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Semiclassical quantization of the periodic Toda chain

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Abstract. Gutzwiller's semiclassical quantization scheme for the trace of Green's function is applied to the periodic Toda chain. We obtain a set of algebraic equations that determine the energy levels arising from a special periodic orbit, namely the single cnoidal wave solution. Our formulae show a simple dependence on the number of particles N in the chain. N merely occurs as a parameter. We perform the soliton limit of our equations and get a semiclassical correction to first order in $\hbar$ to the dispersion relation $E = E(p)$ of a soliton on the infinite chain which is in remarkable agreement with the Bethe ansatz result. The classical data which enter into the semiclassical quantization formula are of interest in their own right. We give a complete treatment of the linear stability analysis of a single cnoidal wave and also some new expressions for its dispersion relation which expresses the frequency ν as a function of the wavenumber k.

1. Introduction

The Toda chain [1] is a chain of identical particles with exponential interaction between nearest neighbours. Supplied with periodic boundary conditions it is an interesting prototype of an integrable N-particle mechanical system.

The integrability of the classical system was proved in [2–4], where N independent integrals of the motion were derived. The decisive step towards a complete solution of the initial value problem [5–7] was done in [8, 9], where the authors introduced new variables which also made it possible to derive the action-angle variables of the system [10]. The general solutions of the equations of motion are the so-called multi-cnoidal wave solutions which can be expressed in terms of the Riemann theta function [11]. They may be imagined as 'nonlinear superpositions' of single cnoidal waves.

The integrability of the quantum Toda chain was proved in [12]. However, in contrast to other integrable systems the (coordinate) Bethe ansatz does not apply because of the finite decay length of the potential. Nevertheless, and quite surprisingly, the asymptotic Bethe ansatz proposed by Sutherland [13] yields the correct ground-state energy and excitation spectrum of the *infinite* chain, and thus also the correct classical limit. Proposed originally as an approximation for low densities, when the system spends most time in regions of the phase space where all particles are well separated, it is still valid for densities of the order of unity [14].

The understanding of the *finite* periodic system, where the Bethe ansatz equations fail to be exact [15], was pioneered by Gutzwiller [16, 17], who was successful in transferring the canonical transformation of Kac and van Moerbeke [8, 9] into quantum mechanics. Gutzwiller's approach makes use of the explicit eigenfunctions of the problem. These are quite difficult to handle, and therefore Gutzwiller only investigated the cases of three and four particles, although, in principle, his results can be generalized to arbitrary N.

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Wavefunctions may be avoided if one uses the quantum inverse scattering method (QISM). This was done by Gaudin [18], Sklyanin [19] and more recently by Pasquier and Gaudin [20], who borrowed methods from the theory of integrable statistical systems. Sklyanin re-derived the integral equations for the elementary excitations of the infinite chain which were known from the asymptotic Bethe ansatz. He also gave an elegant account of the classical periodic system using the classical R-matrix formalism.

In spite of the deep insight into the finite quantum problem which was gained by the work of Gutzwiller, Gaudin and Sklyanin, there is still no effective way to compute the spectrum explicitly. This is probably the reason why the authors of [21–23] used conventional algorithms, starting directly with the Hamiltonian, in their numerical calculations for chains up to $N = 6$ particles. The difficulties in applying Gutzwiller's results numerically were also described in [15]. Hence, it is still desirable to derive effective, practicable methods, and, among these, semiclassical approximations are promising.

It is not possible to apply the standard WKB approximation to the periodic Toda chain, since no coordinate system in position space is known which separates Schrödinger's equation [24]. The action variables are known [10], however, and therefore the Einstein–Brillouin–Keller (EBK) quantization procedure [25] may be applied. This has been done in [15, 22, 23], but it is also numerically quite involved for large N, since there is no explicit formula expressing the Hamiltonian in terms of the action variables. Hence the present paper relies on Gutzwillwer's trace formula [24, 26] which is used preferably in quantizing chaotic motions. We follow the account of Dashen, Hasslacher and Neveu [27], who adapted Gutzwiller's method to field theory, and applied it to the infinite sine-Gordon system. In actual fact, the first attempt on the quantum Toda chain [28] was in this direction. Unfortunately, however, the author failed in at least two aspects when he calculated the classical input data for the formalism. As will become evident in section 4, an incorrect stationary phase condition was applied. Furthermore it was assumed that the stability angles agree with those of the chain at rest. This is only true for a soliton on the infinite chain and only to lowest order in $1/N$, but not for a cnoidal wave on a finite periodic chain, as will be shown in sections 5 and 6.

The trace formula is a semiclassical approximation to the trace of Green's function which is obtained by replacing the propagator with its semiclassical approximation. As Gutzwiller pointed out [26], to first order in $\hbar$ only the classical periodic orbits contribute to the trace. To compute the whole spectrum of a given mechanical system one is faced with the difficult problem of classifying all classical periodic orbits. If they are merely available in part, then only a part of the spectrum is obtained [24]. In the present paper we present a set of algebraic equations for the energy levels arising from a particular family of periodic orbits—the single cnoidal wave solutions.

Our result should be of general interest as one of the relatively few examples where the Gutzwiller trace formula could be explicitly exploited. Because of the complex structure of the periodic orbits in phase space, only very simple few-particle systems, like billiards or the anisotropic Kepler problem, have been investigated in the context of quantizing classically chaotic systems. In field theory, on the other hand, one usually deals with systems that have an infinite number of degrees of freedom (see [29], for example). In the present paper, in contrast, an N-particle system is treated successfully.

In the soliton limit, i.e. when the classical chain turns into an infinite chain bearing a single soliton, it is on first sight not at all clear how to utilize the semiclassical spectrum. In contrast to the sine-Gordon system [27] there remains no discrete part of the spectrum which, in the language of particle physicists, could be interpreted as a mass spectrum of elementary particles in their rest frame. In [27] the authors find the mass corresponding to the kink solution of the sine-Gordon system and a whole mass spectrum corresponding to the breather. But both kink and breather solutions are different in nature to the Toda soliton. The kink is a topological soliton, which means it has a non-zero excitation energy even in the classical case. The breather, on the other hand, is non-topological, but can be interpreted as a bound state of two kinks. In comparison to the Toda soliton it has an internal degree of freedom, which gives rise to the mass spectrum when quantized. In the language of particle physics the Toda soliton must be understood as a massless particle. This might correspond to the fact that there is no classical Toda solitons at rest. That is to say, there is a finite lower limit for the velocity of the Toda soliton.

In the present paper a semiclassically corrected dispersion relation, $E = E(p)$, for the soliton on the infinite chain is proposed. This has become possible, since we found an expression which can be interpreted as the semiclassically corrected momentum of a soliton. We compare the semiclassical dispersion relation, $E = E(p)$, of the soliton with the one following from the asymptotic Bethe ansatz [14] or, equivalently, from the QISM [19]. It is also compared with the dispersion relation following from a different semiclassical approach that is based on the time-dependent variational principle [30]. Indeed, one of the motivations when we first started this work was to find out whether the two semiclassical methods would lead to the same results. The answer is negative.

The paper is organized as follows. In section 2 we elucidate the semiclassical quantization formula in [27] and explain how to obtain semiclassical corrections to the momentum of a soliton. In the following four sections which form the main part of our paper we calculate the classical data that enter into the semiclassical quantization formula. These are the energy and action per particle of a single cnoidal wave and the stability angles of the corresponding linear stability problem. For all this data the soliton limit is carried out in section 6. The boundary conditions are handled with special care, for it was a careless treatment of the boundary conditions that caused a subtle mistake in [28] (see section 4, below). Physically, it is appropriate either to fix the pressure or to fix the length of the chain. It will prove to be possible to switch between these boundary conditions by means of a scale symmetry of the Lagrangian. Our account starts in section 2 with the general solution of the periodic problem in terms of theta functions [5, 7]. It is analogous to the treatment of the periodic KdV equation according to Dubrovin [11], and leads to a set of algebraic relations connecting the parameters of the multi-cnoidal wave solutions with each other, as well as with the length parameter Δl of the system. We call these relations dispersion relations. From the general formula we derive new expressions for the dispersion relation of a single cnoidal wave in section 4, which are simple and beautiful and thus of their own worth. The complete treatment of the linear stability analysis of a single cnoidal wave in section 5 may also be of interest outside the context of semiclassical quantization. Finally, in section 7 the classical data have been used to perform the semiclassical quantization procedure. The semiclassically corrected dispersion relation of the soliton is discussed in detail, whereas a more detailed discussion of the periodic few-particle systems is postponed to a forthcoming publication [31].

2. Semiclassical quantization

The energy levels ε_j of a quantum system with Hamiltonian H may be obtained as poles of the analytic continuation of the trace of Green's function

$$R(\varepsilon) = -\frac{\mathrm{i}}{\hbar}\int_{0+\mathrm{i}\delta}^{\infty+\mathrm{i}\delta} \mathrm{d}t\, \mathrm{e}^{(\mathrm{i}/\hbar)\varepsilon t}\, \mathrm{tr}\{\mathrm{e}^{-(\mathrm{i}/\hbar)Ht}\} = \sum_j \frac{1}{\varepsilon - \varepsilon_j}. \tag{2.1}$$

In [27] a semiclassical approximation to $R(\varepsilon)$ is obtained in three steps. In the first step the propagator $\langle q|\exp(-iHt/\hbar)|q'\rangle$ is replaced by its semiclassical approximation [32]. In the second the trace of the semiclassical propagator is analysed and in the third the time integral in (2.1) is calculated by stationary phase approximation. The second step is crucial. In it, it turns out that only periodic orbits contribute to the trace [26].

Although the so-called trace formula is also favoured for the quantization of chaotic motions [33], no naive use is possible, because in general it fails to converge on the real axis. This has been the subject of recent discussions, and much progress has been made [34, 35].

In the case of the integrable systems however, the result presented in [27] seems now to be well accepted [29]. It is

$$\mathrm{tr}\{e^{-(i/\hbar)HT}\} = \sum_{n,k} \Delta_n \exp\left\{\frac{i}{\hbar}(S_n + \xi_{n,k} - \theta_n)\right\}. \tag{2.2}$$

The expression on the right-hand side is a sum over all periodic orbits (index n) with period T and a sum over contributions arising from the fluctuations around the periodic orbits (index k). It is entirely determined by the following classical data:

(i) S_n, the action per period;

(ii) $\xi_{n,k} := -\sum_\alpha (k_\alpha + 1/2)\hbar\eta_{n,\alpha}$, the sum over the stability angles $\eta_{n,\alpha}$ (k will turn out to be a vector of quantum numbers with the components k_α);

(iii) θ_n, a discrete phase factor depending on the number of critical points of the periodic orbit in phase space; and

(iv) Δ_n, a factor depending on the continuous symmetries of the corresponding orbit.

