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Is the finite-temperature sine-Gordon soliton mass discontinuous?

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Abstract. The integrability of a quantum sine-Gordon model allows finite densities of zero binding energy 'bound states' at finite temperatures for certain values of the coupling constant. At these same coupling strengths, the usual Yang and Yang formulation of Bethe ansatz thermodynamics appears to predict discontinuities in some elementary excitation masses, for example solitons. This is examined in two limits—free fermions and free bosons. The apparent discontinuity turns out to be an artefact of the formalism, common to all cases where zero binding energy bound states exist.

Chung and Chang [1] have recently reiterated their startling claim that, at finite temperatures, the mass of the quantum sine-Gordon soliton changes discontinuously as the coupling parameter passes through the values $\mu=\pi(1-n^{-1})$, where n is an integer. If real, such a soliton mass change could perhaps be observed by, for example, varying the pressure on a suitable quasi-one-dimensional physical system. However, we argue here that there is in fact no physical change in the soliton as the coupling passes through these values, and the apparent discontinuity is merely an artefact of the Bethe ansatz thermodynamic formalism, or, more precisely, of its interpretation by Chung and Chang.

As originally formulated by Yang and Yang [2], the thermodynamic analysis begins with the observation that a single state of an integrable system can be labelled by the set of momenta $\{k_i\}$ of the individual excitations (for technical reasons, it is better to use rapidities α_i in the sine-Gordon system [3]). In the limit of a large system, a state is described by the densities of the different excitations $\rho_j(\alpha)$ in rapidity space, where j labels solitons, breathers, etc. The function $\varepsilon_j(\alpha)$ is defined in terms of the ratio of empty state density $\tilde{\rho}_j$ to ρ_j by

$$\tilde{\rho}_j(\alpha)/\rho_j(\alpha)=\exp(\varepsilon_j(\alpha)/T). \tag{1}$$

In the standard Yang and Yang treatment, one considers a representative state of the thermodynamic ensemble corresponding to given macroscopic particle densities and minimises the free energy to obtain the following equation for $\varepsilon_j(\alpha)$:

$$\varepsilon_j(\alpha)=E_j(\alpha)+\frac{T}{2\pi}\sum_i \operatorname{sgn}(i)\frac{\partial}{\partial\alpha}\Delta_{ij}*\ln[1+\exp(-\varepsilon_i/T)]. \tag{2}$$

Here $E_j(\alpha)$ is the dispersion curve of the j particle in the physical vacuum, and the second term, where the star denotes convolution, gives the shift in the j-particle energy total from the presence of other excitations, usually referred to as the backflow. Thus, $\varepsilon_j(\alpha)$ looks like the total (dressed) excitation energy of the particle at finite temperature. For technical details, such as the sgn(i) term, see [1, 4]. Yang and Yang also showed that, if a particle is moved from rapidity α to rapidity β, the energy change in the system is

$$\Delta E = \varepsilon_j(\beta) - \varepsilon_j(\alpha). \tag{3}$$

One might conclude from equations (2) and (3) (as Chung and Chang [1] did) that $\varepsilon_j(\alpha)$ is always the dispersion curve of a real physical excitation. In fact this is correct at zero temperature—the $\varepsilon_j(\alpha)$ do go precisely to the well known sine-Gordon excitation spectra of solitons, antisolitons and breathers. One also finds that the method predicts a temperature-dependent sine-Gordon soliton mass which in the classical limit agrees with transfer matrix results [5].

However, there is one important special situation where we shall see that the function $\varepsilon_j(\alpha)$ does *not* correspond directly to a physical excitation curve at non-zero temperature. This is the case where a zero binding energy bound state is present. Such a 'bound state', which is really just two (or more) excitations travelling together, can survive in an integrable system (in contrast to any other environment), because the infinite number of conservation laws imply that, in any scattering event, the outgoing set of particle momenta is precisely the same as the ingoing set. At finite temperatures, this survival is less clear—the non-integrable heat bath perturbation would presumably tend to break up these states. We return to this point later, noting here that just dropping these states from consideration would lead to incorrect results in some known limits.

