Modulated Waves in a Semiclassical Continuum Limit of an Integrable NLS Chain

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Abstract

A one-dimensional integrable lattice system of ODEs for complex functions $Q_n(\tau)$ that exhibits dispersive phenomena in the phase is studied. We consider wave solutions of the local form $Q_n(\tau) \sim q\exp(i(kn+\omega\tau+c))$, in which q, k, and ω modulate on long time and long space scales $t=\varepsilon\tau$ and $x=\varepsilon n$. Such solutions arise from initial data of the form $Q_n(0)=q(n\varepsilon)\exp(i\phi(n\varepsilon)/\varepsilon)$, the phase derivative ϕ' giving the local value of the phase difference k. Formal asymptotic analysis as $\varepsilon\to 0$ yields a first-order system of PDEs for q and ϕ' as functions of x and t. A certain finite subchain of the discrete system is solvable by an inverse spectral transform. We propose formulae for the asymptotic spectral data and use them to study the limiting behavior of the solution in the case of initial data $|Q_n|<1$, which yield hyperbolic PDEs in the formal limit. We show that the hyperbolic case is amenable to Lax-Levermore theory. The associated maximization problem in the spectral domain is solved by means of a scalar Riemann-Hilbert problem for a special class of data for all times before breaking of the formal PDEs. Under certain assumptions on asymptotic behaviors, the phase and amplitude modulation of the discrete systems is shown to be governed by the formal PDEs. Modulation equations after breaking time are not studied. Full details of the WKB theory and numerical results are left to a future exposition. © 1999 John Wiley & Sons, Inc.

1 Introduction

1.1 Background

The semiclassical limit of the linear Schrödinger equation of quantum mechanics is supposed to represent one step toward a refinement of the classical approximation. This consists of inserting a fast-oscillating ansatz into the Schrödinger equation and studying the resulting evolution of the amplitude and phase as Planck's constant ε tends to zero:

$$i\varepsilon\psi_t = -\varepsilon^2\psi_{xx}+V(x)\psi, \qquad \psi(x,t)=A(x,t)\exp\left(-\frac{iS(x,t)}{\varepsilon}\right).$$

This conventional analysis may be a good intuitive point of entry into this article, in which we undertake a study of a semiclassical continuum limit of a discrete, nonlinear Schrödinger system of ordinary differential equations. The system is completely integrable and solvable by an inverse spectral transform, and its steady oscillating solutions are subject to a relation between frequency and wave number, or a "dispersion relation." We study the limiting behavior of the system in relation

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to its formal limit. The background and tools of analysis are described in this subsection.

Singular limits of integrable dispersive systems solvable by inverse spectral methods were first understood in a rigorous analytical manner by Lax and Levermore [8] in their study of the Korteweg–de Vries (KdV) equation as a singular perturbation of the inviscous Burgers equation,

$$u_t + uu_x + \varepsilon^2 u_{xxx} = 0\,.$$

They studied its solutions by analyzing the asymptotics of its associated spectral and inverse spectral transforms. They found that, for certain types of initial data, Burgers'equation, before the breaking time of its solution, governs the limit of the solutions of the KdV equation as ε tends to zero. After this breaking time, the solutions develop oscillations emanating from the breaking point of Burgers' equation with wavelength on the order of ε. At this time, there arise systems of partial differential equations in Riemann-invariant form that describe the slow-scale modulation of these waves. A fundamental object in the analysis is the solution of a quadratic variational minimization problem in the spectral domain parameterized by the variables x and t. This variational problem arises from the asymptotics of the inverse spectral transform. The minimizer is posed as the unique solution to a Riemann-Hilbert problem and solved by complex-analytical methods. In [8], the problem was solved for negative initial data $u(x,0)$ that decays sufficiently rapidly as $|x|$ tends to infinity and that has a unique local minimum. Later, Venakides extended the methods to include positive decaying initial data with a unique local maximum [13] and periodic initial data [14].

Similar analysis has since been applied to numerous singular limits of nonlinear dynamical systems: Jin, Levermore, and D. McLaughlin [7] studied the behavior of dispersive waves in the semiclassical limit of the defocusing nonlinear Schrödinger (NLS) equation; Ercolani, Jin, Levermore, and McEvoy [5] treated the dispersion-free limit of the NLS and mKdV hierarchies; Deift and K. McLaughlin [3] carried over the procedures to a continuum limit of a discrete system in their work on the Toda lattice. Essential to the procedure is the complete integrability of the system and an explicit solution by means of inverse spectral theory. Equally important is a knowledge of the asymptotic distribution of eigenvalues and behavior of the associated spectral data. Typically, the formally limiting PDE or system of PDEs describes the limiting behavior of the integrable systems until the breaking time of these formal equations; thereafter, modulation equations for the evolution of locally wavelike solutions arise. These are the modulation equations that have been derived previously by the method of averaged conservation laws by Whitham [15] and developed extensively by Flaschka, Forest, and D. McLaughlin [6] for the KdV equation. Their derivation in the context of singular limits and the passing from the formal limit to these more complicated equations is undertaken, for example, in [8] and [3] and also in [11], in which Tian and Ye study this transition in the semiclassical limit of the defocusing NLS equation.

The present study concerns a semiclassical continuum limit of an integrable discrete version of the defocusing NLS equation (see equation (1.1) below) with boundary conditions $|Q_0| = |Q_N| = 1$. The system is solvable by an inverse spectral transform. A fundamental dichotomy in the nature of the system, its spectral data, and its continuum limit arises. When $|Q_n| < 1$ for $n = 1, \ldots, N-1$, the eigenvalues are unitary complex numbers and the associated norming constants are real and the formal continuum limit is a hyperbolic system of two real PDEs for the modulus and phase. When $|Q_n| > 1$, the eigenvalues and norming constants are unrestricted and the formal PDEs are elliptic. The restriction of the eigendata, which is a consequence of the unitarity of the spectral problem, is crucial both for interpreting the WKB theory to arrive at an understanding of their asymptotics and for subjecting the inverse transform to the procedure of Lax and Levermore. Such is typical of these tractable problems. Also typical is that the formally limiting equations are well-posed and are seen to describe the limit of the inverse spectral solution and thus can be analyzed to reveal information about the singular limit until the breakdown time of their solution. In this paper, we study the semiclassical limit in the case that $|Q_n| < 1$ only before breaking of the formal PDEs. Full details of the WKB analysis and numerical studies of the asymptotics of the spectral transform are left to a later exposition of these issues in their own right.

In the case that $|Q_n| > 1$, the spectral problem is not unitary and its asymptotics are not understood, the singular limit is not amenable to the theory of Lax and Levermore, and the formally limiting system of PDEs is elliptic rather than hyperbolic. This case is to be compared with the non-self-adjoint Zakharov-Shabat spectral problem studied by Bronski [2], who discusses the WKB dilemma and presents numerical results on the distribution of eigenvalues in the complex plane in the light of asymptotic bounds obtained by Deift, Venakides, and Zhou [4].

1.2 The Discrete NLS Chain

We will consider a finite subchain of the following version of the discrete defocusing nonlinear Schrödinger equation (DNLS):[1]

$$i\dot{Q}_n + Q_{n+1} - 2Q_n + Q_{n-1} - |Q_n|^2(Q_{n-1} + Q_{n+1}) = 0\,, \quad n \in \mathbb{Z}\,, \tag{1.1}$$

in which $Q_n(\tau)$ are complex functions of time τ and $\dot{Q}_n$ denotes $dQ_n/d\tau$. We prescribe initial data by fixing two real-valued functions $q \geq 0$ and ϕ of a real variable x and, for each (small) positive value of ε, putting

$$Q_n(0) = q(n\varepsilon)\exp\left(\frac{i}{\varepsilon}\phi(n\varepsilon)\right). \tag{1.2}$$

The DNLS system (1.1) with these intial data will be denoted by $\mathcal{S}_\varepsilon$. We will introduce the finite subchain shortly, but first we study the dispersive properties of the system in general and provide a mathematical motivation for imposing such

[1] D here stands for "discrete," not "defocusing."

initial data, which result in the semiclassical limit when one allows ε to tend to zero.

This DNLS system admits solutions of the form

$$Q_n(\tau) = q \exp(i(kn + \omega\tau + c)),$$

in which the modulus q, the phase difference (or discrete wave number) k, the frequency ω, and the phase shift c are constants. These solutions are subject to the dispersion relation

$$\omega - 2(1 - q^2)\cos k + 2 = 0. \tag{1.3}$$

More generally, if one inserts the form

$$Q_n(\tau) = q_n(\tau) \exp(i(kn + \omega\tau + c))$$

into the system, where the q_n are real-valued and k, ω, and c are constants, the following relations result:

$$\begin{aligned} \omega q_n - (1 - q_n^2)(q_{n-1} + q_{n+1})\cos k + 2q_n &= 0, \\ \dot{q}_n + (1 - q_n^2)(q_{n+1} - q_{n-1})\sin k &= 0. \end{aligned} \tag{1.4}$$

If the q_n are not all equal, then these equations do not have a solution. However, the second equation indicates that, if the q_n vary only very little with the index n, then they are approximately constant in time, and so the first equation, the dispersion relation, is then approximately valid for an appreciable time interval. Indeed, if the q_n are initially all equal, then they are constant in time and the dispersion relation (1.3) is exactly valid for all time. Therefore, given initial values of q_n that vary appreciably only over large variations in n, one may then reasonably inquire about the long-time modulation of the values of q_n and the local phase difference k. One may attempt to describe solutions in which the differences $q_{n+1} - q_n$ are at the order of some small parameter ε as follows: Let $q^\varepsilon(x,t)$ and $\phi^\varepsilon(x,t)$ be real-valued functions that are asymptotic to differentiable real-valued functions $q(x,t)$ and $\phi(x,t)$ as ε tends to zero, and put

$$Q_n(\tau) = q^\varepsilon(\varepsilon n, \varepsilon\tau) \exp\left(\frac{i}{\varepsilon}\phi^\varepsilon(\varepsilon n, \varepsilon\tau)\right). \tag{1.5}$$

One may think of $Q_n(\tau)$ as evolving complex-valued functions defined on a lattice with a spacing of $\Delta x = \varepsilon$ between sites. Given a fixed integer n_0 and a fixed time τ_0, then for integers n sufficiently close to n_0 and times τ sufficiently close to τ_0, this function is approximated by

$$Q_n(\tau) = q_0 \exp(i(kn + \omega\tau + c)),$$

in which $q_0 = q^\varepsilon(\varepsilon n_0, \varepsilon\tau_0)$, $k = \phi_x^\varepsilon(\varepsilon n_0, \varepsilon\tau_0)$, and $\omega = \phi_t^\varepsilon(\varepsilon n_0, \varepsilon\tau_0)$. One may therefore reasonably expect the existence of solutions with the asymptotic form (1.5) in which

$$\phi^{\varepsilon}(x,t) \sim \phi(x,t) + \varepsilon\phi_1(x,t) + \varepsilon^2\phi_2(x,t) + \cdots, \tag{1.6}$$

$$q^{\varepsilon}(x,t) \sim q(x,t) + \varepsilon q_1(x,t) + \varepsilon^2 q_2(x,t) + \cdots. \tag{1.7}$$

The initial data (1.2) for the systems $\mathcal{S}_\varepsilon$ have indeed the asymptotic form of (1.5)–(1.7) at $\tau = 0$; the coefficient functions ϕ_i and q_i for $i \geq 1$ are taken to be zero at time $t = 0$. We expect the solutions of $\mathcal{S}_\varepsilon$ to have the proposed asymptotic form as long as the derivatives of the functions q, ϕ_x, and ϕ_t remain finite.

One can formally insert (1.5), (1.6), and (1.7) into the DNLS system and pass to the slow time variable $t = \varepsilon\tau$. As expected, this asymptotic ansatz is formally consistent, and from the leading term one obtains

$$\begin{aligned} &\phi_t - 2(1-q^2)\cos\phi_x + 2 = 0, \\ &q_t + (1-q^2)\big(2q_x\sin(\phi_x) + q\phi_{xx}\cos(\phi_x)\big) = 0. \end{aligned} \tag{1.8}$$

The first of these equations is the continuum analogue of the dispersion relation (1.3). Differentiating it with respect to x yields a first-order autonomous quasilinear system of partial differential equations for the phase derivative $\phi' = \partial\phi/\partial x$ and q:

$$\begin{aligned} &\phi'_t + 2(1-q^2)\phi'_x\sin(\phi') + 4qq_x\cos(\phi') = 0, \\ &q_t + (1-q^2)\big(2q_x\sin(\phi') + q\phi'_x\cos(\phi')\big) = 0. \end{aligned} \tag{1.9}$$

This system is hyperbolic whenever $q < 1$ and elliptic whenever $q > 1$. In the case that it is hyperbolic, a pair of Riemann invariants is given by

$$\alpha = 2\arcsin(q) - \phi', \qquad \beta = 2\pi - 2\arcsin(q) - \phi'. \tag{1.10}$$

In terms of these, q and ϕ' are recovered by

$$q = \cos\left(\frac{\beta-\alpha}{4}\right), \qquad \phi' = \pi - \frac{\beta+\alpha}{2}. \tag{1.11}$$

The system (1.9) of PDEs in Riemann-invariant form is

$$\alpha_t = f(\alpha,\beta)\alpha_x, \qquad \beta_t = f(\beta,\alpha)\beta_x, \tag{1.12}$$

in which the function f is defined by

$$f(\mu,\gamma) = \sin(\mu) - \sin\left(\frac{\mu+\gamma}{2}\right).$$

In this article, we study the hyperbolic case subject to boundary conditions that give rise to a decoupled finite subchain, which we describe next.

1.3 The Finite Subchain

One observes that, if $Q_0(0)$ and $Q_N(0)$ in equation (1.1) are taken to be unitary complex numbers, then $Q_0(\tau)$ and $Q_N(\tau)$ are independent of their neighbors:

$$Q_0(\tau) = Q_0(0)e^{-2i\tau}\,, \qquad Q_N(\tau) = Q_N(0)e^{-2i\tau}\,.$$

Thus, the evolution of the quantities Q_n for $n = 1,\dots,N-1$ becomes decoupled from the rest of the chain, resulting in a system of $N-1$ ordinary differential equations. This finite system was shown to be integrable by Vekslerchik [12], who also presented a solution by inverse spectral formulae. The spectral theory is presented in Section 2, with the details provided in the appendix.

