Finite-temperature renormalization of sine-Gordon field by variational method

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A variational approach based on the path-integral formulation of the statistical mechanics is applied for calculating the partition function of the sine-Gordon field. This is done by determining an effective potential which includes, in a complete quantum way, the linear modes of the field, while treating variationally the nonlinear excitations. Using this effective potential the temperature renormalization is separately studied both for the vacuum and the one-soliton sector, recovering the total one-loop self-consistent (Hartree-Fock) renormalized approximation. A high-temperature expansion is calculated whose range of applicability is found to be much wider with respect to previous expansions of the same kind. Finally, a comparison with a Monte Carlo simulation is presented, obtaining a very good agreement with the numerical data.

I. INTRODUCTION

The study of the thermodynamical properties of a statistical system in the framework of the path-integral method[1] is reduced to the calculation of the following expression for the partition function Z and, consequently, for the free energy F,

$$Z=e^{-\beta F}=\int_{\Phi(0)=\Phi(\beta\hbar)}\mathcal{D}[\Phi(u)]e^{-S[\Phi(u)]/\hbar}, \tag{1.1}$$

where S is the Euclidean action and $\beta=1/K_BT$. The functional integral is evaluated over all closed paths. In this approach, a variational method based on the well-known Jensen inequality[1]

$$F\leq F_0+\frac{1}{\beta\hbar}\langle S-S_0\rangle_0 \tag{1.2}$$

was developed in previous papers[2-6] for determining the quantum corrections to the partition function of a self-interacting scalar field Φ starting from a trial action S_0 to be optimized. As a result, we were able to calculate an effective potential $V_{\rm eff}$ to be inserted in the classical configurational integral. In particular, in the low-coupling limit, low- and high-temperature expansions of classical statistical mechanics of one-dimensional soliton-bearing systems,[7,8] as well as transfer integral procedures,[9,10] became available and permitted simpler calculations of the quantum thermodynamics of these systems beyond the dilute soliton gas approximation.[11] The improvement of our treatment with respect to the analogous approach described in Ref. 1 has been twofold. In the first place, the quadratic contribution has been taken into account in a fully quantum way, while the quantum corrections due to the remaining nonlinear interactions have been calculated using the variational principle. For the single particle, we performed the detailed calculation of $V_{\rm eff}$ for a double-well potential[4] and the very same results have been later recovered.[12,13] The second improvement concerns the extension of the method to fields. Here the exact treatment of the linear excitations of the field in the partition function allows the zero-temperature limit to be reached without producing the usual nonphysical consequences in thermodynamical quantities, like the specific heat.

A further interesting consequence of our variational method is the different character, at different temperatures, of the physical parameters determined by the minimization of the inequality (1.2). Indeed, at high temperatures, we simply recover the first term of the Wigner expansion, which evidently corresponds to the very tiny influence of the harmonic oscillators in such a range of temperatures. On the other hand, at lowest temperatures, it appears that the above equations can be dealt with in a steepest-descent approximation around the minimum of the effective potential. In Ref. 4, a sketchy computation has been indicated for the vacuum sector of a sine-Gordon (SG) system, and it has been found that the one-loop self-consistent mass renormalization is a direct consequence of the variational principle.

A final achievement of our theory, which we want to stress, is the transparent physical interpretation of the different terms which appear in the low-coupling expansion of the partition function. The latter, in fact, is composed of a factor exactly accounting for the linear modes of the field, while the contribution of the nonlinear interaction is contained in a classical configurational integral involving a potential whose "bare" constants have been replaced by their renormalized counterparts.

This paper treats in detail the SG field in all ranges of temperature. The temperature-dependent renormalization is calculated from our effective potential both for the vacuum and one-soliton sectors, recovering in a unified scheme results of previous semiclassical treatments.[14-16] Moreover, we present in detail a high-temperature expan-

sion with a range of applicability wider than the range of the Wigner series.[17] A comparison with a quantum Monte Carlo simulation, which uses the same separation of the quadratic part of the potential,[18] is finally presented.

II. EFFECTIVE POTENTIAL FOR THE SG CHAIN

The discrete SG chain with lattice constant a and $2N+1$ sites is described by the Lagrangian

$$L=\sum_{i=-N}^{N}\frac{Aa}{2}\dot{\Phi}_i^2-V(\Phi)\ , \tag{2.1}$$

with

$$V(\Phi)=Aa\sum_{i=-N}^{N}\left[\frac{1}{2}\frac{c_0^2}{a^2}(\Phi_i-\Phi_{i+1})^2+\Omega_1^2[e^{-D_{\rm vac}(0)/2}-\cos(\Phi_i)]\right]$$
$$\equiv Aa\left[\tfrac{1}{2}\sum_{i,j=-N}^{N}\Phi_i\mathcal{B}_{ij}\Phi_j+\sum_{i=-N}^{N}\mathcal{U}(\Phi_i)\right]\ , \tag{2.2}$$

where Φ_i is the angular displacement of the ith site, Aa has the dimensions of a moment of inertia, Ω_1 and $\Omega_0=c_0/a$ are frequencies, $\mathcal{B}_{ij}=\Omega_0^2(2\delta_{ij}-\delta_{i,j-1}-\delta_{i,j+1})$ is the matrix defined by the nearest neighbor interaction while $\mathcal{U}(\Phi_i)$ contains the nonlinear interaction term. The meaning of the constant $e^{-D_{\rm vac}(0)/2}$ will be clarified in the following.