In [29] it is shown how to calculate the stationary phase approximation to (2.2) as we need it for the Toda chain.

$$R_s(\varepsilon) \sim \sum_k (1 - \exp\{i(S(\tau) + \varepsilon\tau + \xi_k(\tau) - \theta)/\hbar\})^{-1}. \tag{2.3}$$

This formula is valid in the centre-of-mass system. The centre-of-mass motion can be separated by using the methods developed recently by Creagh and Littlejohn [36]. It turns out to be treated exactly within the frame of semiclassical quantization.

The right-hand side of equation (2.3) is the contribution to $R_s(\varepsilon)$ arising from every family of periodic orbits. We suppressed a subscript labelling the different families, because only a particular one will be considered in the present paper. It is the family of single cnoidal wave solutions which correspond to the most degenerate one-dimensional tori in phase space. These are suspected to give relevant contributions to the semiclassical density of states [37, 38]. Note that in deriving (2.3) the sum over repeated traversals of orbits with basic period τ for one traversal has already been performed.

It is amusing that equation (2.2) can be connected to the work of three different authors leading to three different quantization conditions [26, 29, 39]. The result depends on whether or not the sum over stability exponents ξ_k is included in the stationary phase condition required to calculate the time integral in (2.1). The classical input data, however, agree for all these formulae. They have been listed above. Also, for the Toda chain they will be calculated in the following sections.

A comparison between the different quantization formulae will be given elsewhere [31]. Here we rely on the formulae given by [27–29] for several reasons: they permit a satisfactory physical interpretation; they have been applied successfully to the sine-Gordon system, and they allow for a clear regularization procedure in the soliton limit of the Toda chain.

We now return to the discussion of equation (2.3). The parameter θ in (2.3) is a discrete phase connected to the number $4v$ of critical points on a basic orbit by $4v = 2\theta/\hbar\pi$. $R_s(\varepsilon)$ has poles at

$$S(\tau) + \varepsilon\tau + \xi_k(\tau) = (n + v)2\pi\hbar. \qquad (2.4)$$

The period τ is determined as a function of ε by the stationary phase condition leading to (2.3),

$$-\,\mathrm{d}_\tau S = \varepsilon + \mathrm{d}_\tau \xi_k(\tau) = E. \qquad (2.5)$$

Here we abbreviated the derivative with respect to τ as d_τ. E is the classical energy as a function of the period τ. Note that the last equation is only correct if the Hamiltonian does not depend explicitly on τ. This may occur and is discussed in section 4. We combine (2.4) and (2.5) to get a parametric representation of the energy as a function of the quantum number n:

$$\varepsilon = E(\tau) - \mathrm{d}_\tau \xi_k \qquad (2.6)$$

$$\frac{(n+v)2\pi\hbar}{N} = \frac{S(\tau) + E(\tau)\tau}{N} + \frac{1}{N}(1 - \tau\,\mathrm{d}_\tau)\xi_k. \qquad (2.7)$$

Regarding the definition of ξ_k, the physical interpretation is as follows. Equations (2.6) and (2.7) describe the energy levels corresponding to a cnoidal wave with period τ in the presence of phonons with energies $(k_\alpha + 1/2)\hbar\,\mathrm{d}_\tau\eta_\alpha$. The vector k indicates how many phonons of each energy are excited. For $k = 0$ we get the energy levels corresponding to a cnoidal wave in the absence of phonons. But even then the zero-point motion of the phonons renormalizes the cnoidal wave energies.

We have divided equation (2.7) by N to indicate how the soliton limit works. We assume that there are no phonons excited. Suppose further for a moment that $v = 0$ on the left-hand side of (2.7), then the left-hand side is equal to $p_n := n2\pi\hbar/N$ (the momentum of a free particle on a ring of length N). In the thermodynamic limit $N \to \infty$, p_n turns into a continuous variable p. p does not vanish if $\hbar \to 0$, since the range of p is unbounded. In the soliton limit which includes the thermodynamic limit and is described in section 6, the first term on the right-hand side of (2.7) turns into the well known momentum of a soliton. The second term remains finite for every τ and is proportional to $\hbar$. Note that in (2.6) and (2.7) τ merely plays the role of the curve parameter for the curve $\varepsilon = \varepsilon(n)$. This curve can be reparametrized in an arbitrary manner. In the soliton limit it will prove to be convenient to use the soliton parameter α which will be introduced in section 6 whereby (2.7) will become the form $p = p_{\mathrm{cl}}(\alpha) + \hbar\Delta p(\alpha)$. Analoguously, if we subtract the vacuum energy ε_0 in (2.6) we get an equation of the form $\varepsilon - \varepsilon_0 = E(\alpha) + \hbar\Delta E(\alpha)$.

It is tempting to interpret these two equations as the semiclassically corrected dispersion relation of a soliton. They are investigated in section 7.

3. General solution of the periodic N-particle problem

The Toda chain [1], as we conceive it physically, is a chain of identical particles connected by nonlinear springs. In dimensionless units (see [14], for example) these springs are defined by the potential

$$U(x) = \mathrm{e}^{-(x-l)} + x - l - 1 \qquad (3.1)$$

where l is the equilibrium length of the free spring. If we consider N particles at positions x_n, $n = 1, \ldots, N$, and define $x_{N+1} := x_1 + Nl + \Delta l$ with Δl arbitrary, the total potential energy of the quasi-periodic chain of length $Nl + \Delta l$ is

$$V = \sum_{n=1}^{N} U(x_{n+1} - x_n). \tag{3.2}$$

As usual, we will consider the variables $q_n := x_n - (n-1)l$ instead of x_n. Furthermore we introduce the distances $r_n := q_{n+1} - q_n$ and the shifted potential

$$W(x) := U(x + l) = \mathrm{e}^{-x} + x - 1. \tag{3.3}$$

As a result the Lagrangian of the N-particle quasi-periodic system is

$$L = \sum_{n=1}^{N} \left\{ \frac{\dot{q}_n^2}{2} - W(r_n) \right\}. \tag{3.4}$$

Δl is the total elongation of the chain and is a parameter of the system, not a dynamical quantity. The equilibrium of the chain is characterized by $r_n = \Delta l/N$. The total equilibrium energy as a function of Δl has a minimum at $\Delta l = 0$.

Besides translational invariance, the Lagrangian (3.4) shows a scale symmetry, which will be exploited throughout the remainder of this paper. Consider the transformation

$$t' = \mathrm{e}^{\sigma/2} t \qquad q_n'(t') = q_n(t) + n\sigma \tag{3.5}$$

where σ is an arbitrary real parameter. It affects the equations of motion according to (3.4) only by changing Δl, since

$$\begin{aligned} &L(q_n(t), \dot{q}_n(t), \Delta l) = \mathrm{e}^{\sigma} L(q_n'(t'), \dot{q}_n'(t'), \Delta l') + \Delta l' \mathrm{e}^{\sigma} - \Delta l - N(\mathrm{e}^{\sigma} - 1) \\ &\Delta l' := \Delta l + N\sigma. \end{aligned} \tag{3.6}$$

Note that it is always possible to transform the Lagrangian into a symmetric form by choosing $\sigma = -\Delta l/N$. This is presumably the reason why many other authors start their calculations with $\Delta l = 0$. But leaving Δl unspecified makes it possible to switch between zero-pressure and zero-length boundary conditions at the end of the calculations. This has been clearly seen by Sklyanin [19]. Also the single cnoidal wave solution (see below) in its best known form as originally derived by Toda is a solution of the Toda equations of motion for zero pressure rather than for zero length. It does not follow from (3.4) with $\Delta l = 0$. This led to some confusion in a former article on semiclassical quantization of the periodic Toda chain [28].

The initial-value problem corresponding to (3.4) has been solved by algebraic-geometric methods [5–10]. All solutions are of the same form. They may be understood as 'nonlinear superpositions' of cnoidal waves. Apart from an overall constant shift these nonlinear superpositions are in a centre-of-mass frame of the form

$$q_n(t) = nd + \ln\left(\frac{\theta(nk - \nu t + \gamma | B)}{\theta((n+1)k - \nu t + \gamma | B)} \right) \tag{3.7}$$

where $\theta(z|B)$ is Riemann's theta function of g variables, $g = 1, \ldots, N-1$ is the genus of the Riemann surface constructed from the Riemann matrix B. For a given g equation (3.7) is said to be the g-cnoidal wave solution (or g-zone solution) of the Toda equation of motion. k, ν and γ are g-dimensional vectors of wavenumbers, frequencies and phases and d is a real constant.

$\theta(z|B)$ is usually defined in terms of its Fourier representation:

$$\theta(z|B) := \sum_{n\in\mathbb{Z}^g} \exp\{\pi \mathrm{i}\langle n, Bn\rangle + 2\pi\mathrm{i}\langle n, z\rangle\} \tag{3.8}$$

where $z \in \mathbb{C}^g$ is a complex vector and B is a complex symmetric $g \times g$ matrix with a positive definite imaginary part. B is called a Riemann matrix. The diamond brackets denote the Euclidean scalar product: $\langle x, y\rangle = \sum_{j=1}^{g} x_j y_j$. The fact that B is a Riemann matrix guarantees the series in (3.8) to be absolutely convergent.

For later convenience we introduce a slight generalization of (3.8). Theta functions with characteriztics $[\alpha, \beta]$ will be defined as

$$\theta[\alpha,\beta](z|B) := \sum_{n\in\mathbb{Z}^g} \exp\{\pi\mathrm{i}\langle n+\alpha, B(n+\alpha)\rangle + 2\pi\mathrm{i}\langle n+\alpha, z+\beta\rangle\}. \tag{3.9}$$

Here $\alpha, \beta \in \mathbb{R}^g$, $0 \leqslant \alpha_j, \beta_j \leqslant 1$. For $[\alpha, \beta] = [0, 0]$ the Riemann theta function (3.8) is obviously recovered. If there is no danger of confusion, we write $\theta[\alpha, \beta](z)$ instead of $\theta[\alpha, \beta](z|B)$. The elementary properties of theta functions as far as we need them in the present paper are explained in [11].

The parameters k, ν, γ, B, d in (3.7) are not mutually independent. In [5, 7] the authors show that they are uniquely determined by the initial conditions. It is possible to determine their *explicit* mutual dependence by reinserting the solution (3.7) into the equations of motions. As a result a set of algebraic relations between the parameters is obtained which we call the dispersion relations of the multi-cnoidal waves. The corresponding relations for the KdV equation were derived by Dubrovin [11]. He also indicated the result for the Toda chain. Since it is necessary in our context to identify the physical meaning of the parameters in the dispersion relations, we present a brief derivation. We only show that the dispersion relations to be derived are sufficient for (3.7) to solve the equations of motion. This will be possible without reverting to methods of algebraic geometry.

