Statistical Mechanics of the Sine-Gordon Equation

J. Timonen
Department of Physics, University of Jyväskylä, SF-40100 Jyväskylä, Finland
and
M. Stirland, D. J. Pilling, Yi Cheng, and R. K. Bullough
Department of Mathematics, University of Manchester Institute of Science and Technology, Manchester M60 1QD, United Kingdom
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We give two fundamental methods for evaluation of classical free energies of all the integrable models admitting soliton solutions; the sine-Gordon equation is one example. Periodic boundary conditions impose integral equations for allowed phonon and soliton momenta. From these, generalized Bethe-*Ansatz* and functional-integration methods using action-angle variables follow. Results for free energies coincide, and coincide with those that we find by transfer-integral methods. Extension to the quantum case, and quantum Bethe *Ansatz*, on the lines to be reported elsewhere for the sinh-Gordon equation, is indicated.

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The quantum and classical sine-Gordon (s-G) equations are of fundamental importance: The classical case is integrable by the inverse (spectral-transform, ST) method,[1] and the normally ordered quantum s-G equation is solved for eigenspectra and eigenstates by the Bethe *Ansatz* (BA)[2] and quantum-inverse method (QIM).[3] The statistical mechanics of either case is equally important: The quantum statistical mechanics includes quantum mechanics as a special case; Bose-Fermi equivalence is superbly illustrated[1,2] in different ways[4] in these quantum cases. The classical case has fundamental importance as a test of calculation methods,[4] and both the classical and quantum statistical mechanics (SM) have application to experiment.[5]

In this Letter we draw together the different approaches to the quantum and classical SM of the s-G equation. For simplicity of report we focus primarily on the classical SM. Reference to related work[4] on the quantum and classical SM of the sinh-Gordon (sinh-G) equation indicates the interrelation of the classical and quantum calculations.

The classical s-G equation is

$$\phi_{xx} - \phi_{tt} = m^2 \sin\phi, \tag{1}$$

where $\phi_{xx} \equiv \partial^2\phi/\partial x^2$, etc., and m is a mass ($\hbar = c = 1$). It is Hamiltonian and completely (Liouville[1,6]) integrable, with ($H \equiv H[\phi]$)

$$H \equiv \gamma_0^{-1} \int dx \{ \tfrac{1}{2}\phi_t^2 + \tfrac{1}{2}\phi_x^2 + m^2(1-\cos\phi) \}, \tag{2}$$

Poisson bracket $\{\Pi, \phi\} = \delta(x-x')$ (and $\Pi = \gamma_0^{-1}\phi_t$), and dimensionless coupling constant γ_0, becoming the linear Klein-Gordon (K-G) equation for $\gamma_0 \to 0$ in both the classical[6] and quantum[7] cases. The classical integrability means there are action-angle variables[6,8]

$$\{p_i, q_i; \bar{p}_j, \bar{q}_j; \hat{p}_l, \hat{q}_l; 4\gamma_0^{-1}\theta_l, \Phi_l; P(k), Q(k)\}, \tag{3}$$

with obvious Poisson brackets, such that H can be expressed in action variables alone[6,9] as

$$H[p] = \textstyle\sum_i E(p_i) + \sum_j E(\bar{p}_j) + \sum_l E_b(\theta_l, \hat{p}_l) + \int_{-\infty}^{\infty} \omega(k) P(k)\, dk \tag{4}$$

($1 \le i \le N_k$; $1 \le j \le N_{\bar{k}}$; $1 \le l \le N_b$), where $\omega(k) = (m^2+k^2)^{1/2}$, $E(p) \equiv (M^2+p^2)^{1/2}$, and $E_b(\theta,p) \equiv (4M^2 \sin^2\theta + p^2)^{1/2}$. The phase spaces are known.[6,9] The mass is $M \equiv 8m\gamma_0^{-1}$.