In accordance with these boundary conditions on the discrete systems $\mathcal{S}_\varepsilon$, we restrict the functions q and ϕ of x to the interval $[0,1]$ and put q equal to 1 at the endpoints. The value of $\phi(0)$ is not important, since it only contributes to a constant phase shift in the solutions of the systems $\mathcal{S}_\varepsilon$. Accordingly, it only contributes a constant to the solution ϕ of the formal system of PDEs for q and ϕ. We thus prescribe q and ϕ such that

$$\begin{aligned} &q : [0,1] \to [0,1]\,, \quad 0 \le q(x) < 1 \text{ for } x \in (0,1),\; q(0) = q(1) = 1\,, \\ &\phi : [0,1] \to \mathbb{R}\,, \quad \phi(0) = 0\,. \end{aligned}$$

The following observations about the Riemann invariants then follow: $\alpha(x) \le \beta(x)$, equality holding only at $x = 0$ and $x = 1$, and if q has a nonzero x-derivative at one of the endpoints, then both α and β have infinite slope there. The two functions form a non-self-intersecting closed curve in $\mathbb{R}^2$. See Figure 2.1.

1.4 Overview

The central question in this study asks about the capacity in which the formally limiting PDEs govern the slow-time and long-lattice modulation of the amplitude and phase difference of the discrete systems. The strategy is to investigate the asymptotic behavior of the moduli q_n where εn tends to a fixed value of x as ε tends to zero. The formula for these quantities in terms of the spectral data makes this limit amenable to the theory of Lax and Levermore. For this we need asymptotic descriptions of the spectral density and norming constant in the inverse spectral transform. These are presented in Section 2. We arrive at the problem of maximizing a quadratic functional over positive functions of the spectral variable subordinate to the spectral density. Parameters in this functional are x and t and the spectral data arising from the functions $q(\cdot,t)$ and $\phi'(\cdot,t)$. The solution, the Lax-Levermore maximizer, is presented as the unique solution of a scalar Riemann-Hilbert problem on the unit circle, which is the spectral domain in this study. In the time interval in which the formal PDEs have a solution, this maximizer is characterized by an interval in the spectral domain on which it does not attain either of its constraints. One finds that the endpoints of this interval are equal to the functions $\alpha(x,t)$ and $\beta(x,t)$ given by equations (1.10) (compare [3]). In this manner, the Riemann-Hilbert problem provides a way of inverting the asymptotic spectral transform. We find that, when the spectral data are taken to be the asymptotic form of the data for the discrete systems $\mathcal{S}_\varepsilon$, these endpoints evolve according to the Riemann-invariant form of the formal PDEs. This indicates that the formal PDEs do indeed govern the limiting slow amplitude and phase modulation of the solutions of the discrete systems.

1.5 Remarks on Continuum Limits

The semiclassical continuum limit proposed in this article is to be contrasted with a different sort of continuum limit, which results formally in the continuous defocusing NLS equation for a complex function $P(x,t)$:

$$i\frac{\partial P}{\partial t}+\frac{\partial^2 P}{\partial x^2}-2|P|^2P=0\,. \tag{1.13}$$

The ansatz for an asymptotic expansion of a solution of the DNLS system (1.1) that leads to this result is

$$Q_n(\tau)\sim \varepsilon P(n\varepsilon,\varepsilon^2\tau)+\varepsilon^2P_1(n\varepsilon,\varepsilon^2\tau)+\cdots\,, \tag{1.14}$$

and initial data that are expected to produce solutions with such asymptotics may be prescribed by fixing a complex function P of x and putting

$$Q_n(0)=\varepsilon P(n\varepsilon)\,.$$

One may see that this is reasonable by discretizing the x-variable in the NLS equation, writing

$$\begin{aligned}i\frac{\partial P}{\partial t}+\frac{1}{\varepsilon^2}(P(n\varepsilon+\varepsilon)-2P(n\varepsilon)+P(n\varepsilon-\varepsilon))&\\ -|P(n\varepsilon)|^2(P(n\varepsilon+\varepsilon)+P(n\varepsilon-\varepsilon))&=o\,(\varepsilon)\,,\end{aligned}$$

and then multiplying through by ε^3 and passing to a fast time scale $\tau=t/\varepsilon^2$,

$$\begin{aligned}i\frac{\partial(\varepsilon P)}{\partial\tau}+(\varepsilon P(n\varepsilon+\varepsilon)-2\varepsilon P(n\varepsilon)+\varepsilon P(n\varepsilon-\varepsilon))&\\ -|\varepsilon P(n\varepsilon)|^2(\varepsilon P(n\varepsilon+\varepsilon)+\varepsilon P(n\varepsilon-\varepsilon))&=o\,(\varepsilon^4)\end{aligned}$$

so that the quantities $Q_n(\tau)=\varepsilon P(n\varepsilon,\varepsilon^2\tau)$ approximately satisfy the DNLS system. Observe also that such a discretization of the NLS equation would not resolve the spatial oscillations if initial data of the form

$$Q(x,0)=q(x)\exp\left(\frac{i}{\varepsilon}\phi(x)\right)$$

were taken for some fixed functions q and ϕ of x.

The crucial difference between this ansatz and the semiclassical one is the behavior of the phase difference between sites and the time frequency of oscillation as the lattice spacing $\Delta x=\varepsilon$ tends to zero. This can be seen most clearly by comparing the local wavelike behavior of the two asymptotic forms of solution: According to the ansatz (1.5), solutions are, to leading order in ε, locally asymptotic to a steady oscillation of constant amplitude

$$Q_n(\tau) \sim q\exp(i(kn+\omega\tau+c)) + o(\varepsilon), \quad \varepsilon \to 0,$$

subject to the dispersion relation (1.3). The values of q and k (and therefore also ω) modulate on a long time scale, and this modulation is what the formal PDEs are supposed to describe. In contrast, the ansatz (1.14) implies leading-order local phase asymptotics that are constant in n and τ and a modulus that is asymptotic to a multiple of ε,

$$Q_n(\tau) \sim \varepsilon q \exp(ic) + o(\varepsilon^2), \quad \varepsilon \to 0,$$

in which the oscillations take place only on long space and long time scales. The NLS equation is supposed to describe the slow modulation of the modulus of $Q_n(\tau)/\varepsilon$ and the phase itself, not the phase difference between sites.

One also observes that the ansatz (1.14) is inconsistent with the boundary conditions $|Q_0| = |Q_N| = 1$, which give rise to the finite chain.

The limit from a finite chain to a finite real interval proposed in this article might perhaps be used to approximate the semiclassical continuum limit of an infinite lattice for which the moduli $|Q_n|$ approach 1 as $|n|$ tends to infinity. For example, one may take $1-q(x)$ to be a Gaussian-type function highly localized at $x=\frac{1}{2}$.

2 The Spectral Transform and Its Asymptotics

In this section, we present the spectral method of [12] for the finite DNLS system in the case of subunitary data and propose its leading semiclassical asymptotics. We leave the details of the derivation of the direct and inverse spectral transforms to the appendix. The results in the following outline rely heavily on the material presented there.

2.1 The Spectral Transform

Let $\{Q_n(\tau)\}$ be a solution to the finite DNLS system with $|Q_n(\tau)| < 1$ for $0 < n < N$. Without loss of generality, one may take $Q_0(0) = 1$ and $Q_N(0) = \xi$ with $|\xi| = 1$. Let z be an arbitrary complex parameter, and define the matrices

$$U_n(z,\tau) = \begin{bmatrix} z & \bar{Q}_n(\tau)e^{-2i\tau} \\ Q_n(\tau)e^{2i\tau} & z^{-1} \end{bmatrix}.$$

One forms the so-called transfer matrix

$$T(z,\tau) = \begin{bmatrix} \xi^{1/2} & 0 \\ 0 & \xi^{-1/2} \end{bmatrix} U_N U_{N-1} \cdots U_1,$$

in which $\xi^{1/2}$ is a square root of ξ and considers its trace

$$J(z) = \operatorname{tr} T(z,\tau) = \xi^{\frac{1}{2}} z^{-N} \prod_{k=1}^{N} (z^2 - z_k^2),$$

which is constant in time. The squared roots $\zeta_k = z_k^2$ are the eigenvalues, or "squared eigenvalues," in the spectral transform. They are distinct. Letting $F(z,\tau)$ denote the upper left entry of $T(z,\tau)$, consider the residues $H_k(\tau)$ of $F(z,\tau)/z^2 J(z)$ as a function of z^2:

$$\frac{F(z,\tau)}{J(z)} = z^2 \sum_{k=1}^{N} \frac{H_k(\tau)}{(z^2-\zeta_k)} .$$

These are the associated "norming constants" in the spectral transform. (There is no such object as the reflection coefficient here.) One can show that the set of "unsquared eigenvalues" z_k is equal to the set of values of z for which the following boundary value problem for the discrete evolution of a complex column vector $\vec{u}_n$ has a solution:

$$\vec{u}_{n+1} = U_n \vec{u}_n ; \quad \vec{u}_0 = \begin{bmatrix} z \\ 1 \end{bmatrix}, \quad \vec{u}_{N+1} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

This formulation will be useful in studying the asymptotics of the distribution of eigenvalues.

The inverse spectral transform reconstructs $Q_n(\tau)$ from the eigenvalues and norming constants. It turns out, in the case of subunitary values of Q_n (for $0 < n < N$), that the eigenvalues are unitary and the norming constants are real and positive. Putting $W_k = H_k(0)$, one can define the "tau-functions," which take on a special form in this subunitary case:

$$\Delta_n = \sum_{s\in S_n^N} \prod_{k\in s} W_k \exp[-i(\zeta_k - \zeta_k^{-1})\tau] \prod_{\substack{i\in s,\, j\in s,\\ i\neq j}} |\zeta_i - \zeta_j| , \qquad 1 < n < N ,$$

$$\tilde{\Delta}_n = \sum_{s\in S_n^N} \prod_{k\in s} \zeta_k^{-1} W_k \exp[-i(\zeta_k - \zeta_k^{-1})\tau] \prod_{\substack{i\in s,\, j\in s\\ i\neq j}} |\zeta_i - \zeta_j| , \quad 1 < n < N ,$$

and $\Delta_0 = \tilde{\Delta}_0 = 1$, where S_n^N denotes the set of all order-n subsets of the set of integers $\{1,\ldots,N\}$. In terms of these, the Q_n and their moduli are reconstructed by the formulae

$$Q_n = e^{-2i\tau}(-1)^n \frac{\tilde{\Delta}_n}{\Delta_n}, \quad n = 1,\ldots,N-1, \tag{2.1}$$

$$1 - |Q_n|^2 = \frac{\Delta_{n-1}\Delta_{n+1}}{\Delta_n^2}, \qquad n = 1,\ldots,N-1 . \tag{2.2}$$

In addition, it turns out that

$$W_k = \frac{|F(z_k,0)|}{\prod_{k'\neq k} |\zeta_{k'} - \zeta_k|} , \tag{2.3}$$

and, denoting $|F(z_k,0)|$ by G_k, the expressions for the tau-functions may be rewritten as

$$\Delta_n = \sum_{s\in S_n^N} \prod_{k\in s} G_k \exp[-i(\zeta_k - \zeta_k^{-1})\tau] \prod_{i\in s,\, j\notin s} |\zeta_i - \zeta_j|^{-1}, \tag{2.4}$$

$$\tilde{\Delta}_n = \sum_{s\in S_n^N} \prod_{k\in s} \zeta_k^{-1} G_k \exp[-i(\zeta_k - \zeta_k^{-1})\tau] \prod_{i\in s,\, j\notin s} |\zeta_i - \zeta_j|^{-1}. \tag{2.5}$$

Subsequently, we will be concerned mostly with the quantities

$$G_k \exp[-i(\zeta_k - \zeta_k^{-1})\tau]$$

rather than the W_k. One observes that, since the eigenvalues ζ_k are unitary, these remain positive for all time. It is this property, which holds only in the subunitary case, that makes the formula (2.2) amenable to the theory of Lax and Levermore.

2.2 The Asymptotic Spectral Data

Prescription of the Formulae

In the construction of the continuum limit in Sections 1.2 and 1.3, we prescribed initial data for the DNLS systems $\mathcal{S}_\varepsilon$ by fixing $q(x)$ and $\phi(x)$ and putting $Q_n(0) = q(n\varepsilon)\exp(\frac{1}{\varepsilon}\phi(n\varepsilon))$. Much of the asymptotic analysis, however, is more convenient using the functions $\alpha(x)$ and $\beta(x)$ where (α,β) are related to (q,ϕ') by the transformation (1.10).

We will place the following restrictions on the initial data $\alpha(x)$ and $\beta(x)$: First, $\beta(x) > \alpha(x)$ for $0 < x < 1$ with equality at the endpoints; this is guaranteed by equation (1.10) or (1.11). We assume, in addition, that α attains a local minimum at exactly one point x_1 in $[0,1]$ and that β attains a local maximum at exactly one point x_2 in $[0,1]$. Denoting these extreme values by $\alpha_{\min} = \alpha(x_1)$ and $\beta_{\max} = \beta(x_2)$, we assume in addition that $\beta_{\max} - \alpha_{\min} \le 2\pi$. Thus we may fix a number μ_0 such that $\mu_0 \le \alpha_{\min} < \beta_{\max} \le \mu_0 + 2\pi$. Furthermore, for any value of μ, there exists at most one integer m such that $\alpha_{\min} < \mu + 2m\pi < \beta_{\max}$. If such m exists, then there are exactly two values of x at which either α or β assumes the value $\mu + 2m\pi$. We call these values "turning points" and denote them by $x_-(\mu)$ and $x_+(\mu)$. See Figure 2.1.

