# Thermodynamics of the sine-Gordon field*

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(Received 18 March 1977)

We comment on a recently published paper of Gupta and Sutherland on the thermodynamics of the sine-Gordon chain. We present a short alternative derivation of the various thermodynamic functions in the high- and low-temperature limits. While our mathematical results essentially agree with theirs, we propose a different physical interpretation.

## I. INTRODUCTION

In this Comment, we examine the recent calculation of the classical statistical mechanics of the sine-Gordon field by Gupta and Sutherland[1] (hereafter GS). Using the functional integral approach, GS have calculated a partition function for a field with nonperiodic boundary conditions, or net winding number $N$. This they do by treating $N$ as a thermodynamic variable in a grand canonical ensemble. GS base their interpretation of the results on the behavior of the intensive thermodynamic functions, or densities, such as the internal free energy per unit length, $u$, or on other fields such as the winding-number chemical potential $\mu$. For example, at zero temperature, $\mu$ is essentially the classical energy of formation of a single soliton whose value is 8 in these units, and they conclude, therefore, that solitons are stable. However, since at any finite temperature and vanishing density $N/L$, $\mu \simeq 0$, their localization and stability criteria lead them to conclude that the few-soliton solutions are unstable with respect to thermal fluxtuations.

We calculate the classical statistical mechanics of the sine-Gordon field in the limits of very high and low temperature. Our results do not have as large a range of validity as that of GS, but they suffice for interpretation, and they allow us to express various thermodynamic functions in a transparent form. Our physical interpretation, which is distinct from that of GS, is familiar in the theory of the equilibrium properties of chemical reactions. We distinguish three "reactants": solitons $s$, antisolitons $\bar{s}$, and continuum excitations $C$. We show that in first approximation, the thermodynamics of the sine-Gordon field is equivalent to the thermodynamics of the "chemical reaction"

$$s + \bar{s} \rightleftarrows C.$$

That is, apart from the pair creation mechanism, solitons behave as a classical gas of free particles. This is an important conceptual remark for it suggests how to treat, at least approximately,

the thermodynamics of a large class of nonlinear field models. In the case of the sine-Gordon equation, it will be shown elsewhere that there are other reasons, stemming from the known exact solutions of the equations of motion, to support our interpretation.

In the following we adopt the same notation as GS to facilitate comparison of the results.

## II. CLASSICAL CANONICAL PARTITION-FUNCTION CALCULATION

Gupta and Sutherland set out to calculate, using the transfer integral techniques, the classical canonical partition function $Z$ of the one-dimensional sine-Gordon field $\phi$ which satisfies the following equation and boundary conditions[2]:

$$\phi_{tt} - \phi_{xx} + \sin\phi = 0, \tag{1}$$

$$\phi(0) = 0, \quad \phi(L) = 2\pi N, \tag{2a}$$

$$\dot{\phi}(L) = \dot{\phi}(0) = 0. \tag{2b}$$

It is straightforward to show that $Z$ can be expressed [see Eq. (96) in GS] in the thermodynamic limit as

$$Z = \lim_{L \to \infty} \lim_{M \to \infty} \left(\frac{2\pi}{\beta}\right)^M \int_{-1/2}^{1/2} dk \exp\left[-\beta L\left(\frac{a_0(4\beta^2, k)}{8\beta^2} + 1\right) - 2\pi i N k\right] |\Phi_k(0)|^2, \tag{3}$$

where $M$ is the number of divisions of the length $L$ required by the transfer integral technique, $\Phi_k(\phi)$ is the transfer operator eigenfunction labeled by the Floquet wave vector $k$, $a_0(q, k)$ is the eigenvalue of Mathieu equation in the standard notation,[3] $\beta \equiv T^{-1}$ where $T$ is the temperature ($k_B \equiv 1$). We make the following definitions:

$$n \equiv \left|\frac{N}{L}\right|, \quad f \equiv \frac{-T}{L}\ln(Z), \quad u \equiv \frac{1}{L}\frac{\partial \ln(Z)}{\partial \beta},$$

$$\mu \equiv \left(\frac{\partial f}{\partial n}\right)\text{sgn}(N),$$

where $n$ is the winding number density, $f$ the free energy per unit length, $u$ the internal energy per unit length, and $\mu$ the chemical potential.

Rather than changing to a grand canonical partition function, we shall calculate $Z$ directly. Since $\Phi_k(0)$ is a slowly varying function of $k$, we shall make no error in replacing $\Phi_k(0)$ with $\Phi_{k=0}(0)$ and factoring it from the integrand of Eq. (3). When $T$ is very large, we can approximate $a_0(q,k)$ as[4]

$$a_0(q,k) \approx -\tfrac{1}{2}q^2 + 4(1 - \tfrac{1}{2}q^2)k^2 + O(q^4), \qquad (4)$$

and calculate the thermodynamic functions $f$, $u$, and $\mu$. In this temperature regime, our results agree with those obtained by GS; for example, the internal energy density $u$ is dominated by the energy of $M$ harmonic oscillators each having two degrees of freedom.