The relative simplicity of $H[p]$ suggests that the coordinates (3) are the ones to use in evaluation of both the partition function Z and the correlation functions. In the classical limit Z is the functional integral

$$Z = \int \mathscr{D}\Pi\, \mathscr{D}\phi \exp(-\beta H[\phi]), \tag{5}$$

with $\beta^{-1} \equiv T$ the temperature. Instead, as also in Ref. 4, the idea is to evaluate Z in the form

$$Z = \int \mathscr{D}\mu \exp(-\beta H[p]), \tag{6}$$

where $\mathscr{D}\mu$ is a measure to be determined. It is the quantum form of (6) which relates directly to the methods of BA and QIM, for the coordinates (3) are expressible in terms of the spectral data of the classical ST,[1–4,6] and these data relate in turn to the k-space formulation of the BA method[2] and the operators and operator algebra of the QIM.[3]

Reference 4 calculates $F = -\beta^{-1}\ln Z$ for a large *class* of quantum integrable models in terms of spectral data. Here we extend that work to include all cases admitting soliton solutions and focus on the classical s-G equation as one important physical example.

The essence of the problem (and cf. Ref. 4) is to impose periodic boundary conditions, period $L < \infty$, so that a proper finite-density thermodynamic limit can be taken for $L \to \infty$. We give three methods. The first is a generalized form of the BA, taken here in classical form[4]: In effect this method uses the coordinates (3)[9] and *no Ansatz whatsoever.* The second evaluates (6) by use of the coordinates (3).[9] And the third uses the familiar[4,6] classical transfer-integral method (TIM) on (5). The resultant expressions for FL^{-1}, the free energy per unit length, totally coincide—establishing the two new methods in their classical context and, by implication, bringing together quantum BA,[2] the various generalizations of it that we shall report,[4,10] the QIM,[3] and the quantum functional-integration method which generalizes (6).[4]

The analysis of (5) by the TIM for the s-G equation is well studied[6,11] and *ad hoc* methods for it are also reported,[11,12] so that we shall not give details here. In both of the two new methods that we report, the "classical BA" and the method based on (6), our starting point is a generalization of the periodicity condition given in a simpler form for the no-soliton case in Ref. 4. First we replace $H[p]$ by $H[\tilde{p}]\equiv\tilde{H}$, where

$$\tilde{H}=\sum_i E(\tilde{p}_i)+\sum_j E(\tilde{\bar{p}}_j)+\sum_n \tilde{\omega}_n P_n, \tag{7}$$

with $\tilde{\omega}_n\equiv(m^2+\tilde{k}_n^2)^{1/2}$, and, conveniently, $-\frac{1}{2}N_{\rm ph}\leq n\leq\frac{1}{2}N_{\rm ph}$ and $N_k+N_{\bar{k}}+(N_{\rm ph}+1)=N+1$ ($N_{\rm ph}$ is even, for convenience): $P_n\leftrightarrow 2\pi L^{-1}P(\tilde{k}_n)$, while (8), which follows, shows that $\tilde{p}_i,\tilde{\bar{p}}_j,P(\tilde{k}_n)2\pi L^{-1}\to p_i,\bar{p}_j,P(k)dk$ as $L\to\infty$. Evidently (7) extends the oscillator contributions, which alone survive for the sinh-G equation,[4] to include additional kink and antikink contributions.[13] Work on a lattice form of the s-G equation under periodic boundary conditions[9] shows that (7) is correct to $O(L^{-1})$ for a lattice with $N+1$ lattice points, spacing a, in a period $L=(N+1)a$. Floquet theory[4,6] then shows in this case that to $O(L^{-1})$

$$\begin{aligned}L\tilde{k}_n&=Lk_n-\sum_m{}'\Delta(\tilde{k}_n,\tilde{k}_m)P_m+\sum_i\Delta_k(\tilde{k}_n,\tilde{p}_i)+\sum_j\Delta_{\bar{k}}(\tilde{k}_n,\tilde{\bar{p}}_j),\\ L\tilde{p}_k&=Lp_k-\sum_m\Delta_k(\tilde{k}_m,\tilde{p}_k)P_m-\sum_i{}'\Delta_{kk}(\tilde{p}_k,\tilde{p}_i)-\sum_j\Delta_{k\bar{k}}(\tilde{p}_k,\tilde{\bar{p}}_j),\end{aligned} \tag{8}$$

and a similar expression for $L\tilde{\bar{p}}_l$ $(-\frac{1}{2}N_{\rm ph}\leq m,n\leq\frac{1}{2}N_{\rm ph}$, etc.). The $\sum'$ omits the index on the left-hand sides and $Lk_n=2\pi n$. Other terms $O(1)$ are omitted since they do not contribute as $L\to\infty$.