We need descriptions of the asymptotic distribution of the eigenvalues $e^{i\mu_k}$ and behavior of the corresponding norming exponents G_k as ε tends to zero. Thus we propose a spectral density ρ and an asymptotic norming exponent $\mathcal{E}$, both functions of an angular variable μ. By this we mean that if $\#_\varepsilon[\mu_1,\mu_2]$ denotes the number of eigenvalues located in the interval $[\mu_1,\mu_2]$, then

$$\#_\varepsilon[\mu_1,\mu_2] \sim \frac{1}{\varepsilon}\int_{\mu_1}^{\mu_2} \rho(\mu)\,d\mu, \quad \varepsilon \to 0,$$

and, given μ_* and an eigenvalue μ_{k_ε} for each of the systems $\mathcal{S}_\varepsilon$ with associated norming constants G_{k_ε}, we have

$$\varepsilon \log G_{k_\varepsilon} \to \mathcal{E}(\mu_*) \quad \text{if } \mu_{k_\varepsilon} \to \mu_* \text{ as } \varepsilon \to 0.$$

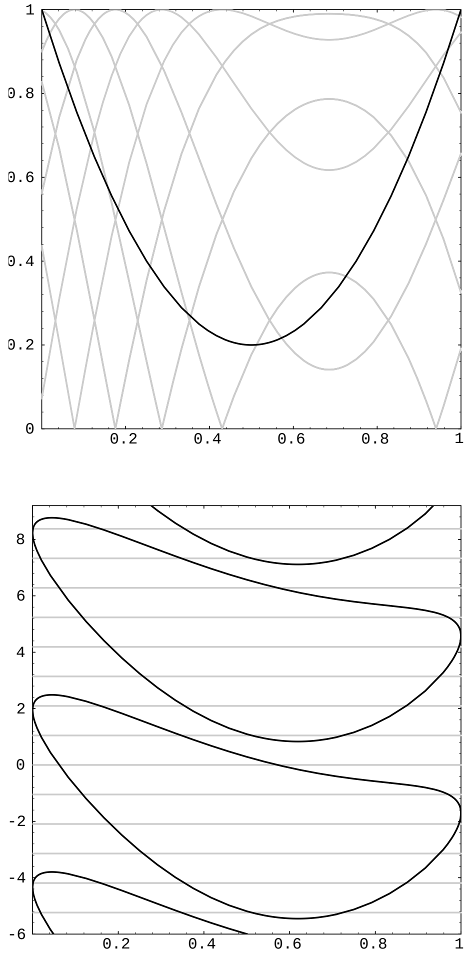

FIGURE 2.1. Riemann invariants and turning points. Top: $q(x)$ is in black and $|\sin((\mu+\phi'(x))/2)|$ in gray for various values of μ. Here q is a parabola and $\phi'(x) = 6\sin(2x+.2)$. Bottom: $\alpha(x)+2\pi m$ and $\beta(x)+2\pi m$ for various integers m in black and the values of μ used above in gray. These data do not satisfy the property that $\beta_{\max}-\alpha_{\min} \leq 2\pi$. For example, there are two turning points for $\mu = 0$ but four turning points for $\mu = 2$.

The reason for expecting the existence of a function $\mathcal{E}$ with this property will be evident from the analysis of the asymptotics of the tau-functions Δ_n in Section 3. The following paragraph gives the proposed prescription for ρ and $\mathcal{E}' = d\mathcal{E}/d\mu$; a brief asymptotic motivation follows it.

We first define a function P of a complex number z and real parameters κ and λ by putting $\chi = (\kappa+\lambda)/2$ and

$$P(\kappa,\lambda;z) = \frac{e^{i\chi}+z}{[(z-e^{i\kappa})(z-e^{i\lambda})]^{1/2}}\,. \tag{2.6}$$

P is defined on the complex plane with a cut from $e^{i\kappa}$ to $e^{i\lambda}$. For points $z = e^{i\mu}$ on the unit circle, P assumes the form

$$P(\kappa,\lambda;e^{i\mu}) = \frac{\cos\left(\frac{\chi-\mu}{2}\right)}{\left[\cos^2\left(\frac{\chi-\mu}{2}\right) - \cos^2\left(\frac{\lambda-\kappa}{4}\right)\right]^{1/2}}\,,$$

and we choose the sign of the square root by taking the denominator to be positive for values of μ in (κ,λ). (Notice that the quantity under the square root sign is positive in this interval.) We now define

$$\rho(\mu) = \frac{1}{2\pi}\int_{x_-(\mu)}^{x_+(\mu)} P\big(\alpha(x),\beta(x);e^{i\mu}\big)\,dx\,, \tag{2.7}$$

$$\mathcal{E}'(\mu) = \frac{i}{2}\left[\int_0^{x_-(\mu)} - \int_{x_+(\mu)}^{1}\right] P\big(\alpha(x),\beta(x);e^{i\mu}\big)\,dx\,, \tag{2.8}$$

for $\mu \in (\alpha_{\min},\beta_{\max})$, and set $\rho(\mu) = 0$ and $\mathcal{E}'(\mu) = 0$ for $\mu \in [\mu_0,\mu_0+2\pi]\setminus(\alpha_{\min},\beta_{\max})$. Since $P(\alpha(x),\beta(x);e^{i\mu})$ is real-valued for $x \in [x_-(\mu),x_+(\mu)]$ and purely imaginary otherwise, these formulae define ρ and $\mathcal{E}'$ as real-valued functions supported on the interval $[\alpha_{\min},\beta_{\max}]$. We will denote their domain by I:

$$I = [\mu_0,\, \mu_0+2\pi]\,.$$

In the asymptotic analysis of the inverse spectral transform, it is $\mathcal{E}'$ that will be needed and not $\mathcal{E}$ itself.

Derivation of the Formulae

We now give a highly abridged account of the derivation of the asymptotic formulae.[2] Recall that the set of values z_k is equal to the set of values of z for which the following boundary value problem has a solution:

$$\vec{u}_{n+1} = U_n\vec{u}_n\,; \quad \vec{u}_0 = \begin{bmatrix} z \\ 1 \end{bmatrix}, \quad \vec{u}_{N+1} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{2.9}$$

where the U_n for initial data in the system $\mathcal{S}_\varepsilon$ are given by

$$U_n = \begin{bmatrix} z & q(n\varepsilon)\exp\left(-\frac{i}{\varepsilon}\phi(n\varepsilon)\right) \\ q(n\varepsilon)\exp\left(\frac{i}{\varepsilon}\phi(n\varepsilon)\right) & z^{-1} \end{bmatrix}.$$

[2] The WKB and numerical analyses of the spectral data are expected to appear in a future paper. One can also refer to [10].

To make the asymptotics of this problem amenable to WKB analysis, one first makes a change of coordinates that eliminates the occurrence of $1/\varepsilon$ in U_n by putting these fast spatial oscillations into the solution vector:

$$\left[u_n^1\ u_n^2\right]^{\mathsf{T}} \mapsto \left[\exp\left(\frac{i\phi(n\varepsilon)}{2\varepsilon}\right)u_n^1\ \exp\left(\frac{-i\phi(n\varepsilon)}{2\varepsilon}\right)u_n^2\right]^{\mathsf{T}} = \check{u}_n\,.$$

In these new coordinates, the matrices U_n are replaced by

$$\check{U}_n(z) = \begin{bmatrix} ze^{i\frac{\psi_n}{2}} & q_n e^{i\frac{\psi_n}{2}} \\ q_n e^{i\frac{\psi_n}{2}} & z^{-1}e^{i\frac{\psi_n}{2}} \end{bmatrix} \tag{2.10}$$

in which $\psi_n = (\phi(n\varepsilon+\varepsilon)-\phi(n\varepsilon))/\varepsilon$ and $q_n = q(n\varepsilon)$. The leading order in ε of $\check{U}_n$ involves the x-derivative ϕ' rather than ϕ itself. (This is favorable since ϕ' is a quantity that naturally appears as one of the functions in the formal system of PDEs.) Since we are only interested in leading-order analysis, we simplify the problem and use only the $o(1)$ part of $\check{U}_n$. Denoting this leading order by V_n, we have $V_n(z) = V(n\varepsilon, z)$, where

$$V(x;z) = \begin{bmatrix} ze^{i\frac{\phi'(x)}{2}} & q(x)e^{i\frac{\phi'(x)}{2}} \\ q(x)e^{-i\frac{\phi'(x)}{2}} & z^{-1}e^{-i\frac{\phi'(x)}{2}} \end{bmatrix}, \tag{2.11}$$

and we consider the approximate problem

$$\vec{v}_{n+1} = V_n\vec{v}_n\,; \quad \vec{v}_0 = \begin{bmatrix} z \\ 1 \end{bmatrix}, \quad \vec{v}_{N+1} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Denoting the eigenvalues of $V(x,z)$ by $\lambda^{\pm}(x,z)$ and corresponding eigenvectors by $\vec{p}^{\,\pm}(x,z)$, we make the crude formal ansatz

$$\vec{v}_n \sim \exp\left(\frac{1}{\varepsilon}S_+(n\varepsilon)\right)\vec{p}^{\,+}(n\varepsilon) + \exp\left(\frac{1}{\varepsilon}S_-(n\varepsilon)\right)\vec{p}^{\,-}(n\varepsilon)\,, \tag{2.12}$$

where S_+ and S_- are functions of x that are to be determined. Letting $\left[c_n^1\ c_n^2\right]^{\mathsf{T}}$ represent the vector $\vec{v}_n$ with respect to the basis $\{\vec{p}^{\,\pm}(n\varepsilon)\}$, the WKB analysis leads to the following asymptotics for the ratio c_n^1/c_n^2:

$$\frac{c_n^1}{c_n^2} \sim \exp\left(\frac{1}{\varepsilon}\int^x \log\frac{\lambda^+(y,z)}{\lambda^-(y,z)}\,dy\right), \quad \varepsilon \to 0\,.$$

Since we have established that the spectrum of the systems $\mathcal{S}_\varepsilon$ is located on the unit circle, we may put $z = e^{i\eta}$. Putting $\sigma = (\alpha+\beta)/2$, the eigenvalues $\lambda^{\pm}(x,e^{i\eta})$ are in this case given by

(2.13)

$$\lambda^{\pm}(x,e^{i\eta}) = \sin\left(\frac{\sigma(x)}{2}-\eta\right) \pm \left[\cos^2\left(\frac{\beta(x)-\alpha(x)}{4}\right) - \cos^2\left(\frac{\sigma(x)}{2}-\eta\right)\right]^{\frac{1}{2}}.$$

One sees that the ratio $[\lambda^+(x,e^{i\eta})]/[\lambda^-(x,e^{i\eta})]$ is unitary if $x \in (x_-(2\eta),x_+(2\eta))$ and positive if $x \notin (x_-(2\eta),x_+(2\eta))$. This gives rise to "oscillatory" and "exponential" x-regions separated by the turning points: Between the turning points, the increment of $\log(c_n^1/c_n^2)$ is imaginary, and outside this interval it is real. This leads one to consider the boundary value problem (2.9) as a condition on the increment of $\arg(c_n^1/c_n^2) \pmod{2\pi}$ over the x-interval $[0,1]$. The asymptotic characterization of the eigenvalues $z_k = e^{i\eta_k}$ thus becomes

$$\frac{1}{\varepsilon}\int_{x_-(2\eta_k)}^{x_+(2\eta_k)} 2\arctan\frac{\left[\cos^2\left(\frac{\sigma(x)}{2}-\eta_k\right)-\cos^2\left(\frac{\beta(x)-\alpha(x)}{4}\right)\right]^{1/2}}{\sin\left(\frac{\sigma(x)}{2}-\eta_k\right)}\,dx \sim 2\pi k\,. \tag{2.14}$$

Replacing η_k with η, differentiating with respect to η, changing to the variable $\mu = 2\eta$, and scaling, one obtains the formula (2.7) for the asymptotic spectral density ρ of (squared) eigenvalues $\zeta_k = z_k^2$ with $\int_0^{2\pi}\rho(\mu)d\mu = 1$.

The formula for the derivative $\mathcal{E}'$ of the asymptotic norming exponent is gotten by integrating the same integrand over the exponential region. At present, there is no argument based on asymptotics that suggests this form for $\mathcal{E}'$. Instead, it is obtained through a formal analogy with results from other problems in asymptotic spectral analysis in which the spectral density and the asymptotic norming exponent are known to be symbolically related; in particular, this is true for the Schrödinger operator (see [8]) and the eigenvalue problem for the Toda lattice (see [3]). Both ρ and $\mathcal{E}'$ display several properties inherited from the properties of the spectral data of the discrete systems. In addition, numerical calculations and some rigorous results have helped to confirm their validity. These are not included in this article. In particular, the following has been established:

PROPOSITION 2.1 *Let $[a,b]$ be an oscillatory interval for data $q(x)$ and $\phi(x)$ and spectral value z, and put $\underline{n} = \lceil a/\varepsilon\rceil$ and $\overline{n} = \lfloor b/\varepsilon\rfloor$. Let $\hat{u}_n$ represent the vector $\check{u}_n$ in eigenvector $\{\vec{p}_n^{\,\pm}\}$ coordinates for the matrix transformation $\check{U}_n$, and let the matrix $\hat{U}_n$ represent $\check{U}_n$ with respect to the bases $\{\vec{p}_n^{\,\pm}\}$ in the domain and $\{\vec{p}_{n+1}^{\,\pm}\}$ in the range so that $\check{u}_{n+1} = \check{U}_n\check{u}_n$ becomes*

$$\hat{u}_{n+1} = \hat{U}_n\hat{u}_n\,.$$

Let $\hat{u}_{\underline{n}} = \left[c_{\underline{n}}^1\; c_{\underline{n}}^2\right]$ be fixed. Then

$$\arg\left(\frac{c_{\overline{n}}^1}{c_{\overline{n}}^2}\right) = \frac{1}{\varepsilon}\int_a^b \arg\frac{\lambda^+(y,z)}{\lambda^-(y,z)}\,dy + o\,(1)\,, \quad \varepsilon \to 0\,.$$

Remarks on the WKB Analysis

A couple of comments comparing the present WKB analysis to that of Bronski [2] might be useful to the reader. Bronski considers the semiclassical scaling of the (continuous) non-self-adjoint Zakharov-Shabat eigenvalue problem

$$i\varepsilon\vec{v}_x = M(x,\lambda)\vec{v}\,.$$

First, a remark on the leading-order results. Bronski uses the ansatz

$$\vec{v} = e^{-i\phi(x,\lambda)/\varepsilon}(\vec{v}^0 + \varepsilon\vec{v}^1 + \cdots)$$

and finds that its formal validity necessarily implies that $v^0(x,\lambda)$ is an eigenvector of $M(x,\lambda)$—in other words, that $\vec{v}$ is, to leading order, an eigenvector of M. Consider, however, the ansatz (2.12) for our discrete problem. Leading-order analysis produces

$$S_\pm(x,z) = \int^x \log\lambda^\pm(y,z)dy\,.$$

Thus, if one of λ^+ or λ^- is larger in magnitude than the other, then the WKB analysis proposes that, to leading order, $\vec{v}_n(z)$ is indeed an eigenvector of $V(n\varepsilon,z)$. However, if λ^+ and λ^- are complex conjugates, as in the oscillatory x-regions in our problem, then this is not the case. Indeed, the fact that the ratio of the eigenvector coordinates of $\vec{v}_n$ is a unitary oscillating scalar function of n is the key to the derivation of the spectral density.

