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Quantum sine-Gordon thermodynamics: The Bethe ansatz method

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We show that the thermodynamic properties of the quantum sine-Gordon system in the zero-charge sector can be found from the appropriate limit of the Takahashi-Suzuki Bethe ansatz analysis of the *XYZ* spin chain. We prove that the rather complex criteria for allowed states in thermodynamic sums in that analysis correspond simply to including only states with normalizable wave functions. The behavior of the *XYZ* phase-shift function in the sine-Gordon limit is discussed.

I. INTRODUCTION

There has been considerable recent interest in the properties of the quantum sine-Gordon (SG) system, which appears to be a suitable model for several one-dimensional spin systems, for example $CsNiF_3$ and $(CD_3)_4$ $NMnCl_3$ (TMMC) (in a magnetic field), at least in appropriate temperature ranges. Our present understanding of the thermodynamics of SG is based in large part on the ideal gas phenomenology pioneered by Krumhansl and Schrieffer,[1] and later refined by Currie *et al.*[2] However, this picture becomes less reliable, and in some ways ambiguous, in the quantum regime. Another method has been developed by Maki and Takayama,[3] who have applied finite-temperature field-theoretical techniques to the problem. They have discussed, for example, the mass spectrum at finite temperatures. Their work has given new insight into the nature of the excitations, but the picture is still far from complete. In particular, many of the results are restricted to weak coupling and/or low temperatures.

A quite different approach to the finite-temperature properties of the system is provided by the Bethe ansatz (BA). In 1972, Takahashi and Suzuki[4] (TS) set up the BA formalism for the spin-$\frac{1}{2}$ (anisotropically coupled) *XYZ* chain at finite temperatures, and it is known from the work of Luther,[5] and Bergknoff and Thacker,[6] that the zero-charge-sector SG system is a particular continuum limit of the *XYZ* chain. This has the implication that the formalism of Takahashi and Suzuki[4] can be developed to give a rather complete quantitative account of quantum sine-Gordon thermodynamics in the zero-charge sector, and will probably answer some of the questions raised by other analyses. The purpose of the present paper is to initiate such a study. A major reason why the very elegant work of Takahashi and Suzuki has been little used so far is that its physical content is not readily discernible, and, furthermore, some of the arguments invoked to restrict sums over states are not very transparent, and hence perhaps rather unconvincing. In the present work, we attempt to clarify the physical picture of the various excitations, first at zero temperature, then at finite temperature. In Sec. II we review briefly the work done so far on the zero-temperature excitation spectrum and discuss, in particular, the "charged vacuum" excitations found by Korepin.[7] These correspond to certain strings (uniformly spaced sets of complex rapidities) whose energy and momenta are completely compensated by backflow in the Fermi sea of negative energy states. Korepin[7] gave a set of criteria for deciding whether a particular string length corresponds to a normalizable wave function. We present a very simple formulation of his ideas.

In Sec. III, we build up a picture of the system at finite temperatures as a gas of interacting excitations, including not only solitons, antisolitons, and breather states, but also excitations corresponding to the "charged vacuum" excitations of Korepin. For nonzero temperatures, these last excitations no longer have zero energy and momentum, essentially because the shielding properties of the "hot" ensemble are different for the ground state. Our main result is that this picture corresponds exactly with the analysis of Takahashi and Suzuki. They restricted the sum over states to certain string lengths, and justified the restriction with arguments concerning exotic states of the system in which all particles were bound in strings of the same length. We show that their restrictions have a simpler and more physical justification—only strings corresponding to normalizable wave functions are allowed. Thus the work of Takahashi and Suzuki, including the criteria for allowed strings in sums over states, can be understood in terms of a rather direct physical picture.

In Sec. IV of the paper, and in the Appendix, we point out that the expression for the phase shift derived from the *XYZ* model in the appropriate limit does not quite coincide with the sine-Gordon phase shift—there is a small linear term, with coefficient inversely proportional to the cutoff. Thus the convergence of one model to the other as the cutoff goes to infinity is not exponentially fast, as one might otherwise have expected.