At low temperatures, only the lowest $k$ band will contribute to Eq. (3), and for this band a tight-binding WKB calculation[5] gives

$$a_0'(k,q) = -8\beta^2 + 4\beta - 8\sigma\beta \cos 2\pi k, \qquad (5)$$

where $\sigma \equiv 8(\beta e)^{1/2}e^{-8\beta}/\pi$. The partition function $Z$ is then easily found to be

$$Z = (2\pi T)^M |\Phi_{k=0}(0)|^2 e^{-L/2} I_N(L\sigma). \qquad (6)$$

We shall consider two important cases. First, suppose $N = 0$ identically. The thermodynamic functions that we calculate should then reflect the behavior of systems for which the winding number $N$ is finite in the thermodynamic limit. We find[6]

$$f = -T[M \ln(2\pi T)/L - \tfrac{1}{2} + \sigma], \qquad (7)$$

$$u = (M/L - \sigma)T + \sigma(8 + \tfrac{1}{2}T), \qquad (8)$$

$$\mu = 0. \qquad (9)$$

The chemical potential vanishes since, as can be seen from GS, $\mu$ must be an odd function of $n$.

If the winding number density $n$ is finite, we can rewrite Eq. (6) as

$$Z = (2\pi T)^M |\Phi_{k=0}(0)|^2 e^{-L/2} I_N(N\sigma/n). \qquad (10)$$

To take the thermodynamic limit, we use the uniform asymptotic expansion[7] for $I_N$ and find for $\sigma \ll n \ll 1$

$$f = -T\{M \ln(2\pi T)/L + n \ln(\sigma/n)$$
$$-n\ln[1 + (1+\sigma^2/n^2)^{1/2}] + n(1+\sigma^2/n^2)^{1/2} - \tfrac{1}{2}\},$$
$$(11)$$

which implies

$$u = (M/L - n - \tfrac{1}{2}\sigma^2/n)T + (n + \tfrac{1}{2}\sigma^2/n)(8 + \tfrac{1}{2}T) \qquad (12)$$

$$\simeq [M/L - (n^2 + \sigma^2)^{1/2}]T + (n^2 + \sigma^2)^{1/2}(8 + \tfrac{1}{2}T), \qquad (13)$$

$$\mu = \{8 - T[\ln(\beta/\pi)^{1/2} + 2\ln 2 - \ln n] + O(T^2 \ldots)\}$$
$$\times \operatorname{sgn}(N) \qquad (14)$$

$$\cong -T \ln\left(\frac{1}{n/\sigma + (1+n^2/\sigma^2)^{1/2}}\right) \operatorname{sgn}(N). \qquad (15)$$

Equations (13) and (15) are approximations to (12) and (14), respectively, that allow us to recover the $n = 0$ results.

We emphasize that in Eqs. (12) and (14), $n$ may not be taken to zero because we have made the approximation $\sigma/n \ll 1$. If a first correction to the tight-binding band approximation, a term proportional to $\cos 4\pi k$, is included in Eq. (5), then the resulting corrections to $f$ are proportional to $n^2$. Thus Eqs. (11) to (15) are valid for $\sigma \ll n \ll 1$. In this range our results agree with those of GS; however, written in this form, the equations suggest a rather different interpretation.

Consider first the internal energy density $u$. At low temperature where $\sigma^2$ is essentially zero, Eq. (12) gives

$$u \sim n(8 + \tfrac{1}{2}T) + (M/L - n)T \qquad T \ll 1, \qquad (16a)$$

$$\sim 8n, \qquad T = 0. \qquad (16b)$$

Expanding the zero-temperature result for $u$ of GS [their Eqs. (40) and (41)] in the small-$n$ limit gives

$$u \sim 8n[1 + e^{-1/2n}(4 + 2/n) + \cdots]. \qquad (17)$$

Our perturbation theory generates a power series in the small quantity $n$ and cannot reproduce the nonanalytic corrections of Eq. (17); however, to leading order, they agree.

In the form (16a), $u$ is the sum of two contributions. The first term is just the number density of solitons times an energy per soliton that would arise at low $T$ if the solitons were free relativistic particles of mass 8 in the units of GS. The second term is the energy density of harmonic or continuum excitations $MT/L$ less an energy $nT$ which means that *for every soliton, one continuum mode* (with two degrees of freedom) *is lost.*[8]

Now consider the role of $\sigma$. Dimensionally, it is a number density just as $n$. It is proportional to the Arrhenius factor, $e^{-E\beta}$, with energy of activation $E$ equal to the rest energy of a soliton. Furthermore, a comparison of Eq. (16a) and Eq. (8) shows that in the internal energy $u$, $\sigma$ plays the same role as $n$. Hence we are led to interpret $\sigma$ as the thermally activated soliton density. Thus in Eq. (13), $(n^2 + \sigma^2)^{1/2}$ plays the role of the effective density of solitons.