Let A be defined as $A := \mathrm{e}^{-d}$, and

$$f_n := -\mathrm{d}_t^2 \ln(\theta(\varphi_n)) + A\theta(\varphi_{n+1})\theta(\varphi_{n-1})/\theta^2(\varphi_n) \tag{3.10}$$

where $\varphi_n := nk - \nu t + \gamma$. Inserting q_n according to (3.7) into the equations of motion following from (3.4) we obtain $f_{n+1} - f_n = 0$. This is obviously true if f_n is a constant f. Then equation (3.10) is equivalent to

$$\mathrm{e}^{-(q_n - q_{n-1})} - 1 = \mathrm{d}_t^2 \ln(\theta(\varphi_n)) + f - 1. \tag{3.11}$$

From this equation we can understand the physical meaning of f. The left-hand side represents the force exerted on the nth spring. We assume all frequencies ν to be real. Then $\mathrm{d}_t \ln(\theta(\varphi_n))$ is bounded as a function of t, and the time-averaged force exerted on each spring is

$$p = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t\, (\mathrm{e}^{-(q_n - q_{n-1})} - 1) = f - 1. \tag{3.12}$$

We call p the pressure. Note that according to our definition it may be negative. It is easy to see that under a scale transformation of type (3.5) f is transformed into $f' = \mathrm{e}^{-\sigma} f$.

We introduce the abbreviation $\theta_{ij...}(z) := (\partial/\partial z_i)(\partial/\partial z_j)\cdots\theta(z)$, and obtain from (3.10)

$$f\theta^2(\varphi_n) + \nu_i\nu_j\theta(\varphi_n)\theta_{ij}(\varphi_n) - \nu_i\nu_j\theta_i(\varphi_n)\theta_j(\varphi_n) - A\theta(\varphi_{n+1})\theta(\varphi_{n-1}) = 0 \tag{3.13}$$

where we agree to sum over double indices. Equation (3.13) yields the desired dispersion relations by the use of an appropriate addition theorem for theta functions. This is explained in appendix A. Using the same abbreviations as in [11],

$$\hat{\theta}[\delta](z) := \theta[\delta, 0](z|2B) \qquad \hat{\theta}[\delta] := \hat{\theta}[\delta](0) \tag{3.14}$$

and denoting partial derivatives of the theta functions again by subscripts we eventually arrive at the desired result

$$f\hat{\theta}[\delta] + 2\nu_i\nu_j\hat{\theta}_{ij}[\delta] - A\hat{\theta}[\delta](2k) = 0. \tag{3.15}$$

Here $\delta \in \frac{1}{2}(Z_2)^g$, i.e. δ is a g-dimensional column with entries $0, \frac{1}{2}$. Equation (3.15) was first given by Dubrovin (see equation (26) in the appendix of [11]). Note that the phase γ in (3.7) does not occur in (3.15) and can therefore be chosen independently.

So far nothing has been said about the restrictions imposed on k by the quasi-periodic boundary condition $q_{n+N} - q_n = \Delta l$. With q_n according to (3.7) it reads

$$\ln\left(\frac{\theta(\varphi_{n+N})\theta(\varphi_{n+1})}{\theta(\varphi_{n+1+N})\theta(\varphi_n)}\right) = \Delta l - Nd. \tag{3.16}$$

This is always true, if

(i) Nk is a quasi-period of the theta function, i.e. $Nk = j + Bl$, $j, l \in \mathbb{Z}^g$; and

(ii) $Nd = \Delta l$.

The second condition determines A as a function of the outer parameter Δl. We claim that the first condition can be restricted further to $k_j = m_j/N$, where m_j is one of the numbers $1, \ldots, N-1$, and all m_j are different. This restricts the maximum number of cnoidal waves to be superposed in (3.7) to $N-1$. The manifold of all physically relevant solutions should be exhausted by solutions of this type. We cannot prove our claim, but at least it is valid for the special examples considered in the remainder of the present paper. It is also valid in the harmonic limit, which is obtained from (3.7), (3.15) considering all the amplitudes $\exp(\mathrm{i}\pi B_{jj})$ to be small.

Regarding (3.7) and (3.15) we can interpret the scale transformation (3.5) as acting on ν instead of t. ν is transformed into $\nu' = \mathrm{e}^{-\sigma/2}\nu$ and A into $A' = \mathrm{e}^{-\sigma}A$. The Riemann matrix is invariant under the above transformation, $B' = B$. Thus the effect of a scale transformation on (3.15) is simply to multiply the whole equation by a factor of $\mathrm{e}^{-\sigma}$. For this reason we can restrict ourselves to the solution for $f = 1$ corresponding to the boundary condition of zero pressure. The boundary condition where Δl is treated as independent is obtained subsequently with the aid of a scale transformation. Thus, from this point of view, our main object of interest will be the equation

$$\hat{\theta}[\delta] + 2\nu_i\nu_j\hat{\theta}_{ij}[\delta] - A\hat{\theta}[\delta](2k) = 0. \tag{3.17}$$

Let us denote the length Δl that follows from (3.17) by Δl_0. For the frequencies at zero pressure following from (3.17) we keep the notation ν. As indicated above, a scale transformation with $\sigma = (\Delta l - \Delta l_0)/N$ yields the pressure and the frequencies as functions of Δl:

$$p(\Delta l) = \exp(-(\Delta l - \Delta l_0)/N) - 1 \tag{3.18}$$

$$\nu(\Delta l) = \exp(-(\Delta l - \Delta l_0)/2N). \tag{3.19}$$

Note that in our notation $\nu = \nu(\Delta l_0)$.

For $g = 1$ equation (3.17) is a system of two equations for the two unknown parameters ν, A. For $g = 2$ we have four equations for four unknown parameters ν_1, ν_2, A, B_{12}. For all higher genera $g \geqslant 3$ the number of equations exceeds the number of unknown parameters (see [11]). The superfluous equations establish a set of identities on the parameters. The case $g = 3$ has been studied numerically by Hirota and Ito [40], but they used a different form of the dispersion relation (3.17) which is not appropriate for analytical calculations.

In the remainder of this paper we restrict ourselves to the cases $g = 1, 2$. The case $g = 1$ is investigated in the following section, where we recover the well known dispersion relation for a single cnoidal wave. In section 5 we investigate the case $g = 2$ in order to solve the linear stability problem for a single cnoidal wave.

There is a remark on equation (3.10): if we considered θ as an unknown function to be determined by the differential equation (3.10), then this differential equation would be called Hirota's form of the Toda equations of motion [41].

4. The single cnoidal wave solution

The purpose of this section is to calculate the physical quantities that characterize a single cnoidal wave and enter into the semiclassical quantization formulae (2.6), (2.7). Some of the results are well known, but we re-derive them in our formulation, starting from the general formula (3.17). This is a check for (3.17) and simultaneously yields some interesting new expressions for ν and A. At the end of this section we discuss the stationary phase condition emerging from semiclassical quantization.

Equation (3.17) with $g = 1$ is linear in the two unknown parameters A and ν^2. To show that ν^2 and A according to (3.17) agree with the familiar results due to Toda [1] we have to express our formulae in terms of Jacobi elliptic functions and complete elliptic integrals. To this end we introduce the four basic one-dimensional theta functions

$$\begin{aligned} \theta_1(z|B) &:= -\theta[\tfrac{1}{2}, \tfrac{1}{2}](z|B) \qquad & \theta_2(z|B) &:= \theta[\tfrac{1}{2}, 0](z|B) \\ \theta_3(z|B) &:= \theta[0, 0](z|B) \qquad & \theta_4(z|B) &:= \theta[0, \tfrac{1}{2}](z|B). \end{aligned} \tag{4.1}$$

The Riemann matrix B is now a single constant. Since it is fixed we leave it out of the argument of the theta functions in the following. In this section, unlike in the previous one, a subscript is the number according to (4.1). Derivatives with respect to z are denoted by a prime, and the argument zero is left out for theta functions and its derivatives. For example, θ_3'' means $\mathrm{d}^2\theta_3(z)/\mathrm{d}z^2|_{z=0}$.

For $g = 1$ the parameter δ in (3.17) takes on the values $0, \frac{1}{2}$. Thus (remember (3.14a)) (3.17) in matrix notation becomes

$$\begin{pmatrix} \hat{\theta}_3(2k) & -2\hat{\theta}_3'' \\ \hat{\theta}_2(2k) & -2\hat{\theta}_2'' \end{pmatrix} \begin{pmatrix} A \\ \nu^2 \end{pmatrix} = \begin{pmatrix} \hat{\theta}_3 \\ \hat{\theta}_2 \end{pmatrix}. \tag{4.2}$$

We invert this equation and obtain the following explicit expressions for ν^2 and A

$$\nu^2 = -\frac{1}{2}\frac{\hat\theta_3\hat\theta_2(2k) - \hat\theta_2\hat\theta_3(2k)}{\hat\theta_3''\hat\theta_2(2k) - \hat\theta_2''\hat\theta_3(2k)} \tag{4.3}$$

$$A = \frac{\hat\theta_3''\hat\theta_2 - \hat\theta_2''\hat\theta_3}{\hat\theta_3''\hat\theta_2(2k) - \hat\theta_2''\hat\theta_3(2k)}. \tag{4.4}$$

Remember the definition of the Jacobi sn function in terms of theta functions (see [42], for example)

$$\mathrm{sn}(2Kz) = \frac{\theta_3}{\theta_2}\frac{\theta_1(z)}{\theta_4(z)} \tag{4.5}$$

where $2K := \pi\theta_3^2$ is a half period of the sn function. K is the complete elliptic integral of the first kind (see [42]). First of all we express $\hat\theta_2(2z)$ and $\hat\theta_3(2z)$ in terms of $\theta_1(z), \theta_4(z)$. We start with the following addition theorem for theta functions with characteristics [11]

$$\theta[\alpha,\gamma](z+w)\theta[\beta,\varepsilon](z-w) = \sum_{2\delta\in(\mathbb{Z}_2)^g} \hat\theta[\tfrac{1}{2}(\alpha+\beta)+\delta, \gamma+\varepsilon](2z)\hat\theta[\tfrac{1}{2}(\alpha-\beta)+\delta, \gamma-\varepsilon](2w) \tag{4.6}$$

which has also been the starting point for deriving (3.17) in appendix A. From (3.9) we see that for all $n, m \in \mathbb{Z}^g$

$$\theta[\alpha+m, \beta+n](z) = \exp(2\pi\mathrm{i}\langle n, \alpha\rangle)\theta[\alpha,\beta](z). \tag{4.7}$$

Using (4.6) and (4.7) we get

$$\theta_1(z+w)\theta_1(z-w) = \hat\theta_3(2z)\hat\theta_2(2w) - \hat\theta_2(2z)\hat\theta_3(2w) \tag{4.8}$$

$$\theta_4(z+w)\theta_4(z-w) = \hat\theta_3(2z)\hat\theta_3(2w) - \hat\theta_2(2z)\hat\theta_2(2w). \tag{4.9}$$