II. ZERO-TEMPERATURE EXCITATION SPECTRUM OF THE SINE-GORDON SYSTEM

The quantum sine-Gordon system is defined by the Lagrangian density

$$\mathcal{L} = \tfrac{1}{2}\partial_\mu\phi\partial^\mu\phi + \frac{\alpha_0}{\beta^2}\cos\beta\phi \ , \tag{2.1}$$

where ϕ is a canonical boson field in $1+1$ dimensions. The corresponding classical theory is well known to have as excitations the soliton and antisoliton, and "breather" states which can be regarded as soliton-antisoliton $(s\bar{s})$ bound states. Dashen, Hasslacher, and Neveu[8] (DHN) used a semiclassical quantization method to derive the discrete set of $(s\bar{s})$ binding energies for the quantum system. Coleman[9] proved the equivalence of the SG system (2.1) to the massive Thirring model (MTM)

$$\mathcal{L} = \bar{\psi}(i\not\partial - m_0)\psi - \tfrac{1}{2}g_0 j_\mu j^\mu \ , \tag{2.2}$$

where $j_\mu = \frac{1}{2}[\bar{\psi}, \gamma_\mu\psi]$ and ψ is a Dirac fermion field. The Hamiltonian of this model can be written

$$H = \int dx\, [-i(\psi_1^\dagger\partial_x\psi_1 - \psi_2^\dagger\partial_x\psi_2) + m_0(\psi_1^\dagger\psi_2 + \psi_2^\dagger\psi_1) + 2g_0\psi_1^\dagger\psi_2^\dagger\psi_2\psi_1] \ . \tag{2.3}$$

It was shown by Luther[5] that the MTM (and hence SG) arose in a certain continuum limit of the XYZ spin chain,[10] described by the Hamiltonian

$$H = -\tfrac{1}{2}\sum_n (J_x\sigma_n^x\sigma_{n+1}^x + J_y\sigma_n^y\sigma_{n+1}^y + J_z\sigma_n^z\sigma_{n+1}^z) \ , \tag{2.4}$$

σ^i being the Pauli matrices. The elementary excitations from the ground state of (2.4) had been previously found by Johnson, Krinsky, and McCoy[11] and they corresponded—in the appropriate limit—precisely with the semiclassical results of DHN, suggesting that the latter had a wider range of validity then the semiclassical regime.

A clear analysis of the MTM excitation spectrum, and a discussion of the XYZ limiting process, has been given by Bergknoff and Thacker.[6] We briefly outline some of their notation and results. The single Dirac fermion eigenstates of the quadratic part of the MTM Hamiltonian (2.3) are conveniently labeled by a rapidity variable β,

$$E = m_0\cosh\beta, \quad k = m_0\sinh\beta \ . \tag{2.5}$$

Thus the real β axis corresponds to positive energies, the line $\mathrm{Im}\beta = \pi$ to negative energies, and in the physical vacuum state of the MTM system these negative energy levels are all filled—the usual Dirac sea. The interaction term in (2.3) is a reflectionless potential and causes a phase shift between particles having relative rapidity β of

$$\phi(\beta) = -i\ln\left(-\frac{\sinh\frac{1}{2}(\beta - 2i\mu)}{\sinh\frac{1}{2}(\beta + 2i\mu)}\right), \quad \mu = \tfrac{1}{2}(\pi + g_0) \ . \tag{2.6}$$

In the standard Bethe ansatz fashion, allowed momenta in any state are given by applying periodic boundary conditions and computing the total phase shift (kinetic plus interactions) for a particle taken around the system, that is

$$Lk_i = Lm_0\sinh\beta_i = -2\pi n_i - \sum_j \phi(\beta_i - \beta_j) \ . \tag{2.7}$$

The density of negative-energy states in the physical vacuum is found by subtracting from (2.7) the corresponding equation for β_{i-1} and going to the $L \to \infty$ limit, yielding a nonsingular integral equation. The bare excitations of the system are holes in the Dirac sea, particles with real β, and certain multiparticle bound states called strings, in which individual particles have complex rapidities. The physical excitation spectrum from the ground state is given by computing the backflow in the Dirac sea caused by the bare excitations—from (2.7), the allowed β_i in the sea are shifted slightly. The integral equations are solved by Fourier methods.