Regarding higher-order results, the difficulty in our discrete problem is the messy dependence of the matrices $\check{U}_n$ on neighboring lattice sites: Recall that V_n is only the leading order; in the exact problem, the matrices, as functions of $x = n\varepsilon$, have local expansions in ε. In fact, the author has studied higher-order WKB-type expansions in the vicinity of a turning point and has come up with no formally valid asymptotics, much less been able to perform matching between regions.

3 Asymptotics of the Inverse Spectral Transform

We now describe the formal details of the construction of the Lax-Levermore maximization problem associated with the asymptotics of the moduli $|Q_n(\tau)|$ in the continuum limit. Let $\lfloor y\rfloor$ denote the largest integer not greater than y. We wish to understand the behavior of $|Q_{\lfloor x/\varepsilon\rfloor}|$ as a function of x as $\varepsilon \to 0$. From formula (2.2), we find that

$$\begin{aligned}\log(1-|Q_n|^2) &= \log\Delta_{n+1} - 2\log\Delta_n + \log\Delta_{n-1}\\ &= \frac{1}{\varepsilon^2}\left(\varepsilon^2\log\Delta_{n+1} - 2\varepsilon^2\log\Delta_n + \varepsilon^2\log\Delta_{n-1}\right),\end{aligned}$$

which suggests that the quantity $\varepsilon^2\log\Delta_{\lfloor x/\varepsilon\rfloor}$ should have a limit, and if this limit is well enough behaved, we may be able to calculate

$$\lim_{\varepsilon\to 0}\log\left(1-|Q_{\lfloor x/\varepsilon\rfloor}|^2\right) = \frac{d^2}{dx^2}\lim_{\varepsilon\to 0}\varepsilon^2\log\Delta_{\lfloor x/\varepsilon\rfloor}\,.$$

In the original theory of Lax and Levermore for the dispersion-free limit of the Korteweg–de Vries equation [8], the quantity analogous to $\varepsilon^2\log\Delta_{\lfloor x/\varepsilon\rfloor}$ is shown to be convex in x, and one can infer weak convergence of the quantity analogous to $\log(1-|Q_{\lfloor x/\varepsilon\rfloor}|^2)$. The analysis there, in fact, indicates strong convergence to the solution of Burgers' equation for as long as it exists as a single-valued function. This will be the goal in our analysis, too, although in our discrete case, we have no such convexity property to guarantee weak convergence. We will proceed below with the formal mathematics nonetheless. In the Riemann-Hilbert problem of Section 4, which arises from this formula for $|Q_n|$ alone, we will see how the convergence of *both* the modulus and phase derivative to the solution of the formal system of PDEs follows from a study of the solution of this Riemann-Hilbert problem. Such is also the case in the continuum limit of the Toda lattice [3].

We now use the expression (2.4) for Δ_n and pass to a slow time scale $t = \varepsilon\tau$:

$$\begin{aligned}\Delta_n\left(\frac{t}{\varepsilon}\right) &= \sum_{s\in S_n^N}\prod_{k\in s} G_k \exp\left[-i(\zeta_k-\zeta_k^{-1})\frac{t}{\varepsilon}\right]\prod_{i\in s,\, j\notin s}|\zeta_i-\zeta_j|^{-1}\\ &= \sum_{s\in S_n^N}\exp\left\{\frac{1}{\varepsilon^2}\left[\varepsilon\sum_{k\in s}\left(\varepsilon\log G_k - i(\zeta_k-\zeta_k^{-1})t\right)-\varepsilon^2\sum_{i\in s,\, j\notin s}\log|\zeta_i-\zeta_j|\right]\right\}\\ &= \sum_{s\in S_n^N}\exp\left(\frac{1}{\varepsilon^2}\mathcal{Q}_s\right),\end{aligned}$$

in which

$$\mathcal{Q}_s = \varepsilon\sum_{k\in s}\left(\varepsilon\log G_k - i(\zeta_k-\zeta_k^{-1})t\right)-\varepsilon^2\sum_{j\in s, i\notin s}\log|\zeta_i-\zeta_j|$$

and S_n^N is the set of all order-n subsets of $\{1,\dots,N\}$.

Observing that each term of the sum giving Δ_n is positive and letting $\mathcal{Q}_n^* = \max_{s\in S_n^N}\{\mathcal{Q}_s\}$, we write the inequalities

$$\exp\left(\frac{1}{\varepsilon^2}\mathcal{Q}_n^*\right)\le \Delta_n \le \binom{N}{n}\exp\left(\frac{1}{\varepsilon^2}\mathcal{Q}_n^*\right),$$

whence

$$\mathcal{Q}_n^* \le \varepsilon^2\log\Delta_n \le \varepsilon^2\log\binom{N}{n}+\mathcal{Q}_n^*,$$

and notice that $\lim_{\varepsilon\to 0}\varepsilon^2\log\binom{N}{n} = 0$. This reduces the problem of finding $\lim_{\varepsilon\to 0}\varepsilon^2\log\Delta_{\lfloor x/\varepsilon\rfloor}$ to finding the limiting behavior of $\mathcal{Q}^*_{\lfloor x/\varepsilon\rfloor}$ for any value of $x\in[0,1]$ that is fixed as $\varepsilon\to 0$. This is really the crux of the argument that Lax and Levermore used to reduce the asymptotic behavior of an analogous tau-function for the KdV equation to a minimization problem.

Following the standard procedure, we next replace the exact spectral data by its leading-order asymptotics proposed by the WKB analysis:

$$\mathcal{Q}_s \sim \varepsilon\sum_{k\in s}\mathcal{E}(\zeta_k,t)-\varepsilon^2\sum_{j\in s,i\notin s}\log|\zeta_i-\zeta_j|,$$

where the time-dependent asymptotic norming exponent is defined by

$$\mathcal{E}(\zeta,t) := \mathcal{E}(\zeta)-i(\zeta-\zeta^{-1})t\,. \tag{3.1}$$

Putting $\zeta = e^{i\mu}$, we can represent $\mathcal{Q}_s$ as an integral with respect to a singular spectral measure on the interval I:

$$\mathcal{Q}_s \sim \int_I \mathcal{E}(\mu,t)\varepsilon \sum_{k\in s}\delta(\mu-\mu_k)d\mu - \int_I\int_I \log|e^{i\mu}-e^{i\gamma}|\varepsilon^2 \sum_{j\in s,\, i\notin s}\delta(\mu-\mu_i)\delta(\gamma-\gamma_j)d\mu\, d\gamma\,.$$

Now,

$$\int_{\mu_1}^{\mu_2}\varepsilon\sum_{j\in s}\delta(\mu-\mu_j)d\mu \le \int_{\mu_1}^{\mu_2}\varepsilon\sum_{j=1}^{N}\delta(\mu-\mu_j)d\mu \sim \int_{\mu_1}^{\mu_2}\rho(\mu)d\mu\,, \quad \varepsilon\to 0\,,$$

for any subinterval $[\mu_1,\mu_2]$ of I (recall that $N=\lfloor 1/\varepsilon\rfloor$), and if for each ε $s_\varepsilon \subset \{1,\dots,N\}$ is chosen such that $|s_\varepsilon| = \lfloor x/\varepsilon\rfloor$ for some fixed $x\in[0,1]$, then

$$\int_I \varepsilon\sum_{j\in s_\varepsilon}\delta(\mu-\mu_j)d\mu \sim x\,, \quad \varepsilon\to 0\,.$$

This suggests the next step (again, [3, 8] are prototypes), which is to replace the spectral measures $\varepsilon\sum_{j\in s}\delta(\mu-\mu_j)d\mu$ with measures $\psi(\mu)d\mu$ where ψ belongs to the set $\mathcal{A}$ of measurable functions defined on I such that

$$0\le\psi\le\rho \quad\text{and}\quad \int_I \psi(\mu)d\mu = x$$

(compare [3]) and to seek ψ_* which maximizes the quantity

$$\mathcal{Q}(\psi;x,t) := \int_I (\mathcal{E}(\mu)+2t\sin(\mu))\psi(\mu)d\mu - \int_I\int_I \log|e^{i\mu}-e^{i\gamma}|(\rho-\psi)(\gamma)\psi(\mu)d\gamma\, d\mu\,,$$

which one may express in the compact form

$$\mathcal{Q}(\psi) = (\mathcal{E}(\cdot,t),\psi) - (\mathcal{P}(\rho-\psi),\psi)\,, \tag{3.2}$$

where the quadratic functional $\mathcal{P}$ is defined by

$$(\mathcal{P}\psi)(\mu) := \int_I \log|e^{i\mu}-e^{i\gamma}|\psi(\gamma)d\gamma \tag{3.3}$$

and (ψ_1,ψ_2) means $\int_I\psi_1(\mu)\psi_2(\mu)d\mu$. Since $\mathcal{P}$ is a negative definite quadratic functional, $\mathcal{Q}$ is strictly concave, and since the set $\mathcal{A}$ is convex in the linear space of all functions on I, $\mathcal{Q}$ can attain its maximal value at only one function in $\mathcal{A}$.

The Euler-Lagrange equation associated to (3.2), subject to the constraint $\int_I\psi(\mu)d\mu = x$, is

$$\mathcal{E}(\mu,T)+\mathcal{P}(2\psi-\rho)(\mu) \equiv l\,, \tag{3.4}$$

the left-hand side being the variational gradient $\delta\mathcal{Q}$ of $\mathcal{Q}$ at ψ and l being any real constant. A function ψ in $\mathcal{A}$ partitions I into four sets, I_0, I_1, I_2, and I_3 such that

$$\begin{cases} \rho(\mu) = 0 & \Rightarrow \mu \in I_0 \\ \psi(\mu) = 0\,,\ \mu \notin I_0\,, & \Rightarrow \mu \in I_1 \\ \psi(\mu) = \rho(\mu)\,,\ \mu \notin I_0\,, & \Rightarrow \mu \in I_2 \\ 0 < \psi(\mu) < \rho(\mu) & \Rightarrow \mu \in I_3\,, \end{cases}$$

and it is elementary to show that ψ maximizes $\mathcal{Q}$ in $\mathcal{A}$ if and only if there exists a number l such that

$$\begin{cases} \delta\mathcal{Q}\,(\psi) \le l & \text{on } I_1 \text{ (a.e.)} \\ \delta\mathcal{Q}\,(\psi) \ge l & \text{on } I_2 \text{ (a.e.)} \\ \delta\mathcal{Q}\,(\psi) = l & \text{on } I_3 \text{ (a.e.)}\,. \end{cases}$$

4 The Riemann-Hilbert Problem

Differentiating the Euler-Lagrange equation (3.4) with respect to the spectral parameter μ, one obtains

$$\mathcal{E}\,'(\mu,t) + \text{P.V.}\,\frac{1}{2}\int_I \frac{\sin(\mu-\gamma)}{1-\cos(\mu-\gamma)}(2\psi(\gamma)-\rho(\gamma))d\gamma = 0\,,$$

and, by setting $\tilde{\psi} = 2\psi - \rho$, this becomes

$$\mathcal{E}\,'(\mu,t) + \pi(\mathcal{H}\,\tilde{\psi})(\mu) = 0\,, \tag{4.1}$$

where $\mathcal{H}$ is the Hilbert transform on the unit circle.

Thus we have a scalar Riemann-Hilbert problem for $\tilde{\psi}$ in which (4.1) must be satisfied on I_3 and $\tilde{\psi}$ is subject to the two constraints

$$-\rho(\mu) \le \tilde{\psi}(\mu) \le \rho(\mu) \quad \text{for all } \mu \in I\,, \tag{4.2}$$

$$\int_I \tilde{\psi}(\gamma)d\gamma = 2x - 1\,. \tag{4.3}$$

Continuing to follow Lax and Levermore, we impose upon $\tilde{\psi}$ the ansatz that I_3 is an interval $(\kappa,\lambda) \subset [\alpha_{\min},\beta_{\max}]$ whose endpoints depend on x and t, with complement $J = (J_0 \cup J_1 \cup J_2) \subset I$ where $J_1 = (\alpha_{\min},\kappa]$ and $J_2 = [\lambda,\beta_{\max})$ such that

$$\begin{cases} (\mathcal{H}\,\tilde{\psi})(\mu) = -\frac{1}{\pi}\mathcal{E}\,'(\mu,t) & \text{for } \mu \in (\kappa,\lambda) \\ \tilde{\psi}(\mu) = \pm\rho(\mu) & \text{for } \mu \in J_1 \\ \tilde{\psi}(\mu) = \pm\rho(\mu) & \text{for } \mu \in J_2\,. \end{cases} \tag{4.4}$$

The choice of the $\pm$ sign is left undetermined at this point. Observe that $J_0 = I_0$, $J_1 \cup J_2 = I_1 \cup I_2$, and $(\lambda,\kappa) = I_3$. Since $\rho = 0$ on J_0 by its definition, $\tilde{\psi} = 0$ on J_0 also. The strategy to construct such a function $\tilde{\psi}$ is to exploit the fact that if

H is a holomorphic function defined on the open unit disk and h is a complex-valued L^p function on the interval I with $p \geq \frac{1}{2}$ such that $h(\mu) = \lim_{r\to 1} H(re^{i\mu})$ and $\operatorname{Im} H(0) = 0$, then $\operatorname{Im} h = \mathcal{H}\,(\operatorname{Re} h)$. H is to be constructed such that

$$\begin{cases} \operatorname{Im} h(\mu) = -\frac{1}{\pi}\mathcal{E}\,'(\mu,t) & \text{for } \mu \in (\kappa,\lambda) \\ \operatorname{Re} h(\mu) = \pm\rho(\mu) & \text{for } \mu \in J_1 \\ \operatorname{Re} h(\mu) = \pm\rho(\mu) & \text{for } \mu \in J_2\,. \end{cases} \tag{4.5}$$

One can write down such a function with the aid of an auxiliary function of z with parameters κ and λ: Putting $\chi = (\kappa+\lambda)/2$, define

$$R(\kappa,\lambda;z) = \frac{e^{i\chi}-z}{[(z-e^{i\kappa})(z-e^{i\lambda})]^{1/2}}\,. \tag{4.6}$$