Perhaps the simplest way to illustrate the role of these zero binding energy states is to consider the particular limit of the quantum sine-Gordon system in which the soliton mass goes to infinity, but the phonon mass stays constant [6]. This is the 'classical limit' $\mu \to \pi$ but with $\hbar$ held fixed and with temperatures also of order $\hbar$. In other words, we are considering only vanishingly small thermal excitation of an ordinary classical sine-Gordon system, so in the sine-Gordon Hamiltonian we can replace cos ϕ by $1 - \frac{1}{2}\phi^2$, giving the Hamiltonian of a free massive boson (phonon) gas. This system is certainly fully understood and, in particular, the phonon mass has no temperature dependence. The standard Bethe ansatz analysis of this limit is, however, surprisingly complicated. There is a whole sequence of breather excitations, the lowest of which is the phonon of mass m at zero temperature; the others are zero binding energy bound states of phonons, having masses $2m$, $3m$, ... Each breather has an $\varepsilon_j(\alpha)$ defined by (1) above, so one might conclude that $\varepsilon_1(0)$ is the phonon mass at finite temperatures. In fact, the limiting set of Yang and Yang thermodynamic equations can be solved analytically, and $\varepsilon_1(0)$ varies rapidly with temperature. Thus it is clear that $\varepsilon_1(\alpha)$ at non-zero temperature is *not* the dispersion curve of the boson! What, then, is its physical significance? Equation (1) is still correct—it gives the ratio of empty states to filled states. But—and this is the crucial point—with the zero binding energy breathers present, the minimisation of the free energy includes arranging the bosons among all these differently labelled but physically equivalent boxes to maximise the entropy, and, as the temperature varies, so does the appropriate optimum distribution of bosons among the breather states. Thus, the bosons present in a small part of momentum space Δk can be arranged into free bosons, 'bound state' of two, three, etc, for Bethe ansatz bookkeeping purposes and entropy maximisation, without affecting the physical nature of the state. Therefore $\varepsilon_1(\alpha)$, which measures the occupancy of the 'free' state, is not a physically accessible dispersion curve but merely an indicator of how the (actually free) bosons are distributed to maximise the entropy term in the Bethe ansatz description.

There is another free gas limit of the sine-Gordon system. At $\mu = \frac{1}{2}\pi$, it is a free-fermion gas of solitons and antisolitons (which for this μ are just holes in the filled Dirac sea of negative-energy soliton states). For μ strictly equal to $\frac{1}{2}\pi$ the Bethe ansatz thermodynamics is exactly that of a free Fermi gas—the scattering phase shifts are zero, so the problem becomes trivial. However, if instead one takes the limit to $\mu = \frac{1}{2}\pi+$ from above, possible excitations include the soliton, antisoliton and breather—there is only one breather, whose binding energy goes to zero in the limit. (There also exist so-called long strings, which we will discuss shortly.) This limit has some resemblance to the one described above. That is to say, the physical situation—the distribution in momentum space of the constituent particles—is the same for $\mu = \frac{1}{2}\pi$ as for $\mu = \frac{1}{2}\pi + \delta$ as $\delta \to 0$, but the same configuration is described by different sets of occupation probabilities. In the latter case ($\mu = \frac{1}{2}\pi+$) an extra zero binding energy breather state is available, so some density of solitons and antisolitons will go into it to maximise entropy. In the case $\mu = \frac{1}{2}\pi$ this state is not there. Thus the actual density of solitons labelled as 'free' will change discontinuously between $\mu = \frac{1}{2}\pi$ and $\mu = \frac{1}{2}\pi+$, but 'free' here, as above, is a Bethe ansatz bookkeeping label, of no physical significance for the soliton involved.

In fact, the full quantitative analysis of the discontinuity in the soliton occupation parameter $\varepsilon_s(\alpha)$ between $\mu = \frac{1}{2}\pi$ and $\mu = \frac{1}{2}\pi+$ is complicated by the presence at $\mu = \frac{1}{2}\pi+$ of so-called long strings (or Korepin excitations [7]). These arise because the phase shift between the Bethe ansatz bare fermion excitations is non-zero and for $\mu = \frac{1}{2}\pi + \delta$ has a 2π discontinuity in the $\delta \to 0$ limit. This discontinuity gives rise to the 'binding' of the zero binding energy breather (which, of course, for finite δ would have finite binding energy) and also that of the long strings of length 3, 5, 7, ...

We now show in detail how the arrangement of particles for $\mu = \frac{1}{2}\pi+$ among these excitations is equivalent to the $\mu = \frac{1}{2}\pi$ free Fermi gas [4]. When periodic boundary conditions are imposed, then, with the usual 'fermionic' choice of branch for the phase shifts, each momentum state k_j available for an entity of type i can be associated with an integer or half-integer quantum number I_j^i. In a particular eigenstate when the momentum corresponding to I_j^i is present we say there is a type-i 'particle' present; conversely, the absence of the momentum (i.e. leaving I_j^i unfilled) is defined as the presence of a 'hole' of type i. In the usual formulation of Bethe ansatz thermodynamics, these quantum numbers I_j^i play a crucial role: the density of type-i particles or holes in k space is defined in terms of the density of occupied or unoccupied quantum numbers. It is in particular the density of holes in the Dirac sea, *defined in this manner*, that is discontinuous as μ changes from $\frac{1}{2}\pi$ to $\frac{1}{2}\pi+$.