Solely from the analytical properties of the transmission coefficient $a(\zeta)$ of the ST we then show that [to $O(L^{-1})]^{4,6}$

$$\Delta(k,k')=\gamma_0 m^2/4[k\omega(k')-k'\omega(k)], \tag{9a}$$

$$\Delta_k(k,p)=-2\tan^{-1}\{m/\gamma[k-v\omega(k)]\}, \tag{9b}$$

with $\Delta_{\bar{k}}(k,p)=\Delta_k(k,p)$, and $\Delta_{kk}(p,p')=\Delta_{\bar{k}\bar{k}}(p,p')=\Delta_{k\bar{k}}=\Delta_{\bar{k}\bar{k}}$ $[\equiv\Delta_{kk}(\alpha,\alpha')]$. It is convenient to work first of all in rapidities α,β, such that $p=M\sinh\alpha$, $k=m\sinh\beta$, $\omega(k)=m\cosh\beta$, etc. Later we use $p=Mv\gamma$, $\gamma\equiv(1-v^2)^{-1/2}$. In rapidities,

$$\frac{\partial}{\partial\alpha}\Delta_{kk}(\alpha,\alpha')=\frac{8}{\gamma_0}\ln\frac{\cosh(\alpha-\alpha')-1}{\cosh(\alpha-\alpha')+1}, \tag{10}$$

and so on for $\Delta_{\bar{k}k}$, etc. Evidently Δ_k $(\Delta_{\bar{k}})$ is the kink (antikink) phonon phase shift[6,14] and, e.g., (9a) is the classical limit $(\gamma_0\to 0)$ of the two-body S-matrix phase shift for the quantum s-G equation.[3,4,15] Likewise the kink (antikink) momenta are "back" phase shifted by the phonons (terms in P_m). The *derivative* (10) is the classical kink-kink coordinate phase shift in rapidity variables[16] and also derives from an S-matrix shift for $\gamma_0\to 0$.[15]

Despite the strictly classical nature of the analysis sketched here it is still important[4,6] to distinguish "Bose" shifts $\Delta_b(k,k')$ and "Fermi" shifts $\Delta_f(k,k')$ related by[4,6] $d\Delta_b/dk=d\Delta_f/dk-2\pi\delta(k-k')$. Evidently,[4] (9a) is Bose; but (9b) will here be interpreted as a Fermi shift[2,4] in the sense that Δ_k is the continuous branch of the $\tan^{-1}$ function such that $\Delta_k\to -2\pi$ for parameter $k\to-\infty$, and $\Delta_k\to 0$ for $k\to+\infty$. The reason for interpretation of the kinks (antikinks) as fermions is that the expressions (4) [i.e., (7)] for $H[\tilde{p}]$ assume that all kinks and antikinks together must necessarily have *distinct* momenta $p_i,\bar{p}_j$[7]: This is a classical property equivalent to the assumption that the spectral datum $a(\zeta)$ has simple zeros.[1,6,8] Transformation to variables (3) is canonical under this condition.[8] In this sense the kinks (antikinks) are classical fermions!

From Eqs. (5) and (6) it is easy to derive integral equations for the corresponding shifted energies which minimize the free energy $FL^{-1}=(E-\beta^{-1}S)L^{-1}$: The procedure is a generalization of that reported in Ref. 4. In rapidities these prove to be

$$\epsilon(x)=\omega(x)+\frac{1}{2\pi\beta}\int_{-\infty}^{\infty}\frac{d\Delta}{dx}\ln[\beta\epsilon(x')]dx'+\frac{2}{2\pi\beta}\int_{-\infty}^{\infty}\frac{d\Delta_k}{dx}e^{-\beta\tilde{E}(x')}dx', \tag{11a}$$