Our particular interest in this section is the sets of complex rapidities called strings. As a preliminary exercise, it is interesting to compare the nature of the (bare) bound-state wave function for two particles with that in another Bethe ansatz system, the nonrelativistic boson gas with a δ-function attractive potential.[12,13] Consider a scattering state of two such bosons—in the center-of-mass frame, this corresponds to a single boson interacting with a fixed δ-function potential. There will be an incident wave, a reflected wave, and a transmitted wave. Continuing the momentum in the complex plane to a pole of the scattering matrix, we find both transmitted and reflected waves have (equal) infinite magnitude—normalizing gives the usual symmetric bound-state wave function $\sim\exp[-(c/2|x|)]$, where c is the strength of the potential, the pole being at $k = i|c|/2$. For the MTM fermions, the picture is rather different. Here there is no reflected wave, so the normalized bound state corresponding to a pole of the S matrix has *only* the "transmitted" wave (no incident wave), the wave function is nonzero on only one side of the potential (of course, subsequent antisymmetrization adds a term in the wave function with the particle orders reversed). Thus, for a certain value of the complex momentum difference, the scattering matrix acts as a θ function, cutting the wave function to zero on one side, thus suppressing the growing exponential and giving a normalizable bound state. From (2.6), the appropriate rapidity difference is $2i(\pi-\mu)$, or $2i\omega$ where $\omega=\pi-\mu$.

The generalization of this two-particle bound state to n particles is straightforward. Suppose we have a wave function

$$\psi=\exp\left[im_0\sum_{i=1}^{n}x_i\sinh\beta_i\right] \quad \text{for } x_1<x_2<\cdots<x_n \tag{2.8}$$

(suppressing the spinor components of the wave function, which are not relevant to the argument). We can ensure that ψ will be identically zero for any other ordering of the x_i's by taking the rapidities to form a string.

$$\beta_1=B+i(n-1)\omega,\quad \beta_2=B+i(n-3)\omega\ ,\ \ldots,\ \beta_n=B-i(n-1)\omega\ , \tag{2.9}$$

where, for the string to have real total energy and momentum, $\text{Im}B=0$ or π. We define the parity v of the string by

$$v=\begin{cases}+1 & \text{if } B \text{ is real}\\ -1 & \text{if } \text{Im}B=\pi\ .\end{cases} \tag{2.10}$$

Thus as any particle moves past its neighbor, ψ goes to zero, using the two-particle argument given above. (The complete wave function for the bound state is given by antisymmetrizing ψ.)

We now show, following Korepin,[7] that (2.8) is not normalizable for all string lengths. Introducing difference coordinates,

$$y_1=x_1,\quad y_2=x_2-x_1,\quad \ldots,\quad y_n=x_n-x_{n-1} \tag{2.11}$$

the wave function must decay for positive $y_2, y_3, \ldots, y_n$. This leads to

$$\begin{aligned}&\text{Im}(\sinh\beta_2+\sinh\beta_3+\cdots+\sinh\beta_n)>0\ ,\\ &\text{Im}(\sinh\beta_3+\cdots+\sinh\beta_n)>0\ ,\\ &\ldots\ ,\\ &\text{Im}\sinh\beta_n>0\ .\end{aligned} \tag{2.12}$$

Substituting the values (2.9) gives a bound state with mass

$$m_0\frac{\sin\omega n}{\sin\omega}\quad \text{if } \sin\omega p\,\sin\omega(n-p)>0\ ,\quad p=1,\ldots,n-1 \text{ for } v=+1 \tag{2.13}$$

$$-m_0\frac{\sin\omega n}{\sin\omega}\quad \text{if } \sin\omega p\,\sin\omega(n-p)<0\ ,\quad p=1,\ldots,n-1 \text{ for } v=-1 \tag{2.14}$$