Setting z, w equal to zero in the last equation, one is led to

$$\theta_4^2 = \hat\theta_3^2 - \hat\theta_2^2. \tag{4.10}$$

Next, we take the second derivative of (4.8) and (4.9) with respect to z at $w = z = 0$. Exploiting the fact that $\theta_1(z)$ is odd and $\theta_4(z)$ is even we obtain

$$\theta_1'^2 = 2(\hat\theta_3''\hat\theta_2 - \hat\theta_2''\hat\theta_3) \qquad \theta_4\theta_4'' = 2(\hat\theta_3''\hat\theta_3 - \hat\theta_2''\hat\theta_2). \tag{4.11}$$

With $w = 0$, equations (4.8), (4.9) read

$$\begin{pmatrix}\theta_1^2(z)\\ \theta_4^2(z)\end{pmatrix} = \begin{pmatrix}-1 & 1\\ -\hat\theta_2/\hat\theta_3 & \hat\theta_3/\hat\theta_2\end{pmatrix}\begin{pmatrix}\hat\theta_2(2z)\hat\theta_3\\ \hat\theta_3(2z)\hat\theta_2\end{pmatrix}. \tag{4.12}$$

Inverting this equation, inserting the result into (4.3) and using (4.10) and (4.11), we arrive at

$$\nu^2 = \frac{\theta_1^2(k)\theta_4^2}{\theta_4^2(k)\theta_1'^2 - \theta_1^2(k)\theta_4\theta_4''}. \tag{4.13}$$

This is an alternative form of the dispersion relation for ν. Using (4.5) and the relations [42, 43] $\theta_1' = \pi\theta_2\theta_3\theta_4$ and

$$\frac{\theta_4''}{\theta_4} = 8\pi^2 \sum_{n=0}^{\infty} \frac{e^{i\pi B(2n+1)}}{(1 - e^{i\pi B(2n+1)})^2} = 4K(K - E) \tag{4.14}$$

equation (4.13) can be rewritten to Toda's familiar result

$$(2K\nu)^{-2} = \mathrm{sn}^{-2}(2Kk) - 1 + E/K. \tag{4.15}$$

Here E is the elliptic integral of the second kind.

Equation (4.8) can also be exploited to derive an expression for the dispersion relation only in terms of $\theta_1(z)$. The numerator of the fraction on the right-hand side of (4.3) equals (4.8) with $z = 0$, $w = k$; the denominator is obtained taking the second derivative of (4.8) with respect to z at $z = 0$, $w = k$. So we see that

$$\nu^{-2} = -\mathrm{d}_k^2 \ln(\theta_1(k)). \tag{4.16}$$

This is already the fourth expression for the dispersion relation for ν as a function of B and k at zero pressure that we encounter in the course of the present section. Because of its simplicity, we prefer to use it in the following.

It is now very easy to also recover Toda's formula for A from (4.4). One just needs (4.11*a*) and the first of the formulae (4.12) to see that

$$\nu^2/A = \theta_1^2(k)/\theta_1'^2. \tag{4.17}$$

Toda uses the constant

$$C = \left(\frac{\theta_4(k)}{\theta_4}\right)^2 \left[1 - \left(1 - \frac{E}{K}\right)\mathrm{sn}^2(2Kk)\right] \tag{4.18}$$

to express the pressure for zero elongation of the chain as $p(\Delta l = 0) = C - 1$. Thus, according to (3.18), we have to show that $C = 1/A$. Equation (4.15) implies that

$$C\nu^2 = (\theta_4(k)/2K\theta_4)^2 \mathrm{sn}^2(2Kk). \tag{4.19}$$

This is easily seen to agree with the right-hand side of equation (4.17). With that, our justification of (4.3), (4.4) is complete.

Finally, according to (3.19), equation (4.17) provides us with a simple formula for ν at fixed length Δl:

$$\nu(\Delta l) = e^{-\Delta l/2N}\theta_1(k)/\theta_1'. \tag{4.20}$$

We choose the positive sign of the square root of the right-hand side of (4.17), because we want the frequency $\nu(\Delta l)$ to be positive for $0 \leqslant k \leqslant 1$. The quantity $\exp(-\Delta l/2N)$ is seen to be the velocity of sound.

As two of the main ingredients of the semiclassical quantization of a single cnoidal wave, we need its energy and its action per period. These quantities have been calculated by Shirafuji [28]. Note however, that his point of view in treating the Toda chain is slightly different from ours. He leaves out the attractive part of the potential (3.3) and uses

$W_{sh} = \exp(-x) - 1$ instead. Physically, this means that he understands the Toda chain as a one-dimensional gas of mutually repulsive particles, constrained on a ring. Although the equations of motion derived from W and W_{sh} are clearly the same, the expressions for energy and action per period differ. Also, with W_{sh} instead of W there is no minimum of the energy of the chain at rest as a function of Δl, i.e. there exists no physical lattice constant.

In the following we denote the time average by angled brackets. Hence, if a function f is periodic with period $\tau = 1/\nu$, its time average is given as

$$\langle f \rangle = \frac{1}{\tau(\Delta l)} \int_0^{\tau(\Delta l)} \mathrm{d}t\, f(t). \tag{4.21}$$

According to (3.12), $p = \langle -W'(r_n) \rangle$, whereas in Shirafuji's treatment the pressure is $p_{sh} = \langle -W'_{sh}(r_n) \rangle$. With this in mind it is readily seen that the single cnoidal wave (3.7), (4.3), (4.4), corresponding to $p = 0$ in our interpretation, corresponds to $p_{sh} = 1$.

Denote the kinetic energy for a moment as T. Then $E = \langle E \rangle = \langle T \rangle + \langle V \rangle$, with potential energy V according to (3.2). For the action we get $S = \tau(\Delta l)\langle L \rangle = \tau(\Delta l)(\langle T \rangle - \langle V \rangle)$. Equation (3.12) implies

$$\langle V \rangle = \sum_{n=1}^{N} \langle W(r_n) \rangle = \Delta l + Np. \tag{4.22}$$

To compute $\langle T \rangle$ we take $\dot{q}_n$ as follows from (3.7) and use the series representation for the logarithmic derivative of $\theta_3(z|B)$ (see [42] p 489). Then $\langle T \rangle = a/\tau(\Delta l)^2$, where a is defined as

$$a = N(2\pi)^2 \sum_{n=1}^{\infty} \operatorname{cosech}^2(\mathrm{i}\pi Bn) \sin^2(\pi nk). \tag{4.23}$$

For $p = 0$ it follows that

$$E = a/\tau^2 + \Delta l_0 \qquad S = a/\tau - \tau \Delta l_0. \tag{4.24}$$

And for $\Delta l = 0$ we get with p according to (3.18)

$$E = a/\tau^2(0) + Np = a/\tau^2(0) + N(\mathrm{e}^{\Delta l_0/N} - 1) \tag{4.25}$$

$$S = a/\tau(0) - N\tau(0)p = a/\tau(0) - N\tau(0)(\mathrm{e}^{\Delta l_0/N} - 1). \tag{4.26}$$

In the context of semiclassical quantization it only makes sense to consider the system with boundary condition of fixed length Δl. This is because the conditions for the vanishing of the pressure are different in classical and quantum mechanics. In quantum mechanics the zero-point motion of the particles causes an additional contribution to the pressure. It is formally possible to quantize the classical $p = 0$ system, although it is not at all clear what the result of such a calculation would mean physically. But this is what Shirafuji [28] tries to do in his calculations. He tries to quantize the single cnoidal wave solution for $p = 0$. Moreover, the stationary phase condition he is applying when he is analysing the time integral in (2.1) is wrong. This will be explained in the following.

There is a relation between S and E which is crucial in the context of semiclassical quantization and which we will now discuss. Recall from Hamilton–Jacobi theory that, given an orbit in configuration space, S is usually understood as a function of starting and end points of the orbit q, q', as well as of the flight time T. We calculated the action per period for a family of periodic orbits parametrized by their period T; i.e. q and q' agree, as well as the corresponding momenta p and p'. By $q^* := q = q'$ we denote the common starting and end point of a periodic orbit.

Consider first the case $\Delta l = 0$. Then $T = \tau(0)$, $S = S(q^*(\tau(0)), q^*(\tau(0)), \tau(0))$ and

$$\frac{\mathrm{d}S}{\mathrm{d}\tau(0)} = \left(\frac{\partial S}{\partial q} + \frac{\partial S}{\partial q'}\right)\frac{\mathrm{d}q^*}{\mathrm{d}\tau(0)} + \frac{\partial S}{\partial \tau(0)} = \frac{\partial S}{\partial \tau(0)} = -E \tag{4.27}$$

where the second equation follows from periodicity [26] and the third one from the Hamilton–Jacobi equation. Inserting (4.25), (4.26) yields

$$\nu^2 = \frac{\mathrm{d}\Delta l_0}{\mathrm{d}a}. \tag{4.28}$$

Equation (4.28) is a consistency condition connecting E and S. On the other hand, we can read it as an alternative form of the dispersion relation for ν at zero pressure. It would be preferable to have direct proof of (4.28), but we did not find it, except in the single soliton limit (see below). However, we checked equation (4.28) numerically, and there is no doubt that it is correct.

In the cases $p = 0$, $p_{\mathrm{sh}} = 1$, respectively, the relation (4.27) between E and S is no longer valid for Shirafuji's choice of potential, W_{sh}, since the Lagrangian now shows an additional dependence on τ through Δl_0. We have

$$\frac{\mathrm{d}S}{\mathrm{d}\tau} = \frac{\partial S}{\partial \Delta l_0}\frac{\mathrm{d}\Delta l_0}{\mathrm{d}\tau} + \frac{\partial S}{\partial \tau} = \frac{\partial S}{\partial \Delta l_0}\frac{\mathrm{d}\Delta l_0}{\mathrm{d}\tau} - E. \tag{4.29}$$

With our choice (3.3) of the potential energy W the additional term vanishes identically, since

$$\frac{\partial S}{\partial \Delta l_0} = \tau\left\langle\frac{\partial L}{\partial \Delta l_0}\right\rangle = \tau\langle \mathrm{e}^{-(q_1+\Delta l_0 - q_N)} - 1\rangle = \tau p = 0. \tag{4.29}$$

But with W_{sh} instead of W we obtain

$$\frac{\partial S_{\mathrm{sh}}}{\partial \Delta l_0} = \tau\left\langle\frac{\partial L_{\mathrm{sh}}}{\partial \Delta l_0}\right\rangle = \tau\langle \mathrm{e}^{-(q_1+\Delta l_0 - q_N)}\rangle = \tau p_{\mathrm{sh}} = \tau. \tag{4.31}$$

Inserting (4.30) and (4.24) into (4.29) yields again the consistency condition (4.28), and likewise inserting $S_{\mathrm{sh}} = a/\tau$ and $E_{\mathrm{sh}} = a/\tau^2$ as well as (4.31) into (4.29). This shows that the stationary phase condition (26) in Shirafuji's paper is indeed incorrect. The total and the partial derivative of S with respect to τ disagree in his case. To be consistent one should use (4.29) instead of Shirafuji's equation (26). But even if one does so, the physical meaning of the result, if used in semiclassical quantization, remains questionable. The appropriate boundary condition for quantizing the N-particle system is $\Delta l = 0$.

