Bound-state effects on the statistical mechanics of solitons in double-sine-Gordon systems

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(Received 20 March 1984)

The bound states of the spectrum of the small oscillations in the neighborhood of soliton solutions may give nontrivial contribution to the partition function when their frequencies tend to zero. We investigate the case of the double-sine-Gordon system, where the soliton solution degenerates into a pair of sine-Gordon kinks at infinite distance with a change of the symmetry of the potentials and a corresponding slowing down for the frequency of the bound state. The latter is found to be the restoring symmetry mode, and some suggestions for its treatment are given.

The statistical mechanics of classical one-dimensional systems with solitonlike solutions has been extensively studied by transfer matrix,[1,2] soliton-gas phenomenology,[1,2] and path-integral method.[3] In the latter two approaches, the study of the small oscillations around the static solitonlike solutions is required. Their spectrum can present bound states in addition to the translation mode ($\omega_0=0$) and the continuum. It was usually asserted that the knowledge of eigenfrequencies and eigenfunctions of these internal modes is unnecessary to obtain the thermodynamical properties of the system.[4] This fact stems from transfer matrix arguments[5] proving that indeed bound states contribute to the internal energy simply as harmonic oscillators. In our opinion this is true only if the frequency of the bound states is confined away from zero. However, this condition is not always verified since in many cases of physical interest, a bound state whose frequency depends on some parameters appears.[5–7] This frequency may vanish in correspondence with certain values of the parameter and may appear to drive the system towards a mode associated with a new symmetry of the potential.

In this paper we analyze the influence of such a bound state on the statistical mechanics of the double-sine-Gordon (DSG) model, which has been the object of several recent investigations.[5,8–10] This model can be used for studying the thermodynamical properties of some one-dimensional systems, such as magnetic chains,[9,11] He^3 (Ref. 12) or polymers.[10] All these systems are characterized by a set of parameters, which, in a suitable limit lead to the sine Gordon (SG) from the DSG model.[10,11]

Let us consider the following classical Lagrangian

$$\mathscr{L}=\frac{m^3}{\lambda}\int_{-l/2}^{l/2}dx\left[\tfrac{1}{2}(\phi_t^2-\phi_x^2)-V(\phi)\right] , \tag{1}$$

where l is the dimensionless length (in unity of the mass m), λ is the coupling constant, and $V(\phi)$ is the potential. Several parametrizations of V were used;[9–11] a particularly convenient one seems to be[13]

$$V(\phi,R)=1-\cos\phi+[3+\cos\phi+4\cos(\tfrac{1}{2}\phi)]/\cosh^2R \tag{2}$$

even if it does not cover all the previously studied cases.[11] At $R=0$, $V(\phi,R)$ represents a SG potential with a period 4π which remains constant as R increases and reproduces the 2π-SG potential only in the limit $R\rightarrow\infty$.

The use of R as parameter has been shown very useful in Ref. 13. Here we point out that, for $l\rightarrow\infty$, the static solutions turn out to satisfy the wave equation in the (R,x) variables. Therefore the static solitonlike solutions can be expressed in the factorized form:

$$\phi_s(x,R)=\psi(x+R)\pm\psi(R-x) , \tag{3}$$

where

$$\psi(z)=4\tan^{-1}e^z \tag{4}$$

is the well known sine-Gordon kink. The negative sign describes stable 4π kinks while the positive signs give unstable bounces, which become stable only in the 2π-SG limit ($R\rightarrow\infty$). It appears from Eq. (3) that the distance between individual 2π kinks is just $2R$ (see also Ref. 11).

Moreover in Ref. 13 the following results were found and numerically verified.

The spectrum of the linearized equation in the neighborhood of the stable solution (3) gives rise to a bound state with frequency $\omega=\omega_1(R)$ in addition to the usual translation mode and the continuum starting from $\omega=1$. The behavior of $\omega_1(R)$ is shown in Fig. 1, and for certain ranges of R, good analytical expressions are available, namely,

$$\omega_1^2(R)\simeq\begin{cases}1-\dfrac{4}{3\pi}\tanh^2 R, & R\leqslant 0.8\\ \dfrac{3}{\sinh^2 R}-\dfrac{1}{\cosh^2 R}\dfrac{\sinh(2R)+2R}{\sinh(2R)-2R}, & R\geqslant 1.2\ .\end{cases} \tag{5}$$

Hence, for $R\rightarrow\infty$,

$$\omega_1^2(R)\simeq 8\exp(-2R)\ , \tag{6}$$

proving that the bound state merges into the continuum for $R=0$ and becomes a pure translation for $R\rightarrow\infty$. In this limit, the height of the relative minimum of the potential $V(\phi=0,R)$ is just $4\omega_1^2(R)$ and tends to become the degenerate absolute minimum of the SG potential.