The conditions (2.13) and (2.14) can be written

$$\cos(n-2p)\omega>\cos n\omega\ ,\quad p=1,\ldots,n-1,\quad v=+1 \tag{2.15}$$

and

$$\cos(n-2p)\omega<\cos n\omega,\quad p=1,\ldots,n-1,\quad v=-1\ . \tag{2.16}$$

Hence for a given ω, (2.15) and (2.16) give the values of n corresponding to bound states with normalizable wave functions. This leads to a simple method of finding allowed string lengths. For example, let us consider which strings of even n satisfy (2.15). In Fig. 1, we mark on a cosine curve the points $\cos 0$, $\cos\omega$, $\cos 2\omega$, $\cos 3\omega$, ... For an allowed string with even n, the point $\cos n\omega$ must be lower than all preceding even points in the sequence. It is easy to see that all points are allowed up to and including the $n\omega$ closest to π. This set of strings corresponds to the quantized SG breathers. (In Bergknoff and Thacker,[6] these are the strings ending in the first zone.) However, there are in general longer strings which satisfy (2.15). Considering still only even values of n, if the closest point of the set $n\omega$ to 3π is closer than the closest point to π was, then the string ending at the point near 3π has a normalizable wave function. This does not correspond to anything in the previously discussed SG spectrum, and in fact, when the energy and momentum of this longer string is evaluated by including the backflow in the Dirac sea, it is found to be zero. This is one of the charged vacuum excitations of Korepin. For irrational ω, there will be arbitrarily large odd integer multiples of π having some even integer multiple of ω closer than any preceding even integer multiple of ω was to an odd multiple of π. A similar argument works for odd n. For strings of negative parity, $\cos n\omega$ must be higher than $\cos(2p-n)\omega$ for $p=1,\ldots,n-1$. This can only be true for odd n, from the case $p=\frac{1}{2}n$. Actually, these negative-parity strings correspond to a charged vacuum plus a soliton. We note that on

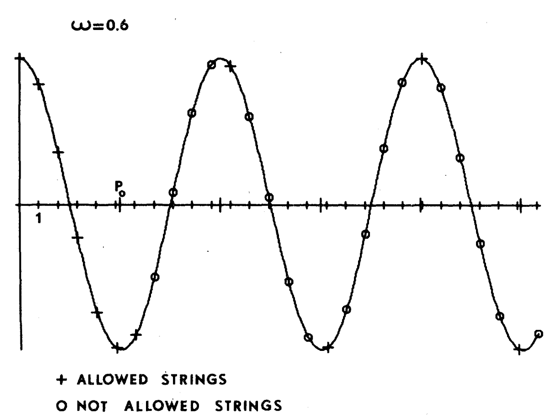

FIG. 1. Allowed and not allowed strings for a given ω. The length scale shown is in units of ω, following Ref. 4, and $p_0=\pi/\omega$.

varying the coupling parameters ω, the set of allowed excitations changes each time ω passes through a rational value—some long strings dissociates into two shorter strings or vice versa.

III. BETHE ANSATZ THERMODYNAMICS

In this section we outline the derivation of the equations describing the thermodynamics for several BA systems, discussing in particular the nature of the excitations appearing in the sum over states.

The first thermodynamic analysis of a BA system was that given by Yang and Yang[14] for the repulsive δ-function boson gas. The basic idea is as follows: for any state of the system, the allowed k values are given by the equation equivalent to (2.7). The canonical ensemble can be represented by assuming that in each small region Δk of momentum space, the allowed k values are randomly filled, so that there is a local density $\rho(k)$ of filled states and $\tilde{\rho}(k)$ of empty states, and a local entropy

$$\Delta S \alpha (\rho+\tilde{\rho})\ln(\rho+\tilde{\rho}) - \rho\ln\rho - \tilde{\rho}\ln\tilde{\rho} \ . \tag{3.1}$$

The energy of the system is simply

$$E = \int_{-\infty}^{\infty} \rho(k)\frac{k^2}{2m}\,dk \ . \tag{3.2}$$

Putting together (3.1) and (3.2) we can construct an expression for the free energy, and minimizing this with respect to $\tilde{\rho}$, say, gives an integral equation connecting ρ and $\tilde{\rho}$. An equation for $\rho+\tilde{\rho}$ in terms of ρ arises from (2.7). These equations can be solved for $\rho, \tilde{\rho}$ and the thermodynamic properties follow.