5. Linear stability analysis for a single cnoidal wave

In this section we investigate the linear stability problem of a single cnoidal wave. As in the previous section we first treat the case of zero pressure. The case of arbitrary length is obtained subsequently by means of the scale transformation (3.5).

For a moment we denote the single cnoidal wave according to (3.7) by $q_n^*(t)$. Its dispersion relation is given by (4.3), (4.4) or one of the alternative forms which have been derived in the previous section. The dynamics of a deviation $\delta q_n(t)$ from $q_n^*(t)$ is given to linear order by the equations of motion

$$\delta\ddot{q}_n = -(\delta q_n - \delta q_{n-1})\mathrm{e}^{-(q_n^*(t)-q_{n-1}^*(t))} + (\delta q_{n+1} - \delta q_n)\mathrm{e}^{-(q_{n+1}^*(t)-q_n^*(t))} \tag{5.1}$$

which define the linear stability problem of $q_n^*(t)$. With $\delta p := \delta\dot{q}$ they may be written as

$$\begin{pmatrix}\delta\dot{q}\\ \delta\dot{p}\end{pmatrix} = A(t)\begin{pmatrix}\delta q\\ \delta p\end{pmatrix} \tag{5.2}$$

where we have combined the N components δq_n and δp_n to column vectors δq and δp, respectively. $A(t)$ is a $2N \times 2N$ matrix, periodic in t with period $\tau = 1/\nu$, i.e. (5.2) is a system of $2N$ linear non-autonomous differential equations with periodic coefficients. Therefore Floquet's theorem applies (see [44], for example) and there is a special fundamental solution to (5.2) of the form

$$\Phi(t) = \Pi(t)\mathrm{e}^{tJ} \tag{5.3}$$

where $\Phi(t)$, $\Pi(t)$, J are $2N \times 2N$ matrices, $\Pi(t+\tau) = \Pi(t)$ and J is a time-independent matrix of Jordan normal form. Since the Toda chain is a Hamiltonian system, the eigenvalues of J must come in complex conjugated pairs, and at least one pair is equal to zero due to the time independence of the Hamiltonian. Suppose that all non-zero eigenvalues $\mathrm{i}\eta_\alpha/\tau$ of J are pairwise distinct. Then the corresponding solutions are of the form

$$\Phi_\alpha(t) = \Pi_\alpha(t)\mathrm{e}^{\mathrm{i}\eta_\alpha t/\tau} \tag{5.4}$$

where $\Phi_\alpha(t)$, $\Pi_\alpha(t)$ are the αth columns of the matrices $\Phi(t)$, $\Pi(t)$, respectively. η_α is called a stability angle. If η_α is real, $\Phi_\alpha(t)$ is bounded and the cnoidal wave is stable against the corresponding perturbation in phase space.

In the present case it is not hard to derive the complete solution of the linear stability problem. It is obtained expanding the two-cnoidal wave solution to linear order in the amplitude of one of the cnoidal waves. For the two-cnoidal wave solution the Riemann matrix B is a two-by-two matrix and φ_n is a two-dimensional vector with components $\varphi_n^j = nk_j - \nu_j t + \gamma_j$, $j = 1, 2$. We abbreviate $\varepsilon := \exp(\mathrm{i}\pi B_{22})$, $\kappa := B_{12}$. Then we expand (3.7) as well as (3.17) to linear order in ε.

From (3.7) we obtain

$$q_n(t) = nd + \ln\left(\frac{\theta_3(\varphi_n^1)}{\theta_3(\varphi_{n+1}^1)}\right) + \varepsilon\left\{\mathrm{e}^{2\pi\mathrm{i}\varphi_n^2}\left(\frac{\theta_3(\varphi_n^1+\kappa)}{\theta_3(\varphi_n^1)} - \frac{\mathrm{e}^{2\pi\mathrm{i}k_2}\theta_3(\varphi_{n+1}^1+\kappa)}{\theta_3(\varphi_{n+1}^1)}\right) + \mathrm{cc}\right\} \tag{5.5}$$

where cc stands for complex conjugate. Here we have supposed B to be purely imaginary and k, ν and γ to be real. Equation (5.5) has already been derived by Shirafuji [28].

The dispersion relations (3.17) for two cnoidal waves are no longer linear in the four dependent parameters ν_1, ν_2, κ, A. They are transcendent with respect to κ. We introduce the notation

$$\delta^1 := \begin{pmatrix}0\\0\end{pmatrix} \qquad \delta^2 := \begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} \qquad \delta^3 := \begin{pmatrix}0\\\frac{1}{2}\end{pmatrix} \qquad \delta^4 := \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$$

and write (3.17) in full as

$$\begin{pmatrix} \hat\theta[\delta^1](2k) & -2\hat\theta_{11}[\delta^1] & -4\hat\theta_{12}[\delta^1] & -2\hat\theta_{22}[\delta^1] \\ \hat\theta[\delta^2](2k) & -2\hat\theta_{11}[\delta^2] & -4\hat\theta_{12}[\delta^2] & -2\hat\theta_{22}[\delta^2] \\ \hat\theta[\delta^3](2k) & -2\hat\theta_{11}[\delta^3] & -4\hat\theta_{12}[\delta^3] & -2\hat\theta_{22}[\delta^3] \\ \hat\theta[\delta^4](2k) & -2\hat\theta_{11}[\delta^4] & -4\hat\theta_{12}[\delta^4] & -2\hat\theta_{22}[\delta^4] \end{pmatrix} \begin{pmatrix} A \\ \nu_1^2 \\ \nu_1\nu_2 \\ \nu_2^2 \end{pmatrix} = \begin{pmatrix} \hat\theta[\delta^1] \\ \hat\theta[\delta^2] \\ \hat\theta[\delta^3] \\ \hat\theta[\delta^4] \end{pmatrix}. \tag{5.6}$$

The theta functions in the first two rows of (5.6), when expanded with respect to ε, yield $\hat\theta[\delta^i](z) = \hat\theta[\delta^i_1](z_1) + \mathcal{O}(\varepsilon^2)$. This means that the upper left-hand quarter of the matrix in (5.6) agrees up to terms of order ε^2 with the matrix in (4.2) and the upper right-hand quarter of the matrix in (5.6) is of order ε^2. Thus we have shown that the terms in curly brackets in equation (5.5) are indeed a solution to the linear stability problem (5.1). The second two rows of equation (5.6) may be expanded as functions of $\varepsilon^{1/2}$. To lowest order we obtain a pair of equations that provides us with the dependent parameters κ, ν_2 of the linear stability problem as functions of k_1, k_2 and B_{11}. To avoid factors of π we rescale k_2 and ν_2, setting $q_2 = 2\pi k_2$, $\omega_2 = 2\pi\nu_2$, and arrive at

$$A(\mathrm{e}^{\mathrm{i}q_2}\hat\theta_j(2k_1+\kappa) + \mathrm{e}^{-\mathrm{i}q_2}\hat\theta_j(2k_1-\kappa)) - 4\nu_1^2\hat\theta_j''(\kappa) - 4\mathrm{i}\nu_1\omega_2\hat\theta_j'(\kappa) + \omega_2^2\hat\theta_j(\kappa) = 2\hat\theta_j(\kappa) \\ (j = 2, 3). \tag{5.7}$$

Here A and ν_1 must be considered as known functions of B_{11} and k_1, given by (4.3) and (4.4). A more convenient form of (5.7) is obtained if we solve it for ω_2:

$$\omega_2 = 2\mathrm{i}\nu_1\,\mathrm{d}_\kappa \ln(\hat\theta_j(\kappa)) \\ \pm\left[2 - A\left(\frac{\mathrm{e}^{\mathrm{i}q_2}\hat\theta_j(2k_1+\kappa)}{\hat\theta_j(\kappa)} + \frac{\mathrm{e}^{-\mathrm{i}q_2}\hat\theta_j(2k_1-\kappa)}{\hat\theta_j(\kappa)}\right) + 4\nu_1^2\,\mathrm{d}_\kappa^2 \ln(\hat\theta_j(\kappa))\right]^{1/2} \\ (j = 2, 3). \tag{5.8}$$

If we subtract these two equations from each other, we are left with a single equation for κ. Unfortunately, we have not been able to solve it analytically except for the cases of the one-soliton limit (see below) and the harmonic limit. On the other hand, however, it is not hard to solve it numerically. Then κ is obtained as a function of k_1, q_2 and B_{11}. Reinserting it in one of the equations (5.8) we obtain the dispersion relation which determines the frequency ω_2 as a function of the wavenumber q_2 for an excitation with small amplitude in the presence of a cnoidal wave characterized by k_1 and B_{11}. For vanishing amplitude $\exp(\mathrm{i}\pi B_{11}) \to 0+$, equation (5.8) (with $j = 3$) turns into the dispersion relation of a harmonic wave, $\omega_2 \to 2|\sin(q_2/2)|$, if we choose the plus sign in equation (5.8). This is what we would have expected.

Because of the linearity of the equations of motion (5.1), not only the whole expression in curly brackets in (5.5) is a solution, but already its first part,

$$\delta q_n(t) = \mathrm{e}^{\mathrm{i}(q_2 n - \omega_2 t)}\left(\frac{\theta_3(\varphi_n^1+\kappa)}{\theta_3(\varphi_n^1)} - \frac{\mathrm{e}^{\mathrm{i}q_2}\theta_3(\varphi_{n+1}^1+\kappa)}{\theta_3(\varphi_{n+1}^1)}\right). \tag{5.9}$$

Clearly, this has to be complemented by equation (5.8). We compare equations (5.9) and (5.4) and see that the stability angles are given as

$$\eta = \omega_2/\nu_1. \tag{5.10}$$

Hence, dividing (5.8) by ν_1 yields directly a pair of equations for the stability angles. For each value of $q_2 = 2\pi j/N$ ($j = 1, \ldots, N-1$, $q_2 \neq 2\pi k_1$) we get a stability angle η_j, as we see explicitly in the harmonic and one-soliton limits. Since the complex conjugate of (5.9) is also a linear independent solution to (5.1), we have a total number of $2N-4$ linear independent solutions that follow from (5.8) and (5.9). For $q_2 = 0$ it is easily seen that $\nu_2 = \kappa = 0$ is a solution of (5.8) for all values of k_1 and B_{11}. But the right-hand side of (5.9) with $q_2 = \omega_2 = \kappa = 0$ is equal to zero and thus does not give a non-trivial solution to the linear stability problem. An analogous statement is true for $k_1 = k_2$.