R is defined on the complex plane minus a cut from $e^{i\kappa}$ to $e^{i\lambda}$. The restriction of this function to the unit circle is

$$R(\kappa,\lambda;e^{i\mu}) = \frac{\sin\left(\frac{\chi-\mu}{2}\right)}{\left[\sin^2\left(\frac{\chi-\mu}{2}\right) - \sin^2\left(\frac{\lambda-\kappa}{4}\right)\right]^{1/2}} \quad \text{for } \mu \in I\,, \tag{4.7}$$

which is purely imaginary whenever $\kappa < \mu < \lambda$ and real for values of μ in J. We choose the sign of the square root by taking values of the denominator of $R(\kappa,\lambda,e^{i\mu})$ to lie on the negative imaginary axis. Using the theory of the Poisson kernel, one can write down the function H that we seek:

$$\begin{aligned} H(z) = R(\kappa,\lambda;z)^{-1}\Bigg\{ &\frac{1}{2\pi}\int_J \pm\rho(\gamma)R(\kappa,\lambda;e^{i\gamma})\left(\frac{e^{i\gamma}+z}{e^{i\gamma}-z}\right)d\gamma \\ &+ \frac{1}{2\pi}\int_\kappa^\lambda \frac{1}{\pi i}\mathcal{E}\,'(\gamma,t)R(\kappa,\lambda;e^{i\gamma})\left(\frac{e^{i\gamma}+z}{e^{i\gamma}-z}\right)d\gamma\Bigg\}\,. \end{aligned} \tag{4.8}$$

The function of z in braces has the property that the limiting values of its real part as z tends to the unit circle are

$$\begin{cases} \frac{1}{\pi i}\mathcal{E}\,'(\mu,t)R(\kappa,\lambda;e^{i\mu}) & \text{for } \mu \in (\kappa,\lambda) \\ \pm\rho(\mu)R(\kappa,\lambda;e^{i\mu}) & \text{for } \mu \in J_1 \\ \pm\rho(\mu)R(\kappa,\lambda;e^{i\mu}) & \text{for } \mu \in J_2\,. \end{cases}$$

Upon multiplying by $R(\kappa,\lambda;z)^{-1}$, one sees that the properties (4.5) of h hold. One can now take the proposed solution $\tilde{\psi}$ of the Riemann-Hilbert problem (4.4) to be equal to $\mathrm{Re}\, h$:

(4.9)
$$\begin{aligned}
&\tilde{\psi}(\mu)\\
&\quad = \mathrm{Re} \lim_{r\to 1} H(re^{i\mu})\\
&\quad = \begin{cases} R(\kappa,\lambda;e^{i\mu})^{-1}\Big\{ \dfrac{1}{2\pi}\displaystyle\int_J \pm\rho(\gamma) R(\kappa,\lambda;e^{i\gamma}) \dfrac{i\sin(\mu-\gamma)}{1-\cos(\mu-\gamma)}\,d\gamma \\ \qquad\qquad + \mathrm{P.V.}\,\dfrac{1}{2\pi}\displaystyle\int_\kappa^\lambda \dfrac{1}{\pi i}\mathcal{E}'(\gamma,t) R(\kappa,\lambda;e^{i\gamma}) \dfrac{i\sin(\mu-\gamma)}{1-\cos(\mu-\gamma)}\,d\gamma \Big\} \\ \quad \text{for } \mu\in(\kappa,\lambda)\,, \\ \pm\rho(\mu) \quad \text{for } \mu\in J\,. \end{cases}
\end{aligned}$$

Its Hilbert transform is

(4.10)
$$\begin{aligned}
&(\mathcal{H}\tilde{\psi})(\mu)\\
&\quad = \mathrm{Im} \lim_{r\to 1} H(re^{i\mu})\\
&\quad = \begin{cases} -\frac{1}{\pi}\mathcal{E}'(\mu,T) \quad \text{for } \mu\in(\kappa,\lambda)\,, \\ \dfrac{1}{i}R(\kappa,\lambda;e^{i\mu})^{-1}\Big\{ \mathrm{P.V.}\,\dfrac{1}{2\pi}\displaystyle\int_J \pm\rho(\gamma) R(\kappa,\lambda;e^{i\gamma}) \dfrac{i\sin(\mu-\gamma)}{1-\cos(\mu-\gamma)}\,d\gamma \\ \qquad\qquad + \dfrac{1}{2\pi}\displaystyle\int_\kappa^\lambda \dfrac{1}{\pi i}\mathcal{E}'(\gamma,t) R(\kappa,\lambda;e^{i\gamma}) \dfrac{i\sin(\mu-\gamma)}{1-\cos(\mu-\gamma)}\,d\gamma \Big\} \\ \quad \text{for } \mu\in J\,. \end{cases}
\end{aligned}$$

Values of κ and λ must now be determined so that the constraints (4.2) and (4.3) are satisfied.

We propose values of κ and λ and a choice of plus or minus sign applied to ρ in the expression for the function $\tilde{\psi}$ and show that the result gives the maximizer we seek. For a fixed value of t, let $\alpha(\cdot,t)$ and $\beta(\cdot,t)$ be data whose asymptotic spectral transform gives rise to the density ρ and the asymptotic norming exponent $\mathcal{E}(\cdot,t)$, if such data exist. Recall that, because of (1.10), $\alpha(x,t)\le\beta(x,t)$ with equality only at $x=0$ and $x=1$. Given values of the parameters x and t in the Riemann-Hilbert problem, we define values of κ and λ in the solution by putting $\kappa=\alpha(x,t)$ and $\lambda=\beta(x,t)$. We then choose the sign applied to ρ in the interval J_i for $i=1,2$ to be positive (respectively, negative) if $x>x_i$ (respectively, $x<x_i$):

$$\rho \text{ in } J_i \quad \text{if } x>x_i\,, \qquad -\rho \text{ in } J_i \quad \text{if } x<x_i\,. \tag{4.11}$$

We will often suppress the t-dependence and refer to $\alpha(\cdot,t)$ as α and to $\beta(\cdot,t)$ as β.

Let us consider the expression in braces in formulae (4.9) and (4.10). Recalling the definitions of ρ, $\mathcal{E}'$, and R, we see that this is a double integral over the shaded region in $y\gamma$-space, illustrated in Figure 4.1. Using the sign of ρ proposed above and reversing the order of integration, the expression takes the form

$$\frac{i}{2\pi}\left[\int_0^x - \int_x^1\right]\text{P.V.}\int_{C_y}\frac{1}{2\pi}P(\alpha(y),\beta(y);e^{i\gamma}) \times R(\alpha(x),\beta(x);e^{i\gamma})\frac{\sin(\mu-\gamma)}{1-\cos(\mu-\gamma)}\,d\gamma\,dy\,.$$

where C_y is the portion of the γ-interval I contained in the shaded region of integration. One observes that C_y is the portion of I on which the integrand is real. Thus the principal value as a function of μ is the Hilbert transform of

$$\operatorname{Re}P(\alpha(y),\beta(y);e^{i\gamma})R(\alpha(x),\beta(x);e^{i\gamma})$$

and is thus equal to

$$\operatorname{Im}P(\alpha(y),\beta(y);e^{i\mu})R(\alpha(x),\beta(x);e^{i\mu})\,.$$

The integration with respect to y for a fixed value of μ now takes place over the non-shaded region in Figure 4.1. Multiplying by $iR(\alpha(x),\beta(x);e^{i\mu})^{-1}$, the proposed solution $\tilde{\psi}$ to the Riemann-Hilbert problem at (x,t) for values of μ in the spectral interval $[\alpha_{\min},\beta_{\max}]$ now takes the simple form

$$\tilde{\psi}(\mu) = \frac{1}{2\pi}\left[\int_0^x - \int_x^1\right]\operatorname{Re}P(\alpha(y,t),\beta(y,t);e^{i\mu})dy\,. \tag{4.12}$$

Indeed, one can check (with the aid of Figure 4.1) that this is valid not only in the interval $(\alpha(x),\beta(x))$ but also in the intervals J_1 and J_2 on which it coincides with either $\rho(\mu)$ or $-\rho(\mu)$ according to the proposed stipulation. The Hilbert transform of this proposed solution is

$$(\mathcal{H}\,\tilde{\psi})(\mu) = \frac{1}{2\pi}\left[\int_0^x - \int_x^1\right]\operatorname{Im}P(\alpha(y,t),\beta(y,t);e^{i\mu})\,dy\,. \tag{4.13}$$

This is also valid in the entire spectral interval.

THEOREM 4.1 *Assume that functions $\alpha(x,t)$ and $\beta(x,t)$ exist as defined in* (4.11), *with α possessing a unique minimum and β possessing a unique maximum for some open time interval. Let $\tilde{\psi}$ be the solution of the Riemann-Hilbert problem posed at point x at time t. Then, for times in this interval, the following statements hold:*

(i) *For $\mu \in (\alpha(x,t),\beta(x,t))$, $-\rho(\mu) < \tilde{\psi}(\mu) < \rho(\mu)$.*
(ii) $\int_I \tilde{\psi}(\gamma)\,d\gamma = 2x-1$.
(iii) $\psi_* = \frac{\tilde{\psi}-\rho}{2}$ *maximizes* $\mathcal{Q}$.
(iv) *$\alpha(x,t)$ and $\beta(x,t)$ evolve according to the differential equations*

$$\alpha_t = f(\alpha,\beta)\alpha_x\,, \qquad \beta_t = f(\beta,\alpha)\beta_x\,,$$

in which

$$f(\mu,\gamma) = \sin(\mu) - \sin\left(\frac{\mu+\gamma}{2}\right).$$

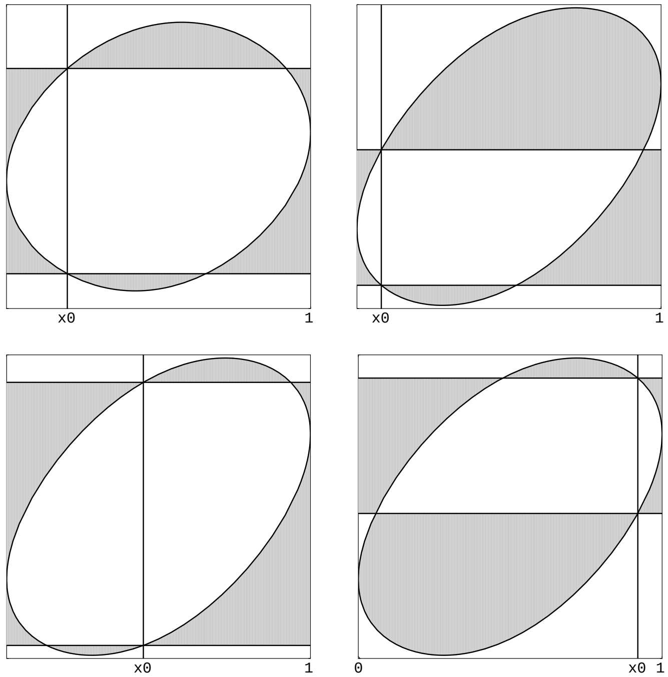

FIGURE 4.1. Real (gray) and imaginary (white) regions for the function $P(\alpha(y),\beta(y),e^{i\mu})R(\alpha(x),\beta(x),e^{i\mu})$ in various scenarios. The lower function is $\alpha(y)$ and the upper is $\beta(y)$. $\alpha(x_0)$ and $\beta(x_0)$ are the proposed values of κ and λ in the solution $\tilde{\psi}$ of the Riemann-Hilbert problem at $x = x_0$.

PROOF: (i) It is evident from formula (4.12) for $\tilde{\psi}$ and the definition of ρ that this constraint is satisfied.

(ii) To compute $\int_I \tilde{\psi}(\mu)\,d\mu$, one uses formula (4.12) and reverses the order of integration:

$$\int_I \tilde{\psi}(\mu)d\mu = \left[\int_0^x - \int_x^1\right]\int_{\alpha(y)}^{\beta(y)} \frac{1}{2\pi}P(\alpha(y),\beta(y);e^{i\mu})d\mu\, dy\,.$$

The inner integral can be done by contour integration, and the result is 1 for any value of y. Integrating with respect to y then gives $2x-1$.

(iii) Recalling that the derivative of the variational gradient $\delta\mathcal{Q}$ of the quadratic functional $\mathcal{Q}$ is equal to

$$\frac{d}{d\mu}\delta\mathcal{Q}\,(\mu) = \mathcal{E}\,'(\mu,t) + \pi(\mathcal{H}\,\tilde{\psi})(\mu)$$

and using the formulae for $\mathcal{E}'$ (2.8) and $\mathcal{H}(\tilde{\psi})$ (4.13), we find that

$$\frac{d}{d\mu}\delta\mathcal{Q}(\mu) = \int_{x_-(\mu)}^{x} \operatorname{Im} P(\alpha(y),\beta(y);e^{i\mu})\,dy\,.$$

($x_-(\mu)$ may be replaced by $x_+(\mu)$ since P is real-valued in $[x_-(\mu),x_+(\mu)]$.) One can check that $\operatorname{Im} P(\alpha(y),\beta(y);e^{i\mu})$ is positive if $\mu\in(\alpha_{\min},\alpha(y))$ and negative if $\mu\in(\beta(y),\beta_{\max})$. Using these facts (and the aid of Figure 4.1), one can verify that

$$\begin{aligned}
&\frac{d}{d\mu}\delta\mathcal{Q}(\mu)<0 \quad \text{if } (x<x_1 \text{ and } \mu<\alpha(x)) \text{ or } (x>x_2 \text{ and } \mu>\beta(x))\,,\\
&\frac{d}{d\mu}\delta\mathcal{Q}(\mu)>0 \quad \text{if } (x>x_1 \text{ and } \mu<\alpha(x)) \text{ or } (x<x_2 \text{ and } \mu>\beta(x))\,,\\
&\frac{d}{d\mu}\delta\mathcal{Q}(\mu)=0 \quad \text{if } \alpha(x)<\mu<\beta(x)\,.
\end{aligned}$$

We may infer from this the existence of a real number l such that, for values of μ in the support of ρ,

$$\begin{aligned}
&\delta\mathcal{Q}(\mu)\le l \quad \text{if } \psi_*(\mu)=-\rho(\mu) \text{ or } \mu\in I_1\,,\\
&\delta\mathcal{Q}(\mu)\ge l \quad \text{if } \psi_*(\mu)=\rho(\mu) \text{ or } \mu\in I_2\,,\\
&\delta\mathcal{Q}(\mu)= l \quad \text{if } -\rho(\mu)<\psi_*(\mu)<\rho(\mu) \text{ or } \mu\in(\alpha(x),\beta(x))\,.
\end{aligned}$$

As already mentioned at the end of Section 3, this proves that ψ_* is the unique maximizer of $\mathcal{Q}$.