Gaudin[15] extended this analysis to the Heisenberg-Ising spin chain ($J_x{:}J_y{:}J_z = 1{:}1{:}\Delta$, $|\Delta| > 1$). For this system, the elementary excitations are magnons, but the magnon-magnon phase shift depends on both momenta, not just the momentum difference. However, transforming to the variable α defined in terms of the momentum by

$$k = -i\ln\left[\frac{\sin\frac{1}{2}(\alpha - i\lambda)}{\sin\frac{1}{2}(\alpha + i\lambda)}\right], \quad \Delta = +\cosh\lambda \ , \tag{3.3}$$

the phase shift has a simple difference form

$$\phi(\alpha,\beta) = -i\ln\left[\frac{\sin\frac{1}{2}(\alpha-\beta-2i\lambda)}{\sin\frac{1}{2}(\alpha-\beta+2i\lambda)}\right] \ . \tag{3.4}$$

It is necessary to go to the α variables to solve the various BA equations by Fourier methods. Comparing (3.4) with (2.6), we notice that the phase shift for this spin chain closely resembles that for the sine-Gordon system. Therefore, by arguments analogous to those in Sec. II, there are allowed strings

$$\alpha_1 = A + i(n-1)\lambda, \quad \alpha_2 = A + i(n-3)\lambda, \quad \ldots, \quad \alpha_n = A - i(n-1)\lambda \tag{3.5}$$

of complex eigenvalues, where A is real. However, the criteria for normalizable wave functions, (2.12) depend on the $k-\alpha$ relationship. When (2.5) is replaced by (3.3), it is easy to check that strings of *any* length correspond to normalizable wave functions. Hence a finite-temperature system will have strings of all lengths present, and has to be described in terms of particle and hole densities $\rho_n(\alpha), \tilde{\rho}_n(\alpha)$ in rapidity space for each n. The appropriate generalization of (2.7) for a given string length, including phase shifting by all the other strings of all lengths, gives integral equations for the $\rho_n(\alpha)+\tilde{\rho}_n(\alpha)$'s in terms of densities of other strings throughout rapidity space. Putting the obvious generalizations of (3.1) and (3.2) into the free energy and minimizing with respect to the $\tilde{\rho}_n$'s gives another set of n equations, so the thermodynamic behavior is formally determined.

We note here the relationship between these strings and the elementary excitations of the spin chain from its ground state.[16] For the ferromagnetic case, the ground state has all spins up, with no magnons present. The sets of strings (3.5) correspond directly to physical excitations, with energy and momenta given simply by summing over the components of the string. In the Ising (large Δ) limit, the n string corresponds to a state having n neighboring spins turned down. For the antiferromagnetic case, the picture is quite different—the ground state has zero total spin and is a Dirac sea of magnons. The backflow in this sea completely compensates the string energy and momentum, so the string does not correspond to a physical excitation—although the presence of a two string causes two holes to appear in the Dirac sea, and these are the "dimer" excitations from the antiferromagnetic ground state.

The next step, taken by Takahashi and Suzuki[4] was to go to the Heisenberg-Ising spin chain with $|\Delta| < 1$. This is closely related to Gaudin's work for $|\Delta| > 1$, but there are important differences. The formulas analogous to (3.3) and (3.4) are

$$k = -i\ln\left[\frac{\sinh\frac{1}{2}(\alpha + i\mu)}{\sinh\frac{1}{2}(\alpha - i\mu)}\right], \quad \cos\mu = -\Delta \ , \tag{3.6}$$

$$\phi(\alpha,\beta) = -i\ln\left[\frac{\sinh\frac{1}{2}(\alpha-\beta+2i\mu)}{\sinh\frac{1}{2}(\alpha-\beta-2i\mu)}\right] \ . \tag{3.7}$$