For the sake of completeness we indicate two pairs of linear independent solutions to (5.1) that correspond to zero stability angle. One is the translational mode $\delta q_n(t) = c_1 + c_2 t$; another one is obtained for example by differentiating the single cnoidal wave solution with respect to its phase γ and its parameter B, respectively.

In the case of arbitrary length Δl the frequencies ν_1, ω_2 change according to equation (3.19). But the stability angles remain unchanged, being the ratio of the two frequencies.

6. Soliton limit of a single cnoidal wave

In our understanding a soliton is a concept which is generically associated with the infinite chain. It corresponds to the discrete part of the spectrum of the inverse scattering transform. We avoid speaking of 'a soliton under cyclic boundary conditions', as for instance Toda [45] does when he means a cnoidal wave consisting of a single peak ($k = 1/N$). As Boyd [46] pointed out, such an object has phonon- or soliton-like properties, depending on the value of the parameter B. However, in a certain limit, such a cnoidal wave turns into the soliton of the infinite chain. In this limit we will compute all the physical quantities which describe the cnoidal wave and which have been derived in the preceding sections. In this connection it seems inevitable to go again briefly through some well known results. We explain for instance how to obtain the shape of a soliton from a cnoidal wave and what is happening with the frequencies ν, $\nu(0)$ and with the length Δl_0 [45]. This is done for the sake of completeness and also to give the reader an idea of how to proceed in the more complex cases when we compute the soliton limit of the linear stability problem and of the sum over the stability angles. The latter is crucial for semiclassical quantization.

We would like to remind the reader that the periodic chain in the soliton limit is not fully equivalent to the infinite chain bearing a soliton (see [45]). For example, a cnoidal wave at zero pressure stretches the chain by an amount $\Delta l_0 > 0$ even in the soliton limit, but the soliton on the infinite chain compresses the chain. Furthermore, the periodic chain with a cnoidal wave of the form (3.7) always has zero momentum [45], whereas the infinite chain bearing a soliton has not [1].

The one-soliton limit is obtained as follows. We want to keep only a single peak and thus set $k = 1/N$. We would also like to reach the limit where all occurring elliptic functions are degenerate. These two claims will be fulfilled consistently if we set $\pi \mathrm{i}/B = \alpha N$, where $\alpha > 0$ will turn out to be the soliton parameter. We further have to replace the phase γ in φ_n by $\frac{1}{2} + \gamma/\alpha N$, where the new γ is again arbitrary. This means we have to use $\theta_4(z|B)$

instead of $\theta_3(z|B)$ to obtain the soliton limit of the equations (3.7) and (5.5). After these substitutions the respective expressions under consideration are expanded for large N.

To start with, consider equations (4.16) and (4.20). With the aid of the formulae (B.3), (B.2) from appendix B, we obtain

$$N\nu = \frac{\sinh(\alpha)}{\alpha}\left(1 - \frac{\sinh^2(\alpha)}{\alpha N} + \mathcal{O}\left(\frac{1}{N^2}\right)\right) \tag{6.1}$$

$$N\nu(0) = \frac{\sinh(\alpha)}{\alpha}\left(1 - \frac{\alpha}{N} + \mathcal{O}\left(\frac{1}{N^2}\right)\right). \tag{6.2}$$

Inserting these two equations into (4.20) and (4.17), we are provided with the expression

$$A = 1 - 2(\sinh^2(\alpha) - \alpha^2)/\alpha N + \mathcal{O}(1/N^2). \tag{6.3}$$

Thus, in the soliton limit, Δl_0 is given as

$$\Delta l_0 = -N\ln(A) \longrightarrow 2(\sinh^2(\alpha) - \alpha^2)/\alpha \tag{6.4}$$

which is always a positive number. To obtain the soliton limit of the energy and of the action per particle we still have to consider the constant a in (4.23). In the soliton limit the right-hand side of (4.23) is equal to

$$a/N^2 \longrightarrow 4\pi\int_0^\infty \mathrm{d}x\ \mathrm{cosech}^2(\pi x/\alpha)\sin^2(x) = 2(\alpha^2\coth(\alpha) - \alpha). \tag{6.5}$$

Using this equation, as well as (6.4) and (6.1) or (6.2), respectively, we get the desired result. Note that, like the frequencies (6.1), (6.2), energy and action per particle agree to leading order in the cases of zero pressure and zero length:

$$E = 2(\cosh(\alpha)\sinh(\alpha) - \alpha) \qquad S/N = 2\alpha\cosh(\alpha) - 4\sinh(\alpha) + 2\alpha^2/\sinh(\alpha). \tag{6.6}$$

In the soliton limit we are also able to verify equation (4.28) to leading order in N:

$$(N\nu)^2 = \frac{\mathrm{d}\Delta l_0}{\mathrm{d}(a/N^2)} \to \frac{\mathrm{d}(\sinh^2(\alpha) - \alpha^2)/\alpha}{\mathrm{d}(\alpha^2\coth(\alpha) - \alpha)} = \frac{\sinh^2(\alpha)}{\alpha^2} \tag{6.7}$$

and thus $\mathrm{d}S/\mathrm{d}\tau = -E$.

Equations (6.1) and (6.2) show that for $p = 0$ as well as for $\Delta l = 0$

$$\varphi_n = \tfrac{1}{2} + (n\alpha - \sinh(\alpha)t + \gamma)/\alpha N + \mathcal{O}(1/N^2). \tag{6.8}$$

We define $\phi_n := n\alpha - \sinh(\alpha)t + \gamma$ and use the first of the equations (B.1) to see that

$$q_n(t) - nd = -\alpha + \ln\left(\frac{1 + \mathrm{e}^{-2\phi_n}}{1 + \mathrm{e}^{-2\phi_{n+1}}}\right) \tag{6.9}$$

to leading order in N. Note that the constant α can be absorbed into $q_n(t)$. Thus the right-hand side of (6.9) is identified as the well known soliton solution for the infinite chain. Recall the meaning of the constant d on the left-hand side. In the case $\Delta l = 0$ it is equal to zero. But for zero pressure it is the change of the lattice constant $d = \Delta l_0/N$ and therefore

nd has no definite soliton limit, since n ranges from 1 to N. On the other hand, since d vanishes as $N \to \infty$, we get a meaningful result even in the case of zero pressure, if we look only at the relative motion. Then

$$e^{-(q_{n+1}-q_n)} - 1 = \sinh^2(\alpha)\,\mathrm{sech}^2(\phi_{n+1}) \tag{6.10}$$

which is the most familiar form of the Toda soliton.

At this point we emphasize the following: the energy and the action per particle can of course be calculated directly for the infinite chain (for the energy see [1]). But since the infinite chain and the periodic chain in the thermodynamic limit are physically different systems, there is no natural reason why the energy and the action per particle should agree in the two cases. Indeed they do for our choice of the potential (3.3), but they do not for Shirafuji's potential W_{sh} in the case $p_{\mathrm{sh}} = 1$. If we calculate the energy E_{sh} in the soliton limit and compare it with the energy calculated directly for the infinite chain with W_{sh}, we see that the two results disagree by an amount $2\sinh^2(\alpha)/\alpha$.

Let us now determine the stability angles following from (5.8) up to terms of the order of $1/N$. The required calculations are quite tedious. We will therefore only give a brief description how to proceed. First we have to calculate the coupling κ to leading order. To this end we eliminate ω from (5.8) by subtracting the two equations from each other and we are left with an equation for κ alone. We introduce the abbreviation

$$\kappa_1 := 2\mathrm{i}\alpha N\kappa. \tag{6.11}$$

For all logarithmic derivatives and all quotients of theta functions occurring in (5.8) we use the representations according to appendix B. The leading terms in the equation for κ_1 are of the order $\exp(-\alpha N/2)$. The factors $\exp(-\alpha N/2)$ cancel out and the remaining equation yields to leading order

$$e^{-\mathrm{i}\kappa_1} = 1 - \frac{(e^{2\alpha} - 1)(e^{\mathrm{i}q_2} - 1)}{(e^{\alpha+\mathrm{i}q_2/2} - 1)^2}. \tag{6.12}$$

Thus κ_1 agrees with the phase shift that a nonlinear phonon suffers due to a soliton [47]. Logarithms must be taken carefully in (6.12), since the solution is not unique. We stipulate κ_1 to be continuous as a function of q_2 for $0 \leqslant q_2 \leqslant 2\pi$, and to vanish as $\alpha \to 0$ for $0 < q_2 \leqslant 2\pi$. Thus we get

$$\tan(\kappa_1/4) = -\tanh(\alpha/2)\cot(q_2/4) \qquad 0 \leqslant q \leqslant 2\pi. \tag{6.13}$$

With that, we are prepared to calculate ω_2. Inserting (6.1), (6.3), (6.11) and (6.13) into one of the equations (5.8) we arrive at

$$\omega_2 = 2\sin\left(\frac{q_2}{2}\right) + \frac{1}{N}\left[\kappa_1\left(\cos\left(\frac{q_2}{2}\right) - \frac{\sinh(\alpha)}{\alpha}\right) - \frac{2\sinh^2(\alpha)}{\alpha}\sin\left(\frac{q_2}{2}\right)\right] + \mathcal{O}\left(\frac{1}{N^2}\right). \tag{6.14}$$

We see that in the soliton limit ω_2 turns into the frequency of a harmonic excitation. This is due to the fact that a soliton is a localized object. The $1/N$ corrections to ω_2 contain the semiclassical corrections to classical energy and momentum of the soliton (see the following section). Using (6.8), (6.11) and (5.9) we obtain the solutions of the linear stability problem in the soliton limit,

$$\delta q_n(t) = \mathrm{e}^{\mathrm{i}(nq_2-\omega_2 t-\kappa_1/2)}\left[\frac{1+\mathrm{e}^{-2\phi_n+\mathrm{i}\kappa_1}}{1+\mathrm{e}^{-2\phi_n}} - \frac{\mathrm{e}^{\mathrm{i}q_2}(1+\mathrm{e}^{-2\phi_{n+1}+\mathrm{i}\kappa_1})}{1+\mathrm{e}^{-2\phi_{n+1}}}\right]. \tag{6.15}$$

Here $\omega_2 = 2\sin(q_2/2)$ and κ_1 is given by equation (6.13). It is merely a matter of patience to substitute (6.15) directly into (5.1) with $\exp(-(q^*_{n+1} - q^*_n))$ given by (6.10), and to see that it is indeed a solution. It would have been possible and also much easier to obtain (6.15) by the method that the authors of [47] used to get the phonon phase shifts due to a soliton. But, unfortunately, this method does not yield the $1/N$ corrections to the frequency ω_2.