(iv) The constraints (4.2) and (4.3) impose relations between κ and λ. First, the constraint that $-\rho(\mu)\le\tilde{\psi}(\mu)\le\rho(\mu)$ implies that $\tilde{\psi}(\chi)<\infty$, and this gives

$$\int_I \pm\rho(\gamma)R(e^{i\gamma})\frac{\sin(\chi-\gamma)}{2\sin^2\left(\frac{\chi-\gamma}{2}\right)}\,d\gamma + \text{P.V.}\int_\kappa^\lambda \frac{1}{\pi i}\mathcal{E}'(\gamma,t)R(e^{i\gamma})\frac{\sin(\chi-\gamma)}{2\sin^2\left(\frac{\chi-\gamma}{2}\right)}\,d\gamma = 0\,.$$

By using the definition (4.7) of R, this condition becomes

$$F(\kappa,\lambda,x,t)=0\,,$$

where F (whose dependence on x is actually trivial) is defined by

(4.14)
$$\begin{aligned}
F(\kappa,\lambda,x,t) = &\int_I \pm\rho(\gamma)\frac{\sin(\chi-\gamma)}{\left[\sin^2\left(\frac{\chi-\gamma}{2}\right)-\sin^2\left(\frac{\lambda-\kappa}{4}\right)\right]^{1/2}\sin\left(\frac{\chi-\gamma}{2}\right)}\,d\gamma\\
&+\int_\kappa^\lambda \frac{1}{\pi i}\mathcal{E}'(\gamma,t)\frac{\sin(\chi-\gamma)}{\left[\sin^2\left(\frac{\chi-\gamma}{2}\right)-\sin^2\left(\frac{\lambda-\kappa}{4}\right)\right]^{1/2}\sin\left(\frac{\chi-\gamma}{2}\right)}\,d\gamma\,.
\end{aligned}$$

Second, we require that $\int_0^{2\pi}\tilde{\psi}(\mu)d\mu = 2x-1$. Thus we compute this integral:

$$\begin{aligned}
&\int_0^{2\pi}\tilde{\psi}(\mu)d\mu \\
&= \int_I \pm\rho(\mu)d\mu \\
&\quad + \int_\kappa^\lambda R(e^{i\mu})\left\{\frac{1}{2\pi}\int_I \rho(\gamma)R(e^{i\gamma})\frac{i\sin(\mu-\gamma)}{1-\cos(\mu-\gamma)}\,d\gamma\right. \\
&\qquad\qquad \left. +\,\text{P.V.}\,\frac{1}{2\pi}\int_\kappa^\lambda \frac{1}{\pi i}\mathcal{E}'(\gamma,t)R(e^{i\gamma})\frac{i\sin(\mu-\gamma)}{1-\cos(\mu-\gamma)}\,d\gamma\right\}d\mu \\
&= \int_I \rho(\mu)d\mu - \int_I \pm\rho(\gamma)R(e^{i\gamma})\frac{1}{2\pi}\int_\kappa^\lambda R(e^{i\mu})^{-1}\frac{i\sin(\gamma-\mu)}{1-\cos(\gamma-\mu)}\,d\mu\,d\gamma \\
&\quad - \int_\kappa^\lambda \frac{1}{\pi i}\mathcal{E}'(\gamma,t)R(e^{i\gamma})\text{P.V.}\frac{1}{2\pi}\int_\kappa^\lambda R(e^{i\mu})^{-1}\frac{i\sin(\gamma-\mu)}{1-\cos(\gamma-\mu)}\,d\mu\,d\gamma\,.
\end{aligned}$$

The inner integrals in the second and third summands of this last expression are identical except that γ is contained in different domains. They can be computed using the theory of the Poisson kernel. Observing that $R(0)=1$, we obtain $\text{Re}\,R(e^{i\mu})^{-1}-1$ for the integral, which, by the properties of R, is equal to $R(e^{i\mu})^{-1}-1$ for $\mu\in I$ and -1 for $\mu\in(\kappa,\lambda)$. The expression thus simplifies to

$$\int_0^{2\pi}\tilde{\psi}(\mu)d\mu = \int_I \pm\rho(\gamma)R(e^{i\gamma})d\gamma + \int_\kappa^\lambda \frac{1}{\pi i}\mathcal{E}'(\gamma,t)R(e^{i\gamma})d\gamma\,.$$

By setting

$$\begin{aligned}
G(\kappa,\lambda,x,t) &= \int_I \pm\rho(\gamma)\frac{\sin\left(\frac{\chi-\gamma}{2}\right)}{\left[\sin^2\left(\frac{\chi-\gamma}{2}\right)-\sin^2\left(\frac{\lambda-\kappa}{4}\right)\right]^{1/2}}\,d\gamma \\
&\quad + \int_\kappa^\lambda \frac{1}{\pi i}\mathcal{E}'(\gamma,t)\frac{\sin\left(\frac{\chi-\gamma}{2}\right)}{\left[\sin^2\left(\frac{\chi-\gamma}{2}\right)-\sin^2\left(\frac{\lambda-\kappa}{4}\right)\right]^{1/2}}\,d\gamma - 2x+1\,,
\end{aligned} \tag{4.15}$$

a second condition on κ and λ becomes

$$G(\kappa,\lambda,x,t)=0\,.$$

One expects the conditions $F=0$ and $G=0$ generically to determine κ and λ as functions of x and t. One may compare these conditions and the subsequent analysis with the results of Deift and McLaughlin [3] for the Toda lattice. Differentiating, one obtains

$$\begin{bmatrix} F_\kappa & F_\lambda \\ G_\kappa & G_\lambda \end{bmatrix}\begin{bmatrix} \kappa_x & \kappa_t \\ \lambda_x & \lambda_t \end{bmatrix} + \begin{bmatrix} F_x & F_t \\ G_x & G_t \end{bmatrix} = 0\,,$$

or, equivalently, solving for $\partial(\kappa,\lambda)/\partial(x,t)$ and observing that $F_x = 0$ and $G_x = -2$,

$$\begin{bmatrix} \kappa_x & \kappa_t \\ \lambda_x & \lambda_t \end{bmatrix} = \frac{-1}{F_\kappa G_\lambda - F_\lambda G_\kappa} \begin{bmatrix} G_\lambda & -F_\lambda \\ -G_\kappa & F_\kappa \end{bmatrix} \begin{bmatrix} 0 & F_t \\ -2 & G_t \end{bmatrix}.$$

We are interested in the relations between κ_x and κ_t and between λ_x and λ_t:

$$[\kappa_x, \kappa_t] \sim [2F_\lambda, F_t G_\lambda - G_t F_\lambda], \tag{4.16}$$

$$[\lambda_x, \lambda_t] \sim [-2F_\kappa, -F_t G_\kappa + G_t F_\kappa]. \tag{4.17}$$

One now needs relations between G_κ and F_κ and between G_λ and F_λ. These are as follows:

$$\begin{aligned} \sin\left(\frac{\lambda-\kappa}{2}\right) G_\kappa &= \sin^2\left(\frac{\lambda-\kappa}{4}\right) F_\kappa, \\ \sin\left(\frac{\kappa-\lambda}{2}\right) G_\lambda &= \sin^2\left(\frac{\kappa-\lambda}{4}\right) F_\lambda. \end{aligned} \tag{4.18}$$

To prove these relations, one first observes that the combinations

$$\sin^2\left(\frac{\lambda-\kappa}{4}\right) F \mp \sin\left(\frac{\lambda-\kappa}{2}\right) G$$

have integrands that are zero at κ (when the minus sign is taken) and at λ (when the plus sign is taken). Thus the differentiation can be carried out inside the integration signs in the formulae for F and G. The calculations are long but finally yield, say for $\partial/\partial\kappa$,

$$\frac{\partial}{\partial\kappa}\left[\sin^2\left(\frac{\lambda-\kappa}{4}\right) F - \sin\left(\frac{\lambda-\kappa}{2}\right) G\right] = \\ -\frac{1}{4}\sin\left(\frac{\lambda-\kappa}{2}\right) F + \frac{1}{2}\cos\left(\frac{\lambda-\kappa}{2}\right) G.$$

On the other hand, the product rule yields

$$\frac{\partial}{\partial\kappa}\left[\sin^2\left(\frac{\lambda-\kappa}{4}\right) F - \sin\left(\frac{\lambda-\kappa}{2}\right) G\right] = \\ \sin^2\left(\frac{\lambda-\kappa}{4}\right) F_\kappa - \frac{1}{4}\sin\left(\frac{\lambda-\kappa}{2}\right) F - \sin\left(\frac{\lambda-\kappa}{2}\right) G_\kappa + \frac{1}{2}\cos\left(\frac{\lambda-\kappa}{2}\right) G.$$

Setting the two results equal to each other, the proposed relation between G_κ and F_κ is obtained. The calculations involving G_λ and F_λ are essentially identical.

We next calculate F_t and G_t. The dependence of F and G on t is linear. The t-coefficient of F is

$$F_t = \frac{1}{\pi}\int_\kappa^\lambda \frac{2i\cos(\gamma)\sin(\chi-\gamma)}{\left[\sin^2\left(\frac{\chi-\gamma}{2}\right) - \sin^2\left(\frac{\lambda-\kappa}{4}\right)\right]^{1/2} \sin\left(\frac{\chi-\gamma}{2}\right)}\, d\gamma. \tag{4.19}$$

By extending the differential being integrated to a meromorphic differential on the complex plane minus a square root branch cut from $e^{i\kappa}$ to $e^{i\lambda}$ (along the unit circle), one can obtain the integral by residue theory of contour integration. The differential is the pullback to the unit circle of the complex differential

$$\pm\frac{2i(z^2+1)(e^{i\chi}+z)}{z^2[(z-e^{i\kappa})(z-e^{i\lambda})]^{1/2}}\,dz\,.$$

Under the change of variables $z=w^{-1}$, it takes the form

$$\pm\frac{2i(1+w^2)(e^{i\chi}w+1)}{w^2[(1-we^{i\kappa})(1-we^{i\lambda})]^{1/2}}\,dw\,.$$

The residues at $z=0$ and $z=\infty$ turn out to be

$$\mathrm{Res}_{z=0}=\pm 4ie^{-i\chi}\cos^2\left(\frac{\lambda-\kappa}{4}\right),\qquad \mathrm{Res}_{z=\infty}=\pm 4ie^{i\chi}\cos^2\left(\frac{\lambda-\kappa}{4}\right).$$

The relative sign of the two residues can be determined by the fact that F_t must be real. The absolute sign can be determined by considering the case when $\chi=\pi$ in the original integral expression (4.19) for F_t. Keeping in mind that the integration is only from $e^{i\kappa}$ to $e^{i\lambda}$ along the inside of the branch cut and multiplying by the factor of $\frac{1}{\pi}$ appearing in (4.19), we obtain

$$F_t=\frac{1}{\pi}\frac{1}{2}(2\pi i)(-4i(e^{i\chi}+e^{-i\chi}))\cos^2\left(\frac{\lambda-\kappa}{4}\right)=8\cos\left(\frac{\lambda+\kappa}{2}\right)\cos^2\left(\frac{\lambda-\kappa}{4}\right).$$

A similar calculation works for G_t, and the result is that

$$G_t=\frac{1}{\pi}\int_\kappa^\lambda\frac{2i\cos(\gamma)\sin\left(\frac{\chi-\gamma}{2}\right)}{\left[\sin^2\left(\frac{\chi-\gamma}{2}\right)-\sin^2\left(\frac{\lambda-\kappa}{4}\right)\right]^{1/2}}\,d\gamma=4\sin\left(\frac{\lambda+\kappa}{2}\right)\sin^2\left(\frac{\lambda-\kappa}{4}\right).$$

Going back to the ratios (4.16) and (4.17) and using the relations (4.18), one finds that

$$[\kappa_x,\kappa_t]\sim\left[2\sin\left(\frac{\lambda-\kappa}{2}\right),-\sin^2\left(\frac{\lambda-\kappa}{4}\right)F_t-\sin\left(\frac{\lambda-\kappa}{2}\right)G_t\right],$$
$$[\lambda_x,\lambda_t]\sim\left[2\sin\left(\frac{\kappa-\lambda}{2}\right),-\sin^2\left(\frac{\kappa-\lambda}{4}\right)F_t-\sin\left(\frac{\kappa-\lambda}{2}\right)G_t\right],$$

and, using the values obtained for F_t and G_t, one calculates that the ratios κ_t/κ_x and λ_t/λ_x are indeed equal to $f(\kappa,\lambda)$ and $f(\lambda,\kappa)$, respectively.

□

Observe that the conditions $F(\alpha,\beta,x,t)=0$ and $G(\alpha,\beta,x,t)=0$ determine the solution $\alpha(x,t)$, $\beta(x,t)$ of the hyperbolic equations (1.12). Thus the solution of the Riemann-Hilbert problem—in particular, the endpoints of the intervals in its presentation—essentially provides an inverse of the asymptotic spectral transform, determining $\alpha(x,t)$ and $\beta(x,t)$ in terms of $\rho(\mu)$ and $\varepsilon(\mu,t)$. After the point of breaking of the hyperbolic equations, one or both of α and β may be multivalued, and the discrete system may exhibit chaotic behavior (waves with wavelength on the order of the lattice spacing). At that point, the present study concludes.

5 Summary and Remarks

We have prescribed functions $q(x)$ and $\phi'(x)$ that, by construction, describe the local limiting modulus and phase difference for initial data in the DNLS system as the lattice spacing tends to zero. We have proposed asymptotic forms $\rho(\mu)$ and $\mathcal{E}'(\mu)$ for the spectral data in the inverse spectral transform for the discrete vector evolution problem $\vec{u}_{n+1} = U_n\vec{u}_n$ in the limit as ε tends to zero. We have also given explicit formulae for the asymptotic form of the time-dependent spectral data $(\rho(\mu), \mathcal{E}'(\mu,t))$ for the solutions of the DNLS systems $\mathcal{S}_\varepsilon$. By means of the Riemann-Hilbert problem arising from the asymptotic analysis of the inverse spectral formula for $|Q_n|$ in the discrete systems, we have shown that, for a time interval in which there exist functions $q(x,t)$ and $\phi'(x,t)$ giving rise to the asymptotic spectral data $\rho(\mu)$ and $\mathcal{E}'(\mu,t)$, these functions are solutions of the slow-time-scale PDEs (1.9) that come out of the formal asymptotic analysis of the continuum limit. This was accomplished by two results (Theorem 4.1): First, the values of κ and λ as functions of x and t that cause the proposed form (4.9) to be a solution to the Riemann-Hilbert problem are equal to the functions $\alpha(x,t)$ and $\beta(x,t)$ that give rise to the spectral data $(\rho(\mu), \mathcal{E}'(\mu,t))$ according to formulae (2.7) and (2.8). In those formulae, α and β are related to q and ϕ' by equations (1.10), which define the Riemann invariants of the formal PDEs. Second, values of κ and λ that do solve the Riemann-Hilbert problem must satisfy $F(\kappa,\lambda,x,t) = 0$ and $G(\kappa,\lambda,x,t) = 0$, F and G defined by equations (4.14) and (4.15), and therefore, as is shown, must evolve according to the Riemann-invariant form (1.11) of the formal PDEs. Assuming that such q and ϕ' are the true limit of the slowly varying modulus and phase difference of the discrete systems as the lattice spacing tends to zero, we conclude that the formal PDEs do indeed describe their space-time modulation in this limit.