We notice that the expression for the phase shift is identical to the SG expression (2.6), so the strings will have the same spacing. [Whether or not a minus sign is included inside the logarithm depends on the convention defining the phase shift in the noninteracting ($\Delta = 0$) case.] To find string lengths corresponding to normalizable wave functions, we must construct conditions analogous to (2.12). This is particularly simple with the logarithmic form of k above, using (3.6),

$$\begin{aligned} &\sinh\tfrac{1}{2}[A + i(n-2\lambda)] > \sinh\tfrac{1}{2}(A - in\lambda) \;, \\ &\sinh\tfrac{1}{2}[A + i(n-4\lambda)] > \sinh\tfrac{1}{2}(A - in\lambda) \;, \\ &\ldots \;, \\ &\sinh\tfrac{1}{2}[A - i(n-2\lambda)] > \sinh\tfrac{1}{2}(A - in\lambda) \;. \end{aligned} \tag{3.8}$$

Since the sinh function is periodic in the imaginary direction with period 2π, it is evident that these conditions are exactly analogous to (2.15) and (2.16) and hence the same lengths of strings (for a given spacing) are allowed. In fact, these same criteria hold for the general XYZ model, for in this case the hyperbolic functions are replaced with η functions having the same periodicity (and maxima, minima) in the appropriate direction.

Thus, the thermodynamic equations for both the Heisenberg-Ising chain with $|\Delta| < 1$ and the general XYZ chain as written down by Takahashi and Suzuki are straightforward extensions of Gaudin's work, the only new feature being the restriction to strings with normalizable bare wave functions.

It is interesting to note that Takahashi and Suzuki (TS) arrived at the allowed string lengths by quite a different route and appeared to be unaware of the simple physical reasoning given above. They argue [their Eq. (5.3)] that if all the magnons (that is, $\frac{1}{2}N$ for an N-spin system) are bound in states of a particular size n, then there is no room to put in more n-particle bound states. This seems reasonable, because if one could add another bound state, it would appear to give a lowest-energy state in some sense for the system having spin n—but that would also be the state given by removing one bound state, and reversing all spin, which clearly has a quite different wave function. In any case, their argument leads eventually to their equation (A3) which is equivalent to our Eqs. (2.14) and (2.15). They go on to give a very elegant formulation of the condition for bound states in terms of continued fractions.

It is easy to show that our conditions for bound states (2.13) and (2.14) are equivalent to TS equation (A3), which reads in our notation

$$\left[\frac{j\omega}{\pi}\right] + \left[(n-j)\frac{\omega}{\pi}\right] = \left[(n-1)\frac{\omega}{\pi}\right] \quad \text{for } j = 1, \ldots, n-1 \tag{3.9}$$

Since $\omega < \pi$, this equation is trivially true for $j = 1$. Taking $[\omega j/\pi]$ as a function of a continuous variable j, it increases stepwise by unity each time $\omega j/\pi$ is an integer, that is, each time $\sin j\omega$ changes sign. Similarly, $[(n-j)\omega/\pi]$ decreases by unity each time $\sin(n-j)\omega$ changes sign. Thus for our (3.9) to be true for $j = 2, \ldots, n-1$ it must be that between each $j, j+1$ both $\sin j\omega, \sin(n-j)\omega$ change sign, or neither does. This immediately leads to our conditions (2.13) and (2.14).

IV. DISCUSSION

We have shown that the criteria of Takahashi and Suzuki for allowed strings correspond simply to those having normalizable wave functions. Little purpose would be served by reproducing here the thermodynamic equations from Takahashi and Suzuki—they are of standard Bethe ansatz type, and are rather cumbersome simply because of the variety of allowed strings. The limiting process giving the sine-Gordon system from the XYZ chain has been analyzed by Bergknoff and Thacker. It can be shown that the bare and dressed excitation spectra, and thermodynamic properties such as the specific heat gap, go to the correct sine-Gordon values.

One minor puzzle connected with the limiting process is perhaps worth mentioning—the MTM expression for the phase shift (2.6) goes from -2μ at $-\infty$ to $+2\mu$ at $+\infty$, a total change of 4μ. For the cutoff theory, this change takes place between $-\Lambda$ and $+\Lambda$ (cutoffs) with exponential accuracy. Yet if the model is regarded as a limit of the XYZ chain, $\pm\Lambda$ are equivalent points in β space, so the total change in phase over 2Λ must be zero (modulo 2π). The resolution of this problem is given in the Appendix, where it is shown that in a careful derivation of the MTM phase shift from the XYZ chain, there is an additional small linear term.