We have previously shown, however, that physically indistinguishable 'gaps' in the Dirac sea can be created in an entirely different way—by the phase shifts between sea particles and strings. For example, in the limit $\mu = \frac{1}{2}\pi+$, a 1-string with rapidity β induces a local depletion in the Dirac sea at rapidity $\beta + \mathrm{i}\pi$, with the lost density adding up to one fermion. Thus when $\mu = \frac{1}{2}\pi+$, the real-rapidity fermion is equivalent to a *free* ($\mu = \frac{1}{2}\pi$) fermion (soliton) plus a hole (antisoliton), which is to say a sine-Gordon breather (of zero binding energy). We emphasise that the 'gap' opened by the phase shift is indistinguishable from a 'hole', defined as above; however the former does *not* arise from leaving a sea-particle quantum number unpaired. Gaps in the Dirac sea are also opened by long strings. In the limit $\mu = \frac{1}{2}\pi+$, the fermions forming these strings lie on the real axis or the $i\pi$ line in rapidity space (mod $2\pi i$). By its phase shifts with the sea, a string introduces a gap of one sea particle; hence a string of length $2l+1$ becomes equivalent to l free fermions and l free sea particles. In the equilibrium thermodynamic state, a portion of the holes in the Dirac sea will be filled in by these extra particles, and in fact it turns out that exactly one half of the holes are so filled. Thus one can say that in the limit $\mu = \frac{1}{2}\pi+$ half of the sea holes combine with long strings to leave free positive-energy particles (i.e. solitons), while the other half remain unpaired and correspond to free antisolitons.

If we add together all of the indistinguishable antifermions (the unpaired holes plus the gaps induced by 1-strings, the total density of antifermions in the limit $\mu = \frac{1}{2}\pi+$ is

$$\rho^{\delta}_{\text{total}} = \rho^{\delta}_{1} + \tfrac{1}{2}\rho^{\delta}_{\text{h}} \tag{4}$$

which turns out to be exactly equal to the density of holes ρ^0_{h} found in the case $\mu = \frac{1}{2}\pi$. That is, the apparent discontinuity in the antifermion density as μ goes from $\frac{1}{2}\pi$ to $\frac{1}{2}\pi+$ is a consequence of including only the 'holes' (corresponding to unfilled quantum numbers) and overlooking the indistinguishable 'gaps' induced by the strings. Because the density of sea fermions and (it turns out) fermions with real rapidity do not change in going from $\mu = \frac{1}{2}\pi$ to $\frac{1}{2}\pi+$, neither would the wavefunction of a system in the equilibrium state. The actual density of excitations in rapidity space is related to ε by

$$\rho \propto \frac{\partial}{\partial T} \ln[1+\exp(-\varepsilon/T)]. \tag{5}$$

To find a physical dispersion relation in light of equations (4) and (5), a reasonable definition for the ε function for antifermions in the case $\mu = \frac{1}{2}\pi + \delta$, $\delta \to 0$, is

$$\ln[1+\exp(-\varepsilon^{\delta}_{i}/T)] + \tfrac{1}{2}\ln[1+\exp(-\varepsilon^{\delta}/T)] = \ln[1+\exp(-\varepsilon^{\delta}_{\text{h}}/T)] \tag{6}$$

which leads immediately to the result that $\varepsilon^{\delta} = \varepsilon^{0}$, i.e. the antifermion (or antisoliton) mass is continuous. This same analysis easily explains the discontinuity at any value $\mu = \pi(1-1/n)$. For all these values the discontinuity is generated by zero binding energy bound states.

Finally, we should like to make some comments on the general question of the thermodynamics of integrable systems, discussed by Chung and Chang. A particular quantum state of an integrable system can be labelled $\{k_i\}$. Naturally, the heat bath interaction is not diagonal in this basis, and the overall state of system plus bath is represented as a mixed state of the system, expressed in the standard (density matrix) way as a sum over eigenstates of the system Hamiltonian alone. This is the same technique as for any other system. It has been remarked [1] that the intrinsic interaction of an integrable system does not bring about thermal equilibrium, but in fact no intrinsic interaction does. A complicated system in a single quantum state, if isolated, remains in that state. The special feature of an integrable system is that the single quantum state is much easier to describe and visualise. Of course, a sufficiently large interaction between an integrable system and the outside world (heat bath) might distort the system sufficiently that the standard analysis based on unperturbed eigenstates is no longer useful. In this case, the Yang and Yang analysis would no longer be valid. To find quantitatively how big an interaction gives what deviation would be mathematically very difficult, but it is clear that in fact the analysis based on integrability is not as fragile as it might seem. For example, in the classical limit of sine-Gordon thermodynamics, the Bethe ansatz analysis gives a result indistinguishable from numerical analysis of a discretised chain, yet the discretisation used certainly destroys the integrability. Another example is provided by the Kondo system. For iron impurities in copper, the Yang and Yang analysis yields results for the temperature-dependent specific heat and susceptibility indistinguishable from experiment (i.e. within ~1% or so), yet the Hamiltonian describing an iron impurity certainly differs significantly from the simple Kondo model used. These results may be further examples of Araki's theorem [8] that for one-dimensional systems at finite temperatures the free energy and its derivatives vary smoothly with coupling parameters, in particular with the strength of the non-integrable perturbation. In any event, the integrable Yang and Yang thermodynamics evidently describes successfully the properties of systems having significant non-integrable perturbations.

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