7. Main results and discussion

In this section we gather all the information about the classical periodic Toda chain which we have obtained in the preceding sections and insert them into the semiclassical quantization formulae (2.6), (2.7).

In the case of the finite chain we cannot go analytically beyond (5.8). For the physically most appropriate boundary condition, $\Delta l = 0$, we take energy and action per particle according to equations (4.25) and (4.26). The sum over stability angles is obtained from (5.8) and (5.10). Thus the right-hand sides of equations (2.6) and (2.7) are completely specified. There remains a single unknown quantity, v, which can take on the values 0, $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$. By comparison with the harmonic limit it turns out that $v = \frac{1}{2}$. It seems noteworthy that, in the equations for the spectrum, the number of particles N is merely playing the role of a parameter. This means that the numerical effort to compute the spectrum does not increase with increasing number of particles.

We think that our results are a good test for the method in general. In a forthcoming publication [31] which is now in preparation they will be compared numerically to the results obtained by Gutzwiller's exact quantization of the three- and four-particle chains [15–17], as well as to the results of direct numerical methods [21, 22]. Furthermore, it seems quite interesting to compare our result with the result arising from EBK quantization, which in the case of the periodic Toda chain has been considered in [15, 21]. First numerical calculations for the three-particle chain show that the semiclassical energy levels obtained with the quantization procedure of section 2 differ from the EBK results. Moreover, the quantization formulae (2.6) and (2.7) break the discrete symmetries of the Hamiltonian which have recently been shown explicitly to be conserved by EBK quantization [48]. On the other hand, the ground-state levels for the three- and four-particle chains are obtained more accurately than with the EBK method.

We now discuss the soliton limit. With the aid of the formulae (6.1), (6.6), (6.13) and (6.14) we are prepared to calculate the semiclassically corrected dispersion relation $E = E(p)$ for a soliton on the infinite chain, as explained in section 2. The details of the calculation are presented in appendix C. The following parametric representation of the semiclassically corrected dispersion relation for $\Delta l = 0$ is obtained:

$$\varepsilon = E - 2\hbar\alpha/\pi \tag{7.1}$$

$$p = p_{\mathrm{cl}} - \frac{2\hbar}{\pi}\int_0^\alpha \mathrm{d}x\,\frac{x}{\sinh(x)}. \tag{7.2}$$

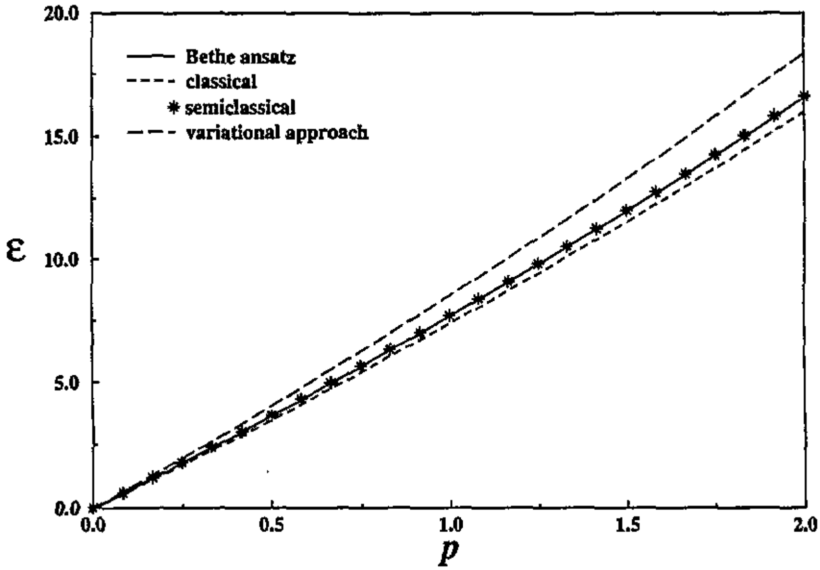

Figure 1. Comparison between the different results for the dispersion relation of a soliton for fixed length $\Delta l = 0$ and $\hbar = 1$. ε in units of $\hbar/2$ and p in units of $\pi\hbar$.

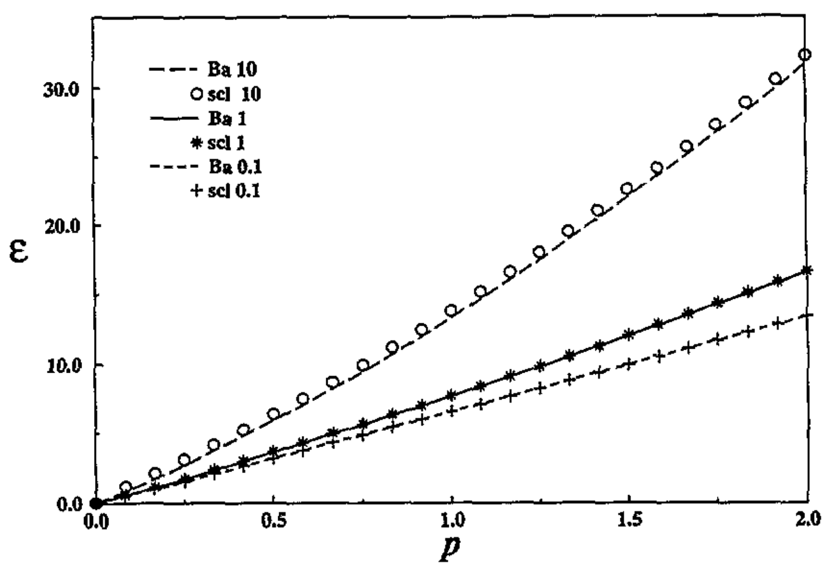

Figure 2. Dispersion relation derived semiclassically (scl) and as follows from the Bethe ansatz (Ba) for $\hbar = 0, 1; 1; 10$. ε in units of $\hbar/2$ and p in units of $\pi\hbar$.

E and $p_{\rm cl}$ are the classical energy and momentum of a soliton:

$$E = 2(\sinh(\alpha)\cosh(\alpha) - \alpha) \qquad p_{\rm cl} = 4(\alpha\cosh(\alpha) - \sinh(\alpha)). \tag{7.3}$$

The result is shown in figure 1 and is compared with the classical result, the Bethe ansatz result and the result following from a time-dependent variational approach [30]. Our semiclassical result is in almost absolute agreement with the Bethe ansatz result even in the full quantum mechanical regime $\hbar = 1$, and in this regime it is quite different from the variational-approach result. Figure 2 shows the remarkable fact that the semiclassical dispersion relation is still in good agreement with the one from Bethe ansatz even if $\hbar = 10$; that is, even if $\hbar$ is two orders of magnitude larger than the value for which the semiclassical approximation is suspected to be applicable.

The important thing about our results as far as they concern the soliton dispersion curve is that our intuitive picture of a soliton as a particle over a vacuum state, which leads us to the definition of the semiclassical momentum, is consistent with the Bethe ansatz. Therefore the two very different approaches support each other. This is of some importance, for all soliton dispersion curves as they are shown in figure 1 contain the soliton momentum as a phenomenological concept. This is especially true for the momentum obtained from Bethe's ansatz by analogy to the δ-function Bose gas.

Let us finally remark that the semiclassical dispersion relation may be computed with arbitrary lattice constant $d = \Delta l/N$ and thus also at zero pressure. This will be explained in appendix D.

Acknowledgments

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Appendix A. Dispersion relations

To derive the dispersion relations (3.17) we use the same formalism as Dubrovin in his work on the KdV equation (see [11], ch 4). The starting point of this calculation is equation (3.13) with $f = 1$ and z instead of φ_n:

$$\theta^2(z) + \nu_i\nu_j\theta(z)\theta_{ij}(z) - \nu_i\nu_j\theta_i(z)\theta_j(z) - A\theta(z+k)\theta(z-k) = 0. \qquad (A.1)$$

We define the infinitesimal shift operator $T_z := \nu_j\partial/\partial z_j$ and the finite shift operator S_z by $S_z f(z) = f(z+k)$. Then the inverse of S_z is given by $S_z^{-1} f(z) = f(z-k)$ and (A.1) reads

$$(1 + T_{z^1}^2 - T_{z^1}T_{z^2} - AS_{z^1}S_{z^2}^{-1})\theta(z^1)\theta(z^2)|_{z^1=z^2} = 0. \qquad (A.2)$$

We now introduce new coordinates

$$\begin{pmatrix} w^1 \\ w^2 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} z^1 \\ z^2 \end{pmatrix} \Leftrightarrow \begin{pmatrix} z^1 \\ z^2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} w^1 \\ w^2 \end{pmatrix}. \qquad (A.3)$$

In these new coordinates (A.2) turns into

$$(1 + 2T_{w^1}T_{w^2} + 2T_{w^2}^2 - AS_{w^2}^2)\theta(\tfrac{1}{2}(w^1 + w^2))\theta(\tfrac{1}{2}(w^1 - w^2))|_{w^2=0} = 0. \qquad (A.4)$$

For the Riemann theta function the addition theorem (4.6) reads

$$\theta(z+w)\theta(z-w) = \sum_{2\delta\in(Z_2)^g} \hat{\theta}[\delta](2z)\hat{\theta}[\delta](2w) \qquad (A.5)$$

(see section 3 for the notation). $\hat{\theta}[\delta](z)$ is an even function for all $\delta \in \frac{1}{2}(Z_2)^g \Rightarrow T_z\hat{\theta}[\delta](z)|_{z=0} = 0$. Also, equation (A.4) implies

$$\sum_{2\delta\in(Z_2)^g} \hat{\theta}[\delta](w^1)(1 + 2T_{w^2}^2 - AS_{w^2}^2)\hat{\theta}[\delta](w^2)|_{w^2=0} = 0. \tag{A.6}$$

Since all the functions $\hat{\theta}[\delta](w)$ are linear independent (see [11])

$$(1 + 2T_w^2 - AS_w^2)\hat{\theta}[\delta](w)|_{w=0} = 0. \tag{A.7}$$

This is the desired result (3.17).

Appendix B. Series representations for the soliton limit

The Fourier representation (3.9) of a theta function with characteriztic $[\alpha, \beta]$ is not the only possible representation. In fact, there is a whole transformation theory dealing with the various equivalent representations of theta functions (see [11] and the literature cited therein). As Boyd [49, 50] pointed out and elaborated in case of the KdV equation, one of these representations is especially convenient to perform the soliton limit of a multi-cnoidal wave. It is called the Gaussian representation and is simply obtained by Poisson re-summation [1] of the Fourier series (3.9), i.e.

$$\begin{aligned}\theta[\alpha, \beta](z|B) &= (\det(-\mathrm{i}B))^{-1/2}\sum_{n\in\mathbf{Z}^g}\exp\{-\pi\mathrm{i}\langle n+\beta+z, B^{-1}(n+\beta+z)\rangle - 2\pi\mathrm{i}\langle n, \alpha\rangle\}\\ &= (\det(-\mathrm{i}B))^{-1/2}\exp\{-\pi\mathrm{i}\langle z, B^{-1}z\rangle + 2\pi\mathrm{i}\langle\alpha,\beta\rangle\}\theta[\beta, -\alpha](-B^{-1}z| - B^{-1}).\end{aligned} \tag{B.1}$$

This is valid at least if $\mathrm{i}B$ is real. For our purposes we only need to consider one-dimensional theta functions. Then (B.1) is the same as what is called Jacobi's imaginary transformation (see [42], p 474).