Note added in proof. The thermodynamic analysis presented here has to be modified for the strongly repulsive quantum sine-Gordon system ($\mu < \frac{1}{3}\pi$). As noted by Bergknoff and Thacker,[6] the equivalence to the XYZ chain breaks down in this region. However, Korepin has given an elegant BA analysis of the ground-state and elementary excitations for $\mu < \frac{1}{3}\pi$, and it appears that a thermodynamic analysis analogous to that above is feasible. We should like to thank V. Korepin for sending us copies of his recent work [Commun. Math. Phys. 76, 165 (1980)].

APPENDIX

In this appendix, we derive the massive Thirring-model phase shift as a limit of the XYZ phase shift, and show that it is of the form (2.6) but with a small linear term added, which goes to zero as the cutoff goes to infinity.

From Takahashi and Suzuki, changing notation to correspond to that used in this paper (that is, $2\zeta \to \pi$

$-\mu$, $\zeta x \to \frac{1}{2}\beta$, a minus sign inside the log, which adds π to ϕ)

$$\phi_{XYZ}(\beta) = -i \ln \left(-\frac{H[\frac{1}{2}(\beta - 2i\mu)]}{H[\frac{1}{2}(\beta+2i\mu)]} \right) , \quad (A1)$$

where H is the elliptic η function. These η functions have modulus l', that is, real period $4K_{l'}$ and imaginary quasiperiod $2K_l$. For convenience we shall denote $K_{l'}$ by K, K_l by K' so that formulas from Whittaker and Watson,[17] and Abramowitz and Stegun[18] can be used directly. Using $H(u) = \theta_1(\pi u/2K)$,

$$\phi_{XYZ}(\beta) = -i \ln \left[\theta_1 \left(\frac{\pi}{4K}(\beta - 2i\mu) \right) \Big/ \theta_1 \left(\frac{\pi}{4K}(\beta + 2i\mu \right) \right] . \quad (A2)$$

The MTM limit is $K \to \infty$, $q = e^{-\pi K'/K} \to 1$ so the usual q expansion is not useful—we need to invert the modulus, using the imaginary transformation

$$\sqrt{-i\tau}\,\theta_1(z) = -i \exp(i\tau' z^2/\pi)\,\theta_1(z\tau'|\tau') , \quad (A3)$$

where $\tau = iK'/K$, $\tau' = -1/\tau = iK/K'$. The exponential multiplier then contributes to the phase-shift function a term

$$\frac{i\tau'}{\pi} \left(\frac{\pi}{4K} \right)^2 [(\beta - 2i\mu)^2 - (\beta + 2i\mu)^2] = +\frac{\pi\mu}{2KK'}\beta . \quad (A4)$$

For $K \to \infty$, $K' \to \frac{1}{2}\pi$, this phase contribution becomes $+\mu\beta/K$ and changes by $+4\mu$ from $\beta = -2K$ to $+2K$, that is, between the two cutoffs. Thus the phase shift is

$$\phi_{XYZ}(\beta) = \frac{+\mu\beta}{K} - i \ln \left[\theta_1 \left(\frac{\pi}{4K'}(i\beta + 2\mu) \right) \Big/ \theta_1 \left(\frac{\pi}{4K'}(i\beta - 2\mu) \right) \right] , \quad (A5)$$

where the θ_1's have $\tau' = iK/K'$.

In the $K \to \infty$ limit, we have

$$\phi_{XYZ}(\beta) = \frac{+\mu\beta}{K} - i \ln \left(\frac{\sinh\frac{1}{2}(\beta - 2i\mu)}{\sinh\frac{1}{2}(\beta + 2i\mu)} \right) \quad (A6)$$

from which the total phase change between the cutoffs $-2K, 2K$ is zero (or 2π, depending on the sheet convention for the logarithm).

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