantum bound states and classical solitons is described in Ref. [4]. For the case of DNLS model, the classical solitons are localized solutions of the equation

$$i\hbar \; \frac{\partial \psi}{\partial t} \;=\; -\,\hbar^2 \; \frac{\partial^2 \psi}{\partial x^2} \;+\; i4\hbar\eta \; \psi^* \psi \; \frac{\partial \psi}{\partial x} \; , \tag{27}$$

with $\int_{-\infty}^{\infty} dx \psi^* \psi = \hbar N$. These solitons are known to exist only if $0 < |\eta| < \pi/N$ [6,13], and they can be obtained by taking the $\hbar \to 0$, $N \to \infty$ limit of the quantum bound states [6]. Another way of relating the classical solitons and quantum bound states of DNLS model is indicated in the first paper in Ref. [11]. There it is argued that the classical soliton mass, with one-loop quantum corrections, is given by

$$M_{\rm cl} \;=\; \frac{1}{2} \; [\; N \;+\; \frac{\eta^2}{3} \; (N^3 - N) \;] \; . \tag{28}$$

Comparing this to the mass of the N-body bound state in Eq. (10), we see that the two agree up to order η^2 for small η. An interesting problem for future study may be to see if there is a classical version of the bound states in the higher bands which we have found in this paper. Since the ranges of values of η for which these bound states exist depend sensitively on N, going to the limit $N \to \infty$ with a fixed value of η may turn out to be a rather subtle problem.

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