$$\tilde{E}(x)=E(x)-\frac{2}{2\pi\beta}\int_{-\infty}^{\infty}\frac{d\Delta_{kk}}{dx}e^{-\beta\tilde{E}(x')}dx'-\frac{1}{2\pi\beta}\int_{-\infty}^{\infty}\frac{d\Delta_k}{dx}\ln[\beta\epsilon(x')]dx', \tag{11b}$$

with, now, $\omega(x)\equiv m\cosh x$ and $E(x)\equiv M\cosh x$, while, in rapidities, $\Delta\equiv\Delta(x-x')$, etc. In the calculations for the entropy S the kinks and antikinks are treated separately as Maxwell-Boltzmann particles—explaining the $e^{-\beta\tilde{E}(x)}$ forms. Since the energies and relevant phase shifts are the same for both kinks and antikinks it is unnecessary to distinguish the two contributions further. Still, it is also possible to carry through the analysis as though both of these particles are fermions and then, as expected,[10] $2e^{-\beta\tilde{E}(x)} \to 2\ln(1+e^{-\beta E(x)})$. Similarly the phonons are most easily treated as bosons, so that,[4] in classical limit, $\ln(1-e^{-\beta\epsilon(x)}) \to \ln[\beta\epsilon(x)]$; but they can be fermions too, or classical (Maxwell-Boltzmann) particles. If all soliton contributions are dropped, (11a) is exactly the boson integral equation in classical limit found for the sinh-G equation[4] except $\Delta \to -\Delta(\gamma_0 \to -\gamma_0)$ and rapidities are now used.

The free energy is found to be

$$\frac{F}{L} = \frac{1}{2\pi\beta}\int_{-\infty}^{\infty}\omega(x)\ln[\beta\epsilon(x)]\,dx - \frac{2}{2\pi\beta}\int_{-\infty}^{\infty}E(x)e^{-\beta\tilde{E}(x)}dx. \tag{12}$$

The coupled system (11) is solved by iteration and the result substituted in (12) to yield $F/L = (F^{(1)} + F^{(2)} + \ldots) + F_{\rm KG}$, where

$$F^{(1)} = -\beta^{-1}m\left(\frac{8}{t\pi}\right)^{1/2} e^{-1/t}[1 - \tfrac{7}{8}t - \tfrac{59}{128}t^2 - \tfrac{897}{1024}t^3 - \ldots] - \beta^{-1}m[\tfrac{1}{4}t + \tfrac{1}{8}t^2 + \tfrac{3}{16}t^3 + \tfrac{53}{128}t^4 + \ldots], \tag{13a}$$

$t \equiv (M\beta)^{-1}$, and $F_{\rm KG} = \beta^{-1}a^{-1}(\ln\beta a^{-1} + \frac{1}{2}ma)$ for a (classical) lattice of spacing a exactly as for the sinh-G equation.[4] The result for FL^{-1} is actually the analytical continuation in γ_0 from the classical free energy of the sinh-G equation[4] as $-\gamma_0 \to \gamma_0$. This is most easily seen by using the TIM on (5), with Hamiltonian (2), and performing a matched asymptotic expansion analysis—as we have done.[11] For $F^{(1)}$ the result of the TIM is exactly (13a), while both of (11) with (12) *and* the TIM independently show that

$$F^{(2)} = \frac{8m}{\pi}Me^{-2/t}\left\{\ln\frac{4C}{t} - \frac{5}{4}t\left[\ln\frac{4C}{t} + 1\right] - \frac{t^2}{32}\left[13\ln\frac{4C}{t} + 2\right] + \ldots\right\}, \tag{13b}$$

and agree at $F^{(3)}$, and apparently on all $F^{(q)}$ $(q = 4, \ldots)$ which are $O(e^{-q/t})$; C is Euler's constant. Note that the power series in (13a) has been thought of[6,7,11,12,17] as the contribution of the classical s-G breather solutions. Instead, the line of argument through (7) and (8) interprets this as large-amplitude phonon contributions.

These results demonstrate the power of the "generalized BA method" reported in this Letter: Plainly it applies to all of the classical integrable models in 1+1 dimensions. But we have also derived[18] the coupled systems (11) with (12) as the classical limit of the published forms[17] of the quantum BA for the s-G equation; and (compare Ref. 4 for the sinh-G equation) these quantum forms can themselves be found from the condition (8) (and apparently can be in Bose, Fermi, or mixed Bose-Fermi forms). Chen, Johnson, and Fowler[19,20] report a derivation of (13) from quantum BA: They obtain integral equations in a form different from but equivalent to our (11) and (12)—iterating these to the result (13).