Many of the formulae that we study in the soliton limit contain logarithmic derivatives of theta functions instead of theta functions. For these it will prove to be convenient to derive certain series representations. Equation (B.1) implies

$$\frac{\theta'[\alpha,\beta](z|B)}{\theta[\alpha,\beta](z|B)} = -\frac{2\pi\mathrm{i}z}{B} - \frac{1}{B}\frac{\theta'[\beta,-\alpha](-z/B|-1/B)}{\theta[\beta,-\alpha](-z/B|-1/B)}. \tag{B.2}$$

On the right-hand side of (B.2) we again have a logarithmic derivative. So we can use some well known formulae (see [42] p 498, for instance) which yield for the four basic theta functions (4.1)

$$\frac{\theta_1'(z|B)}{\theta_1(z|B)} = \frac{\pi\mathrm{i}}{B}\left(-2z + \coth\left(\frac{\pi\mathrm{i}z}{B}\right) - 4\sum_{n=1}^{\infty}\frac{\sinh(2n\pi\mathrm{i}z/B)}{\mathrm{e}^{2n\pi\mathrm{i}/B}-1}\right) \tag{B.3}$$

$$\frac{\theta_2'(z|B)}{\theta_2(z|B)} = \frac{\pi\mathrm{i}}{B}\left(-2z - 2\sum_{n=1}^{\infty}\operatorname{cosech}\left(\frac{n\pi\mathrm{i}}{B}\right)\sinh\left(\frac{2n\pi\mathrm{i}z}{B}\right)\right) \tag{B.4}$$

$$\frac{\theta_3'(z|B)}{\theta_3(z|B)} = \frac{\pi\mathrm{i}}{B}\left(-2z - 2\sum_{n=1}^{\infty}(-1)^n\operatorname{cosech}\left(\frac{n\pi\mathrm{i}}{B}\right)\sinh\left(\frac{2n\pi\mathrm{i}z}{B}\right)\right) \tag{B.5}$$

$$\frac{\theta_4'(z|B)}{\theta_4(z|B)} = \frac{\pi\mathrm{i}}{B}\left(-2z + \tanh\left(\frac{\pi\mathrm{i}z}{B}\right) - 4\sum_{n=1}^{\infty}(-1)^n\frac{\sinh(2n\pi\mathrm{i}z/B)}{\mathrm{e}^{2n\pi\mathrm{i}/B}-1}\right). \tag{B.6}$$

Appendix C. Semiclassically corrected dispersion relation

Starting with (2.6) and (2.7) we calculate the semiclassically corrected dispersion relation $E = E(p)$ of a soliton on a chain of fixed length $\Delta l = 0$. In order to keep the energies in (2.6) finite in this limit we must subtract the vacuum energy: $\varepsilon \to \varepsilon - \sum_q \hbar \sin(q/2)$. Since the soliton limits of E and $(S + E\tau(0))/N$ have already been calculated (6.1), (6.6), we only have to determine $\mathrm{d}_{\tau(0)}\xi + \hbar \sum_{q_2} \sin(q_2/2)$ and $(1 - \tau(0)\mathrm{d}_{\tau(0)})\xi/N$ in the soliton limit. From (6.1) we obtain

$$\mathrm{d}_{\tau(0)} = \frac{\sinh^2(\alpha)}{\sinh(\alpha) - \alpha\cosh(\alpha)} \frac{\mathrm{d}_\alpha}{N} + \mathcal{O}\left(\frac{1}{N^2}\right) \tag{C.1}$$

and, further, from (6.2) and (6.14) we obtain, up to terms of the order of $1/N^2$,

$$\omega_2(0) = \frac{\omega_2}{\sqrt{A}} = 2\sin\left(\frac{q_2}{2}\right) + \frac{1}{N}\left[\kappa_1\left(\cos\left(\frac{q_2}{2}\right) - \frac{\sinh(\alpha)}{\alpha}\right) - 2\alpha\sin\left(\frac{q_2}{2}\right)\right]. \tag{C.2}$$

It thus follows that

$$\mathrm{d}_{\tau(0)}\xi + \hbar\sum_{q_2}\sin(q_2/2) = -\left(\frac{\hbar}{2}\right)\mathrm{d}_{\tau(0)}\sum_{q_2}\left(\omega_2(0) - 2\sin\left(\frac{q_2}{2}\right)\right)\Big/\nu_1(0) \tag{C.3}$$

$$= -\frac{\hbar}{4\pi}\frac{\sinh^2(\alpha)}{\sinh(\alpha) - \alpha\cosh(\alpha)}\mathrm{d}_\alpha\sum_{q_2}\frac{2\pi}{N}\left[\kappa_1\left(\frac{\alpha\cos(q_2/2)}{\sinh(\alpha)} - 1\right)\right.$$
$$\left. - 2\frac{\alpha^2}{\sinh(\alpha)}\sin\left(\frac{q_2}{2}\right)\right] + \mathcal{O}\left(\frac{1}{N}\right) \tag{C.4}$$

with κ_1 according to (6.13). We abbreviate the sum on the right-hand side as Σ and denote the derivative with respect to α by a prime. It follows that

$$(1 - \tau(0)\mathrm{d}_{\tau(0)})\xi/N = -\frac{\hbar}{4\pi}\Sigma + \frac{\hbar}{4\pi}\frac{\alpha\sinh(\alpha)}{\sinh(\alpha) - \alpha\cosh(\alpha)}\Sigma' + \mathcal{O}\left(\frac{1}{N}\right). \tag{C.5}$$

In the soliton limit the sums Σ and Σ' are replaced by integrals with $0, 2\pi$ as limits of integration. Using the relations

$$\frac{\partial\kappa_1}{\partial\alpha}\Big/\frac{\partial\kappa_1}{\partial q_2} = -\frac{2\sin(q_2/2)}{\sinh(\alpha)} \qquad \frac{\partial\kappa_1}{\partial q_2} = \frac{\sinh(\alpha)}{\cosh(\alpha) - \cos(q_2/2)} \tag{C.6}$$

Σ' is calculated by integrating by parts.

$$\Sigma' = 8\left(\frac{\alpha}{\sinh(\alpha)} - \mathrm{d}_\alpha\frac{\alpha^2}{\sinh(\alpha)}\right) = -\frac{8\alpha(\sinh(\alpha) - \alpha\cosh(\alpha))}{\sinh^2(\alpha)}. \tag{C.7}$$

Σ follows from integration with respect to α. Regarding the original integral representation for Σ as an integral over q_2, the integration constant is seen to be zero. In summary we have obtained

$$-\mathrm{d}_{\tau(0)}\xi - \hbar\sum_{q_2}\sin(q_2/2) = -\frac{2\hbar\alpha}{\pi} =: \Delta E \tag{C.8}$$

$$(1 - \tau(0)\mathrm{d}_{\tau(0)})\xi/N = -\frac{2\hbar}{\pi}\int_0^\alpha \mathrm{d}x\,\frac{x}{\sinh(x)} =: \Delta p. \tag{C.9}$$

Using these equations, as well as (6.6), we arrive at (7.1), (7.2).

Appendix D. The cases of arbitrary length and zero pressure

We consider a finite dilation $d = \Delta l/N$ of the chain. Then according to (4.20)

$$\nu(\Delta l) = e^{-d/2}\nu(0). \tag{D.1}$$

The energy turns out to be (see (4.22) and below)

$$\begin{aligned} E(\Delta l) &= a\nu^2(\Delta l) + \Delta l + Np \\ &= e^{-d}(a\nu^2(0) + N(e^{\Delta l_0/N} - 1)) + N(e^{-d} + d - 1) \\ &= e^{-d}E(0) + E_0 \end{aligned} \tag{D.2}$$

where $E(0)$ is the energy in the case $\Delta l = 0$ according to (4.25), and $E_0 := N(e^{-d} + d - 1)$ is the classical ground-state energy. Equation (D.1) further implies that

$$d_{\tau(\Delta l)} = e^{-d/2}d_{\tau(0)} \qquad \tau(\Delta l)d_{\tau(\Delta l)} = \tau(0)d_{\tau(0)}. \tag{D.3}$$

Since ξ is invariant under scale transformations, it follows that

$$\varepsilon = e^{-d}E(0) + E_0 - e^{-d/2}d_{\tau(0)}\xi. \tag{D.4}$$

Hence in this case the proper renormalization of ε in the soliton limit is achieved by the replacement

$$\varepsilon \longrightarrow \varepsilon - E_0 - e^{-d/2}\sum_q \hbar\sin(q/2). \tag{D.5}$$

Because of the second equation (D.3) *the second term on the right-hand side of equation* (2.7) stays invariant under scale transformations. Concerning the first term, we obtain (see (4.22) and below)

$$\begin{aligned} S(\Delta l) + E(\Delta l)\tau(\Delta l) &= 2a\nu(\Delta l) = e^{-d/2}2a\nu(0) \\ &= e^{-d/2}(S(0) + E(0)\tau(0)). \end{aligned} \tag{D.6}$$

This means that the semiclassically corrected dispersion relation for arbitrary d is given as

$$\varepsilon = e^{-d}E + e^{-d/2}\Delta E \tag{D.7}$$

$$p = e^{-d/2}p_{\mathrm{cl}} + \Delta p \tag{D.8}$$

where E and p_{cl} are classical soliton energy and momentum according to (7.3), and ΔE, Δp are the corrections as calculated in the previous appendix.

The vacuum state according to (D.7), (D.8) is characterized by $\varepsilon = p = 0$. Regarding (D.5) we see that in the thermodynamic limit the ground-state energy per particle approaches

$$\varepsilon_0 = e^{-d} + d - 1 + \frac{2\hbar}{\pi}e^{-d/2}. \tag{D.9}$$

The zero-pressure lattice constant d is now determined by stipulating ε_0 to be minimal. With $g := \hbar/2\pi$ it turns out to be

$$d_0 = -\ln\left(1 + 2g^2 - 2g\sqrt{1+g^2}\right) = \hbar/\pi + \mathcal{O}(\hbar^2). \tag{D.10}$$

Note that d_0 agrees to linear order in $\hbar$ with the corresponding quantity obtained from the variational approach [30].

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