We examine now the chemical potential $\mu$. Equation (14) is a form appropriate for a small, but finite $n$ in the limit $T \to 0$, while Eq. (15) is for small but finite $T$ in the limit $n \to 0$. Thus

$$\lim_{n \to 0} \lim_{T \to 0} \mu = 8 \operatorname{sgn}(N), \qquad \lim_{T \to 0} \lim_{n \to 0} \mu = 0. \qquad (18)$$

The $T = 0$ result [Eq. (14)] is just the rest mass,

8, of the solitons plus corrections proportional to $T \ln n$ and $T \ln T$ as one would expect for a noninteracting gas of particles of mass 8 and density $n$. The solitons do, of course, interact via a short-range force, and the first virial corrections come from an inclusion of $\cos 4\pi k$ in the approximation Eq. (5).

At any finite $T$, $\mu$ vanishes with $n$. In order to understand this, we propose the following model. Imagine solitons $s$, antisolitons $\bar{s}$, and continuum excitations $C$, to be in thermal equilibrium. We treat each of these three excitations as reactants in a chemical equilibrium problem. Moreover, we postulate that the $s$ and $\bar{s}$ reactants are free except for a pair creation and destruction mechanism through which they are in equilibrium with the $C$ reactant

$$s + \bar{s} \rightleftharpoons C. \qquad (19)$$

(This is, of course, analogous to the electron-positron gas in thermal equilibrium with a photon gas.[9]) The condition for equilibrium is

$$\mu_s + \mu_{\bar{s}} = \mu_C. \qquad (20)$$

Since the chemical potential $\mu_C$ for the harmonic continuum excitations vanishes, we have

$$\mu_s + \mu_{\bar{s}} = 0. \qquad (21)$$

Now if we take $n \to 0$, there will be no net winding number, and so the number of $s$ and $\bar{s}$ are equal, or $\mu_s = \mu_{\bar{s}}$. Combining this with Eq. (21), we see

$\mu_s = \mu_{\bar{s}} = 0.$

It is now easy to see why the limits $n \to 0$, and $T \to 0$ cannot be interchanged in the calculation of $\mu$. Taking $n$ to zero enforces an additional chemical constraint on $\mu_s$ and $\mu_{\bar{s}}$, which when taken together with the condition $\mu_s = -\mu_{\bar{s}}$, causes $\mu$ to vanish. That is $n = 0$ is an intrinsically different thermodynamic (chemical) equilibrium than $n \neq 0$. Hence, since the chemical potential is precisely the measure of this difference, we should not expect

$$\lim_{n \to 0} \lim_{T \to 0} \mu = \lim_{T \to 0} \lim_{n \to 0} \mu.$$

Finally, we note that these interpretations are consistent with those of Krumhansl and Schrieffer[10] in the "$\varphi^4$" problem; there, however, the winding number $N$ is not physically relevant.

## III. CONCLUSION

We have presented an alternative derivation and interpretation of the thermodynamics of the sine-Gordon chain of GS. In our picture, the solitons appear as important excitations of the system at low temperature and behave much like a gas of noninteracting particles. To a first approximation, the thermodynamics of the sine-Gordon equation is that of a chemical reaction in which the nonlinear excitations (solitons and antisolitons) are in equilibrium, via a pair creation mechanism, with the linear or continuum excitations.

*Work supported by the ERDA Contract No. EY-76-S-02-3161, Technical Report No. COO-3161-55.

[1]N. Gupta and B. Sutherland, Phys. Rev. A 14, 1790 (1976).

[2]Note, if we choose the boundary conditions $\phi(L) - \phi(0) = 2\pi N$, then the $|\Phi_K(0)|^2$ would not appear in Eqs. (3), (6), and (10).

[3]M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (U.S. Dept. of Commerce, Washington, D.C., 1972), Chaps. 9 and 20.

[4]See Eq. (20.3.15) of Ref. 3.

[5]See Eq. (20.2.30) of Ref. 3. Details of this WKB calculation will appear in a future publication by J. F. Currie, A. R. Bishop, and J. A. Krumhansl.

[6]Use was made of Eq. (9.7.1) of Ref. 3.

[7]See Eq. (9.7.7) of Ref. 3.

[8]K. Kawasaki, Prog. Theor. Phys. 55, 2029 (1976).

[9]L. D. Landau and E. M. Lifshitz, Statistical Physics, 2nd ed. (Addison-Wesley, Reading, Mass., 1970), see Sec. 107.

[10]J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B 11, 3535 (1974).