The bound-state eigenfunction, for $R\geqslant 1.2$, is very well approximated by

$$\eta_1=N^{-1}\frac{\partial\phi_s}{\partial R} \tag{7}$$

with the normalization factor given by

$$N=4[1-2R/\sinh(2R)]^{1/2}\ . \tag{8}$$

When the functional integral approach is used in order to calculate the partition function[3,8] this mode should be simply inserted in the Coleman determinant[14] together with all the continuum modes. From the behavior of $\omega_1(R)$, as shown in Fig. 1 and in Eqs. (5) and (6), one can note that this insertion can be safely performed only for low values of R. When R becomes larger and larger, this simple procedure leads to uncontrolled exponential divergences so that a separate treatment,[15] with a careful procedure similar to the one used for the translation mode,[14] is required.

Following the analysis of Ref. 15, the ratio of one soliton to vacuum contribution of the partition function Z is found to be

$$\mathscr{Z}_1=e^{-\beta E[\phi_s]}e^{-H}G_0(\beta)G_1(\beta)\ , \tag{9}$$

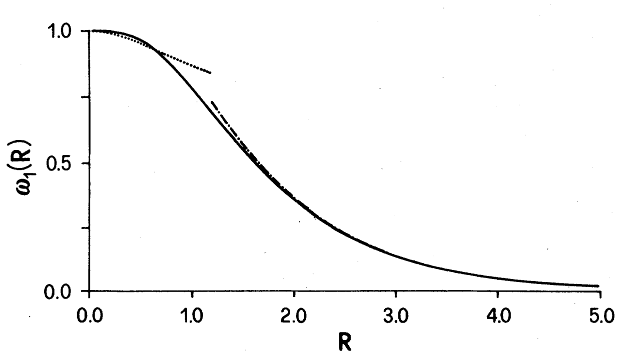

FIG. 1. Frequency of the bound state vs R. Full line, numerical calculations. Dotted line, small-R approximation. Dashed line, large-R approximation. [See Eq. (5).]

where the contributions of the zero mode and the bound state are separately given by the last two factors. The energy functional can be calculated and reads

$$E[\phi_s]=2M[1+2R/\sinh(2R)]\ , \tag{10}$$

where $M=8m^3/\lambda$ is the usual mass of the 2π-SG soliton.

The factor $\exp(-H)$ represents the scattering effect of the continuum and is evaluated according to the Coleman's method, but for the fact that the bound state $\omega_1(R)$ has been removed from the determinant. We find

$$e^{-H}=\left(\frac{\det(-\partial_x^2+1)}{\det[-\partial_x^2+V''(\phi_s)]}\right)^{1/2}\omega_0\omega_1(R) = \frac{2\sqrt{2}\cosh(R)\omega_1(R)}{[1+2R/\sinh(2R)]^{1/2}}\ . \tag{11}$$

We stress that formula (11) is valid and finite for any value of R, since the singularity due to the vanishing of the bound state has been removed.

The usual contribution of the translation mode turns out to be, from Eqs. (3) and (4),

$$G_0(\beta)=4\left(\frac{\beta m}{2\pi}\right)^{1/2} l(1+2R/\sinh 2R)^{1/2}\ . \tag{12}$$

As far as the bound state is concerned, when R is sufficiently small, $\omega_1(R)$ is sufficiently large in order to perform a simple Gaussian integration, at least at low temperatures. In this case

$$G_1(\beta)=[\omega_1(R)]^{-1} \tag{13}$$

leading to

$$\mathscr{Z}_1=4l\left(\frac{\beta M}{2\pi}\right)^{1/2}\cosh(R)\exp\{-2\beta M[1+2R/\sinh(2R)]\} \sim 2l\left(\frac{4\beta M}{2\pi}\right)^{1/2}e^{-4\beta M}\ \text{as}\ R\rightarrow 0\ , \tag{14}$$