We now show how the same periodicity conditions (8) imposed on the functional integral (6) lead to exactly the same (classical) results. We have shown already[6] that the proper measure $\mathscr{D}\mu$ in the classical limit is

$$\mathscr{D}\mu = Z_{\rm KG}\sum(N_k!N_{\bar{k}}!)^{-1}\prod\nolimits_i(2\pi)^{-1}dp_i\,dq_i\prod\nolimits_j(2\pi)^{-1}d\bar{p}_j\,d\bar{q}_j\lim\{\ldots\}, \tag{14}$$

where $0 \leq N_k, N_{\bar{k}} < \infty$, $\lim\{\ldots\} = \lim_{N\to\infty}\{\prod_n(2\pi)^{-1}dP_n\,dQ_n/Z_{\rm KG}(N)\}$ with, after relabeling against (7), $N - N_k - N_{\bar{k}} \geq n \geq 1$, and $Z_{\rm KG}(N)$ is the partition function for N linear K-G modes $[Z_{\rm KG} = \lim_{N\to\infty}Z_{\rm KG}(N)]$; $\omega(k)$ is given by (4). We then use (7) for $H[p]$ in (6) and impose (8). This means that $H[\tilde{p}]$ is not separable; and (compare Ref. 4) formal iteration of (8) leads exactly to the integral equations (11) with FL^{-1} given by (12). Apparently the quantum case goes through similarly, establishing the map from the classical action and the classical spectral data[3,6,8] to the quantum results. We give details elsewhere.[10] In using the measure (14) it is crucial to keep the phase-shift terms of (8) which are $O(L^{-1})$ on $\tilde{k}_n, \tilde{p}_i$. The lattice analysis[9] then shows that (11) with (12) are exact in thermodynamic limit.

However, the expansions (13) are only *asymptotic:* They are found by the functional-integration method by iterating (8) and carrying out the "phonon" integrals followed by the continuum limit $N \to \infty$ at finite density NL^{-1}. This way we arrive at

$$Z = Z_{\rm KG}Z_B\exp\left\{2L(2\pi)^{-1}\int_{-\infty}^{\infty}dp\exp[-\beta E(p) + \sigma_1 + \sigma_2 + \sigma_3 + \ldots]\right\}, \tag{15}$$

where $-\beta^{-1}\ln Z_B$ is ultimately identified as the "breather" (phonon) series in (13a). The "dressings" σ_i on the kink (antikink) energies $E(p)=(M^2+p^2)^{1/2}$ prove to be $\sigma_1=\ln(m\beta)$ and $\sigma_2=\ln(\gamma+1)-v\ln\bar{\gamma}$, while

$$\sigma_3=t\left[\frac{v^2\gamma-1}{\gamma+1}+\frac{1-v}{\gamma}-\ln\bar{\gamma}-\frac{2}{\gamma^3}(\ln\bar{\gamma})^2\right], \qquad (16)$$

where $\bar{\gamma}\equiv\gamma(1+v)$. These dressings yield the remaining (kink + antikink) contributions to the free energy (13). We have thus given a rigorous demonstration of a "dressing method" within the functional-integration method, in result rather like the *ad hoc* so-called "ideal gas phenomenology" for the classical s-G equation[11,12] which was able to produce expressions not too dissimilar from (16). This "dressing method" also justifies first work on the quantum s-G equation.[21]

To conclude, the two methods of calculation based on (8), "generalized BA" and "functional integration on (6)" (classical or quantum), appear quite generally to lead to the same systems of coupled integral equations and hence the same results—which include the quantum eigenspectra at $\beta^{-1}=0$. Thus both of the methods, here described for the classical s-G equation, apply to all of the quantum and classically integrable systems in $1+1$ dimensions with or without soliton solutions. Note that action-angle variables are available for all of these systems[1,6,8] and periodicity conditions like (8) can be deduced in each case.

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