Appendix: The Direct and Inverse Discrete Spectral Transforms

In this appendix, we make the change of dependent variable $Q_n \mapsto Q_n e^{-2i\tau}$, which converts the DNLS system (1.1) to the system

$$\text{(A.1)} \qquad i\dot{Q}_n + (1 - |Q_n|^2)(Q_{n-1} + Q_{n+1}) = 0, \quad n \in \mathbb{Z}.$$

which we will denote by (DNLS$'$). Using initial data with $|Q_0(0)| = |Q_N(0)| = 1$, we see that $Q_0(\tau)$ and $Q_N(\tau)$ remain constant in time, and we may take $Q_0(0) = 1$ and $Q_N(0) = \xi$ with $|\xi| = 1$ without losing generality.

Remark. The ansatz (1.14) is formally inconsistent with the DNLS$'$ system, whereas the ansatz (1.5) is consistent with both the DNLS and the DNLS$'$ systems. This is to be expected since the change of variable is made in the fast-time-scale oscillations. Using the ansatz (1.5) in the DNLS$'$ system (which differs from the DNLS system only by the lack of the $-2Q_n$ term) only changes the dispersion relations: Equations (1.3), (1.4), and (1.8) become, respectively,

$$\omega - 2(1-q^2)\cos k = 0\,,$$
$$\omega q_n - (1-q_n^2)(q_{n-1}+q_{n+1})\cos k = 0\,,$$
$$\phi_t - 2(1-q^2)\cos\phi_x = 0\,,$$

whereas the first equation in the system (1.9) for ϕ' remains unaltered.

The infinite DNLS′ system is a special case of more general discrete systems considered by Ablowitz and Ladik [1], in which the authors studied systems of differential equations using the language of matrices. In that context, the present system is expressed as follows: Let z be an arbitrary complex number, and define the matrices

$$U_n(z;\tau) = \begin{bmatrix} z & \overline{Q}_n(\tau) \\ Q_n(\tau) & z^{-1} \end{bmatrix}, \tag{A.2}$$

$$B_n(z;\tau) = -i\begin{bmatrix} z^2 - Q_{n-1}(\tau)\overline{Q}_n(\tau) & -z^{-1}\overline{Q}_{n-1}(\tau) + z\overline{Q}_n(\tau) \\ zQ_{n-1}(\tau) - z^{-1}Q_n(\tau) & z^{-2} + \overline{Q}_{n-1}(\tau)Q_n(\tau) \end{bmatrix}; \tag{A.3}$$

then the system (1.1) is equivalent to the matrix evolution system

$$\dot{U}_n = B_{n+1}U_n - U_nB_n \tag{A.4}$$

for any fixed value of z. In addition, (A.4) is the compatibility condition for the following associated discrete-space and continuous-time evolution prescription for a two-dimensional complex vector $\vec{u}_n(z;\tau)$:

$$\vec{u}_{n+1} = U_n\vec{u}_n\,, \tag{A.5}$$

$$\dot{\vec{u}}_n = B_n\vec{u}_n\,. \tag{A.6}$$

In [9], Miller et al. studied the spatially twist-periodic Ablowitz-Ladik equations. A twist period of N means that $Q_{n+N} = Q_n\xi$ for some unitary complex number ξ. The finite system obtained by requiring that Q_0 and Q_N be unitary, say $Q_0 = 1$ and $Q_N = \xi$, can evidently be extended to an infinite system with spatial twist period N. An important object in the theory is the "twist-periodic transfer matrix"

$$T(z;\tau) = \begin{bmatrix} \xi^{\frac{1}{2}} & 0 \\ 0 & \xi^{-\frac{1}{2}} \end{bmatrix} U_NU_{N-1}\cdots U_1\,,$$

in which $\xi^{1/2}$ may be either square root of ξ. It is simple to show that the time evolution equation for T is the commutation relation

$$\dot{T} = B_1T - TB_1\,, \tag{A.7}$$

by using (A.4) and the fact that

$$B_{N+1} = \begin{bmatrix} \xi^{-\frac{1}{2}} & 0 \\ 0 & \xi^{\frac{1}{2}} \end{bmatrix} B_1 \begin{bmatrix} \xi^{\frac{1}{2}} & 0 \\ 0 & \xi^{-\frac{1}{2}} \end{bmatrix}.$$

Equation (A.7) shows that the trace $J(z)$ of $T(z;\tau)$ is constant in time, and therefore its roots as a function of z are also constant in time.[3] In the inverse spectral reconstruction of Vekslerchik, the upper left entry $F(z;t)$ of the transfer matrix and the quotient $F(z;\tau)/J(z)$ are central. One finds that J has the form

$$J(z) = \operatorname{tr} T(z;\tau) = \bar{\xi}^{-\frac{1}{2}} z^{-N} \prod_{k=1}^{N} (z^2 - \zeta_k)\,.$$

One then shows that

$$\frac{F(z;\tau)}{J(z)} = \frac{W(z;\tau)}{W(\infty;\tau)}\,, \tag{A.8}$$

in which

$$W(z;\tau) = z^2 \sum_{k=1}^{N} \frac{W_k \exp[-i(\zeta_k - \zeta_k^{-1})\tau]}{z^2 - \zeta_k}\,, \tag{A.9}$$

$\{W_k\}$ are constant in time with $\sum_{k-1}^{N} W_k = 1$, and

$$W(\infty;\tau) = \sum_{k=1}^{N} W_k \exp[-i(\zeta_k - \zeta_k^{-1})\tau]\,.$$

The formulae for reconstructing the solution $Q_n(t)$ from the data are as follows:[4] One first defines the quantities

$$\omega_j = \sum_{k=1}^{N} W_k \zeta^{-j} \exp[-i(\zeta_k - \zeta_k^{-1})\tau] \tag{A.10}$$

and the so-called tau-functions

$$\Delta_n = \det \begin{bmatrix} \omega_0 & \cdots & \omega_{n-1} \\ \vdots & \ddots & \vdots \\ \omega_{1-n} & \cdots & \omega_0 \end{bmatrix}, \tag{A.11}$$

$$\tilde{\Delta}_n = \det \begin{bmatrix} \omega_1 & \cdots & \omega_n \\ \vdots & \ddots & \vdots \\ \omega_{2-n} & \cdots & \omega_1 \end{bmatrix}, \tag{A.12}$$

and $\Delta_0 = 1$, and, in terms of these, one has

$$Q_n = (-1)^n \frac{\tilde{\Delta}_n}{\Delta_n}\,, \qquad n = 1, \ldots, N-1\,, \tag{A.13}$$

$$1 - |Q_n|^2 = \frac{\Delta_{n-1}\Delta_{n+1}}{\Delta_n^2}\,, \quad n = 1, \ldots, N-1\,. \tag{A.14}$$

---

[3] Vekslerchik [12] showed that this finite system is Hamiltonian and exhibited a Poisson bracket and N first integrals of the flow that are in involution.

[4] Concise derivations were presented in [12]; details can be found in [10].

The data $\{W_k\}$ may be multiplied by a common factor, and the formulae are not changed. In fact, one can define the time-dependent quantities

$$W_k(t) = W_k \exp[-i(\zeta_k - \zeta_k^{-1})\tau], \tag{A.15}$$

and it turns out that $\sum_{k=1}^{N} W_k(\tau) = W(\infty;\tau) = \exp(2\,\mathrm{Im}\int_0^t Q_1(\tau')d\tau')$.

We now study the case in which the data $\{Q_n\}$ for $n = 1,\ldots,N-1$ are subunitary (that is, $|Q_n| < 1$). One observes, first of all, that the DNLS$'$ flow preserves subunitarity. Two consequences of such data which we will establish are that the eigenvalues ζ_k are unitary and the norming constants W_k are positive. These results will be crucial for characterizing the asymptotic behavior of the quantities Δ_n in the continuum limit. To begin, we appeal to an observation made by Miller et al. [9] that the spatial evolution of the vector $\vec{u}_n(z)$ given by (A.5) can be understood as the solution of a genuine eigenvalue problem. Assuming that $|Q_n| \neq 1$, one makes the change of variables

$$\vec{u}_n(z) = \prod_{k=1}^{n-1} \sqrt{1-|Q_n|^2}\,\vec{w}_n(z), \tag{A.16}$$

considers the first row of the linear system

$$\begin{bmatrix} z & \bar{Q}_n \\ Q_n & z^{-1} \end{bmatrix} \begin{bmatrix} w_n^{(1)} \\ w_n^{(2)} \end{bmatrix} = \sqrt{1-|Q_n|^2} \begin{bmatrix} w_{n+1}^{(1)} \\ w_{n+1}^{(2)} \end{bmatrix}$$

and the second row of the inverted system

$$\begin{bmatrix} z^{-1} & -\bar{Q}_n \\ -Q_n & z \end{bmatrix} \begin{bmatrix} w_{n+1}^{(1)} \\ w_{n+1}^{(2)} \end{bmatrix} = \sqrt{1-|Q_n|^2} \begin{bmatrix} w_n^{(1)} \\ w_n^{(2)} \end{bmatrix},$$

and sees that (A.5) is equivalent to

$$\Lambda\vec{w}(z) = z\vec{w}(z), \tag{A.17}$$

where the infinite matrix Λ is defined by

$$\Lambda = \begin{bmatrix} \sqrt{1-|Q_n|^2}\Delta & -Q_n \\ \bar{Q}_{n-1} & \sqrt{1-|Q_{n-1}|^2}\Delta^{-1} \end{bmatrix}. \tag{A.18}$$

$\vec{w}$ is the concatenation of the vectors $\vec{w}_n$ into a single vector, which is in general infinite; and Δ is the shift operator $\Delta w_n^{(i)} = w_{n+1}^{(i)}$ for $i = 1,2$. The effect of imposing unitary boundary conditions $Q_0 = 1$ and $Q_N = \xi$ is that both of the quantities $\sqrt{1-|Q_0|^2}$ and $\sqrt{1-|Q_N|^2}$ become zero and a $2N\times 2N$ block A within the infinite matrix Λ becomes decoupled. By setting $a_n = \sqrt{1-|Q_n|^2}$ and taking $N = 4$ as an illustration, the truncated eigenvalue problem

$$A\vec{w} = z\vec{w}$$

assumes the form

$$
\left[\begin{array}{cc|cc|cc|cc}
0 & -\overline{Q}_1 & a_1 & & & & & \\
1 & 0 & & 0 & & & & \\
\hline
0 & & 0 & -\overline{Q}_2 & a_2 & & & \\
 & a_1 & Q_1 & 0 & & 0 & & \\
\hline
 & & 0 & & 0 & -\overline{Q}_3 & a_3 & \\
 & & & a_2 & Q_2 & 0 & & 0 \\
\hline
 & & & & 0 & & 0 & -\overline{\xi} \\
 & & & & & a_3 & Q_3 & 0
\end{array}\right]
\begin{bmatrix} w_1^{(1)} \\ w_1^{(2)} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ w_4^{(1)} \\ w_4^{(2)} \end{bmatrix}
= z \begin{bmatrix} w_1^{(1)} \\ w_1^{(2)} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ w_4^{(1)} \\ w_4^{(2)} \end{bmatrix} . \tag{A.19}
$$

We have introduced this point of view because of the following useful connection between the two formulations (A.5) and (A.17) of the spatial linear problem:

LEMMA A.1 *The set of roots of $J(z)$ is equal to the set of eigenvalues of A.*

PROOF: One observes first that if $\vec{u}_n$ satisfies (A.5) for $n = 0, \ldots, N$ and $\vec{u}_0$ is not in the kernel of U_0, then, for $n = 1, \ldots, N$, $\vec{w}_n$ satisfies (A.19). First, since

$$
U_0 = \begin{bmatrix} z & 1 \\ 1 & z^{-1} \end{bmatrix} ,
$$

$\vec{u}_1$ is a multiple of $[z\ 1]^{\mathsf{T}}$. Then, looking at the second row of the linear system (A.19), one finds that $\vec{w}_1$ is also proportional to $[z\ 1]^{\mathsf{T}}$. The change of variables (A.16) then applies for $1 \le n \le N-1$. Now looking at the penultimate row, one finds that $\vec{w}_N$ and therefore $\vec{u}_N$ must be proportional to $\left[-\overline{\xi}\ z\right]^{\mathsf{T}}$, that is,

$$
\vec{u}_N \propto U_{N-1} \cdots U_1 \begin{bmatrix} z \\ 1 \end{bmatrix} \propto \begin{bmatrix} -\overline{\xi} \\ z \end{bmatrix} . \tag{A.20}
$$

Seeing that $U_N = \begin{bmatrix} z & \overline{\xi} \\ \xi & z^{-1} \end{bmatrix}$, this means that

$$
\vec{u}_{N+1} \propto U_N \cdots U_1 \begin{bmatrix} z \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} , \tag{A.21}
$$

or, equivalently, that

$$
\left[\xi\ z^{-1}\right] U_{N-1} \cdots U_1 \begin{bmatrix} z \\ 1 \end{bmatrix} = 0
$$

since the rows of U_N are proportional. This is then equivalent to the condition

$$
\operatorname{tr}\left(\begin{bmatrix} z \\ 1 \end{bmatrix} \left[\xi\ z^{-1}\right] U_{N-1} \cdots U_1 \right) = 0 . \tag{A.22}
$$

Finally,

$$\begin{bmatrix} z \\ 1 \end{bmatrix} \begin{bmatrix} \xi & z^{-1} \end{bmatrix} = \begin{bmatrix} z\xi & 1 \\ \xi & z^{-1} \end{bmatrix} = \xi^{\frac{1}{2}} \begin{bmatrix} \xi^{\frac{1}{2}} & 0 \\ 0 & \bar{\xi}^{\frac{1}{2}} \end{bmatrix} \begin{bmatrix} z & \bar{\xi} \\ \xi & z^{-1} \end{bmatrix} = \xi^{\frac{1}{2}} \begin{bmatrix} \xi^{\frac{1}{2}} & 0 \\ 0 & \bar{\xi}^{\frac{1}{2}} \end{bmatrix} U_N ,$$

which shows that the left side of (A.22) is simply $\xi^{1/2}J(z)$. □

We will use this lemma in Theorem A.3 to show that the roots of $J(z)$ are unitary and distinct for subunitary data $\{Q_n\}$. In addition, in handling the continuum limit, it will be crucial to know that the quantities $\{W_k\}$ are real and positive. It is easy to show that they are real, but to see that they are positive requires more understanding of the function $F(z)$ in the transfer matrix. We first present some information concerning the structure of the transfer matrix $T(z;0)$. Since we are now dealing with the spatial problem at time $t = 0$, it will be convenient to denote $T(z;0)$ simply by $T(z)$ and $F(z;0)$ by $F(z)$. Parts (i) and (ii) hold assuming only that Q_0 and Q_N are unitary; in part (iii), it is essential that $|Q_n|$ be less than 1 for $n = 1,\dots,N-1$.