which reproduces the result of Refs. 8–10. As already pointed out by these authors, Eq. (14) cannot be extended to large values of R due to its exponential growth. Using a transfer matrix method in the WKBJ approximation with two turning points, the exponential growth is related to the approaching of the height of the relative minimum to the fundamental level of the deepest potential wells and eventually to the degenerate SG picture.[10] Indeed this situation occurs for $\beta M\omega_1^2(R)<1$. On the other hand, from a functional integral standpoint, this is due to the fact that the bound state is becoming a pure translation for large values of R and therefore a simple Gaussian integration is no longer allowed. Physically, this slowing down is related to the breaking of the 2π symmetry of the SG system when R becomes finite and the bound state is associated with deformations of the 4π-DSG soliton which try to restore this symmetry. This can be easily seen from the knowledge of the explicit form of the eigenfunction η_1 at least for $R\geqslant 1.2$ as given by Eq. (7). As a matter of fact, by perturbing the classical static soliton with the mode η_1 in the range of R, where this mode gives rise to an approximate collective coordinate R, we find

$$\phi(x,R)=\phi_s(x,R)+c_1\eta_1\simeq\phi_s\left(x,R+\frac{c_1}{N}\right)\ . \tag{15}$$

Moreover, Eq. (15) suggests a method to improve the evaluation of the bound-state contribution by treating the collective coordinate R in the same way as done for the soliton center in the case of the translation mode.[14,15] This can be realized by looking for an upper bound of the integration over c_1. As the bound state becomes a translation for $R \to \infty$, its contribution must diverge linearly in this limit, implying an asymptotic linear dependence on R for the upper bound of the c_1 integration. Furthermore, a simple bound can be proposed again by Eq. (15), namely,

$$|c_1| \leq RN \ . \tag{16}$$

Then $G_1(\beta)$, in the range of R where the eigenfunction η_1 is well represented by Eq. (7) and where Eq. (15) is valid, is given by

$$G_1(\beta) = \left[\frac{\beta M}{4\pi}\right]^{1/2} \int_0^{RN} dc_1 \exp - \tfrac{1}{16}\beta M \omega_1^2(R) c_1^2 = \frac{1}{\omega_1(R)} \Phi \left[R\sqrt{\beta M}\, \omega_1(R) \left[1 - \frac{2R}{\sinh 2R}\right]^{1/2}\right] , \tag{17}$$

leading to

$$\mathscr{Z}^{(1)} = 4l \left[\frac{\beta M}{2\pi}\right]^{1/2} \cosh(R) e^{-\beta E[\phi_s]} \Phi \left[R\sqrt{\beta M}\, \omega_1(R) \left[1 - \frac{2R}{\sinh 2R}\right]^{1/2}\right] , \tag{18}$$

where Φ is the error function.[16]

When $R \to \infty$, a relationship between R and l must be determined. Since in this limit the DSG soliton degenerates into a pair of 2π-SG solitons which can be considered as independent (dilute gas approximation) the correct choice turns out to be $R = l/4$.

Equation (18) indeed becomes

$$\mathscr{Z}^{(1)} = 4 l^2 \frac{\beta M}{2\pi} e^{-2\beta M} = [\mathscr{Z}_{SG}^{(1)}]^2 \ , \tag{19}$$

where $\mathscr{Z}_{SG}^{(1)}$ is the one-soliton contribution of a SG system.[2,3] Equation (19) shows that in this limit the DSG degenerates into a pair of SG systems. The prefactor β indicates the presence of two translation modes. This occurs also in systems with different symmetries[17] but in our case, each translation mode is associated with a single sine-Gordon kink as shown by the exponential factor. We also note that for higher dimension the change of symmetry of domain walls can be associated with the softening of some frequency.[18]

The right expression for the two-SG-soliton contribution in dilute gas approximation is $\mathscr{Z}_{SG}^{(2)} = [\mathscr{Z}_{SG}^{(1)}]^2/2$. The factor $\frac{1}{2}$ is recovered by noting that each 2π kink acquires a proper individuality, so that the appropriate permutations must be accounted for. Furthermore, for a correct evaluation of the partition function, one should take into account the sector due to the bounce solutions, which become stable for $R \to \infty$ and contribute to the partition function with SG soliton-antisoliton pairs. Similar situations have been met and described in a different context.[19,20] In real systems damping terms must be inserted[21,22] and the bounce solutions give rise to metastable states, which are to be considered for a correct evaluation of the partition function.

Let us conclude with a word of care about the procedure for evaluating the free energy from the knowledge of $\mathscr{Z}^{(1)}$. This implies that the dilute gas approximation should be used or, equivalently, that the excluded volume should be much less than unity (roughly $2R\eta << 1$, η being the soliton density). Therefore for small R, a dilute gas of DSG solitons is allowed, whereas—accounting for the right number of permutations—a dilute gas of SG solitons represents a valid approximation for large R. In the intermediate domain of the parameter R, the interaction among DSG solitons is expected to be non-negligible, in connection with the large size of the excluded volume.

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