LEMMA A.2 (i) *$T(z)$ has the form*

$$\begin{bmatrix} F(z) & z\hat{F}(z) \\ z^{-1}F(z) & \hat{F}(z) \end{bmatrix}$$

where $\hat{F}(z) = \overline{F(\bar{z}^{-1})}$.

(ii) *$F(z)$ is a Laurent polynomial in z that is either even or odd and whose first and last terms are $\xi^{1/2}z^N$ and $\bar{\xi}^{1/2}Q_1 z^{-N+2}$.*

(iii) *All roots of F are in the interior of the unit disk. Given the form in* (ii)*, this means that the winding number of F as z traverses the unit circle is equal to N.*

PROOF: The proof is by induction on the matrices

$$T_k(z) = \begin{bmatrix} \xi^{\frac{1}{2}} & 0 \\ 0 & \bar{\xi}^{\frac{1}{2}} \end{bmatrix} U_N \cdots U_k.$$

The transfer matrix $T(z)$ is $T_1(z)$, and the lemma is just the following induction hypothesis with $k = 1$:

(i_k) $T_k(z)$ has the form $\begin{bmatrix} F_k(z) & z\hat{F}_k(z) \\ z^{-1}F_k(z) & \hat{F}_k(z) \end{bmatrix}$.

(ii_k) $F_k(z)$ is a Laurent polynomial in z that is either even or odd and whose first and last terms are $\xi^{1/2}z^{N-k+1}$ and $\bar{\xi}^{1/2}Q_k z^{-(N-k+1)+2}$.

(iii_k) The winding number of F_k as z traverses the unit circle is equal to $N-k+1$.

First, we calculate

$$T_N(z) = \begin{bmatrix} \xi^{\frac{1}{2}} & 0 \\ 0 & \overline{\xi}^{\frac{1}{2}} \end{bmatrix} \quad \text{and} \quad U_N = \begin{bmatrix} \xi^{\frac{1}{2}} z & \overline{\xi}^{\frac{1}{2}} \\ \xi^{\frac{1}{2}} & \overline{\xi}^{\frac{1}{2}} z^{-1} \end{bmatrix}.$$

We see that the hypothesis holds for $k = N$. Next, assuming the hypothesis for some k such that $N \geq k > 1$, we will prove it with k replaced by $(k-1)$. Using (i$_k$), one can write out $T_{k-1} = T_k U_{k-1}$:

$$\begin{aligned} T_{k-1}(z) &= \begin{bmatrix} F_k(z) & z\hat{F}_k(z) \\ z^{-1}F_k(z) & \hat{F}_k(z) \end{bmatrix} \begin{bmatrix} z & \overline{Q}_{k-1} \\ Q_{k-1} & z^{-1} \end{bmatrix} \\ &= \begin{bmatrix} zF_k(z) + zQ_{k-1}\hat{F}_k(z) & \overline{Q}_{k-1}F_k(z) + \hat{F}_k(z) \\ F_k(z) + Q_{k-1}\hat{F}_k(z) & z^{-1}\overline{Q}_{k-1}F_k(z) + z^{-1}\hat{F}_k(z) \end{bmatrix}. \end{aligned}$$

By inspection, (i$_{k-1}$) and (ii$_{k-1}$) hold with

$$F_{k-1}(z) = zF_k(z) + zQ_{k-1}\hat{F}_k(z).$$

To prove that the winding number $\omega(F_{k-1})$ of F_{k-1} is equal to $N-(k-1)+1$, we observe that $|\hat{F}_k(z)| = |F_k(z)|$ whenever z is on the unit circle and that $|Q_{k-1}| < 1$. An application of Rouche's theorem then yields $\omega(F_{k-1}) = \omega(zF_k) = \omega(F_k)+1 = N-k+2$. □

THEOREM A.3 *Given subunitary data* $\{Q_n\}$ *for* $n = 1, \ldots, N-1$,

(i) *The roots* $\{z_k\}$ *of* $J(z)$ *are unitary and distinct.*
(ii) *The quantities* $\{W_k\}$ *are positive.*

PROOF: (i) Referring to the formulation (A.19) for any fixed eigenvalue z, we observe that $\vec{w}_1 \propto [z\ 1]^{\mathsf{T}}$. It is evident, then, from formulation (A.5) that $\vec{u}_n$ and therefore $\vec{w}_n$ is uniquely determined up to a scalar multiple, and therefore the eigenspace of A (recall that A is the decoupled $N \times N$ block of Λ) for the eigenvalue z is one-dimensional. In [9], the authors also compute Λ^{-1} and the adjoint $\Lambda^\dagger$ of Λ:

$$\Lambda^{-1} = \begin{bmatrix} a_{n-1}\Delta^{-1} & \overline{Q}_{n-1} \\ -Q_n & a_n\Delta \end{bmatrix}, \qquad \Lambda^\dagger = \begin{bmatrix} \overline{a}_{n-1}\Delta^{-1} & \overline{Q}_{n-1} \\ -Q_n & \overline{a}_n\Delta \end{bmatrix}.$$

When the data $\{Q_n\}$ are subunitary, the quantities a_n are real and thus $A^{-1} = A^\dagger$, and we conclude that the eigenvalues of A, which are shown in Lemma A.1 to be equal to the roots of $J(z)$, are unitary. In addition, seeing now that A is diagonalizable and that for a given eigenvalue z, a unique one-dimensional eigenspace is determined by (A.19), we conclude that A has N distinct eigenvalues so that the roots of $J(z)$ are indeed distinct.

(ii) First, by the definition of W_k provided by equations (A.8) and (A.9), one has

$$W_k = \lim_{z \to z_k} \frac{F(z)}{F(z) + \hat{F}(z)} \frac{(z^2 - z_k^2)}{z^2},$$

where z_k is a square root of ζ_k, and, using L'Hôpital's rule and the fact that $\hat{F}'(z) = -z^{-2}\widehat{F'}(z)$, one finds that

$$W_k = \frac{2F(z_k)}{z_k F'(z_k) - z_k^{-1}\widehat{F'}(z_k)}. \tag{A.23}$$

In addition, whenever z is unitary, $\hat{F}(z) = \overline{F(z)}$ and $\widehat{F'}(z) = \overline{F'(z)}$, so any unitary number z is a root of $J = F + \hat{F}$ if and only if $F(z) = -\overline{F(z)}$, or whenever $F(z)$ is purely imaginary. Therefore, using (A.23), we find that

$$W_k^{-1} = \frac{\mathrm{Im}(z_k F'(z_k))}{-iF(z_k)} = \mathrm{Im}\left(\frac{z_k F'(z_k)}{-iF(z_k)}\right) = \mathrm{Im}\left(iz_k \frac{F'(z_k)}{F(z_k)}\right), \tag{A.24}$$

which is a real quantity equal to the angular derivative of F as a function of $\arg(z)$ at $z = z_k$.

To see that the quantities $\{W_k\}$ are in fact positive, we use part (iii) of Lemma A.2 and the result (A.24) to deduce that the number of times that $F(z)$ crosses the imaginary axis in the positive angular direction as z traverses the unit circle is at least $2N$. It must cross transversally since W_k^{-1} cannot be zero. Since each crossing accounts for a root of $J(z)$ of which there are exactly $2N$, we conclude that there are only $2N$ crossing points z_k, for each of which W_k is positive.

□

By using the multilinearity of the determinant and then writing W_k in place of $W_k \exp[-i(\zeta_k - \zeta_k^{-1})\tau]$, we get

$$\begin{aligned}
\Delta_n &= \sum_{(k_1,\dots,k_n)} \begin{vmatrix} \zeta_{k_1}^0 W_{k_1} & \cdots & \zeta_{k_n}^{1-n} W_{k_n} \\ \vdots & \ddots & \vdots \\ \zeta_{k_1}^{n-1} W_{k_1} & \cdots & \zeta_{k_n}^0 W_{k_n} \end{vmatrix} \\
&= \sum_{(k_1,\dots,k_n)} \prod_{j=1}^n W_{k_j} \begin{vmatrix} \zeta_{k_1}^0 & \cdots & \zeta_{k_n}^{1-n} \\ \vdots & \ddots & \vdots \\ \zeta_{k_1}^{n-1} & \cdots & \zeta_{k_n}^0 \end{vmatrix} \\
&= \sum_{(k_1,\dots,k_n)} \prod_{j=1}^n W_{k_j} \prod_{j=1}^n \zeta_{k_j}^{-j} \begin{vmatrix} \zeta_{k_1}^1 & \cdots & \zeta_{k_n}^1 \\ \vdots & \ddots & \vdots \\ \zeta_{k_1}^n & \cdots & \zeta_{k_n}^n \end{vmatrix} \\
&= \sum_{k_1 < \cdots < k_n} \prod_{j=1}^n W_{k_j} \begin{vmatrix} \zeta_{k_1}^1 & \cdots & \zeta_{k_n}^1 \\ \vdots & \ddots & \vdots \\ \zeta_{k_1}^n & \cdots & \zeta_{k_n}^n \end{vmatrix} \sum_{\sigma \in S_n} s(\sigma) \prod_{j=1}^n \zeta_{k_{\sigma(j)}}^{-j}
\end{aligned}$$

$$= \sum_{k_1<\cdots<k_n} \prod_{j=1}^{n} W_{k_j} \begin{vmatrix} \zeta_{k_1}^1 & \cdots & \zeta_{k_n}^1 \\ \vdots & \ddots & \vdots \\ \zeta_{k_1}^n & \cdots & \zeta_{k_n}^n \end{vmatrix} \begin{vmatrix} \zeta_{k_1}^{-1} & \cdots & \zeta_{k_n}^{-1} \\ \vdots & \ddots & \vdots \\ \zeta_{k_1}^{-n} & \cdots & \zeta_{k_n}^{-n} \end{vmatrix}$$

$$= \sum_{k_1<\cdots<k_n} \prod_{j=1}^{n} W_{k_j} \prod_{i<j} (\zeta_{k_i}^{-1} - \zeta_{k_j}^{-1}) \prod_{i<j} (\zeta_{k_i} - \zeta_{k_j})$$

$$= \sum_{k_1<\cdots<k_n} \prod_{j=1}^{n} W_{k_j} \prod_{i<j} |\zeta_{k_i} - \zeta_{k_j}|^2 .$$

At time τ, one then has

$$\Delta_n = \sum_{k_1<\cdots<k_n} \prod_{j=1}^{n} W_{k_j} \exp[i(\zeta_{k_j} - \zeta_{k_j}^{-1})\tau] \prod_{i<j} |\zeta_{k_i} - \zeta_{k_j}|^2 . \tag{A.25}$$

Similarly,

$$\tilde{\Delta}_n = \sum_{(k_1,\ldots,k_n)} \begin{vmatrix} \zeta_{k_1}^{-1} W_{k_1} & \cdots & \zeta_{k_n}^{-n} W_{k_n} \\ \vdots & \ddots & \vdots \\ \zeta_{k_1}^{n-2} W_{k_1} & \cdots & \zeta_{k_n}^{-1} W_{k_n} \end{vmatrix}$$

$$= \sum_{(k_1,\ldots,k_n)} \prod_{j=1}^{n} \zeta_{k_j}^{-1} W_{k_j} \begin{vmatrix} \zeta_{k_1}^{0} & \cdots & \zeta_{k_n}^{1-n} \\ \vdots & \ddots & \vdots \\ \zeta_{k_1}^{n-1} & \cdots & \zeta_{k_n}^{0} \end{vmatrix}$$

$$= \sum_{k_1<\cdots<k_n} \prod_{j=1}^{n} \zeta_{k_j}^{-1} W_{k_j} \prod_{i<j} |\zeta_{k_i} - \zeta_{k_j}|^2 .$$

The time-dependent form is

$$\tilde{\Delta}_n = \sum_{k_1<\cdots<k_n} \prod_{j=1}^{n} \zeta_{k_j}^{-1} W_{k_j} \exp[-i(\zeta_{k_j} - \zeta_{k_j}^{-1})\tau] \prod_{i<j} |\zeta_{k_i} - \zeta_{k_j}|^2 . \tag{A.26}$$

We now go a step further and recall that

$$\frac{F(z)}{J(z)} = z^2 \frac{z^{N-2} \xi^{\frac{1}{2}} F(z)}{\prod\limits_{k=1}^{N} (z^2 - \zeta_k)} = z^2 \sum_{k=1}^{N} \frac{W_k}{(z^2 - \zeta_k)} ,$$

from which we find that

$$W_k = \frac{z_k^{N-2} \xi^{\frac{1}{2}} F(z_k)}{\prod\limits_{k' \neq k} (\zeta_{k'} - \zeta_k)} .$$

Knowing from Theorem A.3 that these quantities are positive, it follows that

$$W_k = \frac{|F(z_k)|}{\prod\limits_{k' \neq k} |\zeta_{k'} - \zeta_k|} .$$

Inserting this expression into formulae (A.25) and (A.26) for Δ_n and $\tilde{\Delta}_n$, one arrives at the expressions

$$\Delta_n = \sum_{s\in S_n^N} \prod_{k\in s} |F(z_k)| \exp[-i(\zeta_k - \zeta_k^{-1})\tau] \prod_{j\in s,\, i\notin s} |\zeta_i - \zeta_j|^{-1}, \tag{A.27}$$

$$\tilde{\Delta}_n = \sum_{s\in S_n^N} \prod_{k\in s} \zeta_k^{-1} |F(z_k)| \exp[-i(\zeta_k - \zeta_k^{-1})\tau] \prod_{j\in s,\, i\notin s} |\zeta_i - \zeta_j|^{-1}, \tag{A.28}$$

where S_n^N denotes the set of all order-n subsets of the set of integers $\{1,\dots,N\}$.

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