The energy scale is fixed by the classical mass of the static kink $E_S=8Ac_0\Omega_1$; its length in lattice units is determined by $R=\Omega_0/\Omega_1$ (Refs. 8 and 19) and the quantum character of the system is ruled by the coupling parameter $Q=\hbar\Omega_1/E_S$. It is also worthwhile to define the reduced temperature $t=K_BT/E_S$. To perform in a convenient way in the continuum limit,[16] we find it useful to introduce the variable $\Psi=\lambda^{-1}\Phi$, with $\lambda^{-1}=c_0\sqrt{A}$. Letting then $a\to 0$ and $R\to\infty$ with constant product $aR=m^{-1}$, the continuum Lagrangian reads

$$L_c=\int_{-L}^{+L}dx\left[\frac{1}{2c_0^2}\dot{\Psi}^2-\frac{1}{2}\left[\frac{\partial\Psi}{\partial x}\right]^2-\frac{m^2}{\lambda^2}[e^{-D_{\rm vac}(0)/2}-\cos(\lambda\Psi)]\right]\ , \tag{2.3}$$

and the soliton energy acquires the usual form $E_S=8m/\lambda^2$.

Our main interest will be devoted to the discrete case for large values of R, which is referred to as the "displacive limit." Sometimes, however, we shall be concerned with the continuum limit of the theory.

According to the general procedure explained in Refs. 2 and 4 and assuming periodic boundary conditions, we take a trial Euclidean action S_0 of the form

$$S_0[\Phi(u)]=Aa\int_0^{\beta\hbar}du\left[\sum_{i=-N}^{N}\frac{1}{2}\dot{\Phi}_i^2+w(\overline{\Phi})+\tfrac{1}{2}\sum_{i,j=-N}^{N}[\Phi_i(u)-\overline{\Phi}_i]w_{ij}(\overline{\Phi})\times[\Phi_j(u)-\overline{\Phi}_j]\right]\ , \tag{2.4}$$

where

$$\overline{\Phi}_i=\frac{1}{\beta\hbar}\int_0^{\beta\hbar}du\ \Phi_i(u)\equiv\varphi_i\ . \tag{2.5}$$

The calculation of the right-hand side of (1.2) is done by first making a (formal) diagonalization of the matrix w_{ij}, namely,

$$\sum_{i,j=-N}^{N}U_{ki}w_{ij}U_{lj}=\omega_k^2\delta_{kl}\ , \tag{2.6}$$

defining the frequencies $\omega_k=\omega_k(\varphi)$ and the orthogonal matrix $U_{ki}=U_{ki}(\varphi)$. For each eigenmode we find it useful to introduce the dimensionless frequency $f_k=\frac{1}{2}\beta\hbar\omega_k$, and the parameter

$$\frac{\alpha_k}{2}=\frac{\hbar^2\beta}{4Aaf_k}\left[\coth f_k-\frac{1}{f_k}\right] \tag{2.7}$$

measures the quantum spread of the kth mode,[4] being the difference between the total mean square displacement $\langle\Phi_k^2\rangle$ minus the classical counterpart of the transformed field $\Phi_k=\sum_i U_{ki}\Phi_i$. A straightforward calculation gives

$$e^{-\beta F_0}=\left[\frac{Aa}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\int d\varphi\, e^{-\beta Aaw(\varphi)}\times\prod_{k=-N}^{N}\frac{f_k(\varphi)}{\sinh f_k(\varphi)} \tag{2.8}$$

and

$$\frac{\langle S-S_0\rangle_0}{\beta\hbar}=e^{\beta F_0}\left[\frac{Aa}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\int d\varphi\, e^{-\beta Aaw(\varphi)}\prod_{k=-N}^{N}\left[\left[\frac{\hbar^2\beta}{6Aa\alpha_k}\right]^{1/2}\frac{f_k}{\sinh f_k}\right]\times\left[\mathcal{H}(\varphi)-\left[\prod_{k=-N}^{N}\frac{6Aa\alpha_k}{\hbar^2\beta}\right]^{1/2}\times\left[Aaw(\varphi)+\sum_{k=-N}^{N}\frac{Aa\alpha_k f_k^2}{\hbar^2\beta^2}\right]\right]\ , \tag{2.9}$$

with

$$\mathcal{K}(\varphi)=\left[\frac{6Aa}{\pi\hbar^2\beta}\right]^{(2N+1)/2}\int d\eta\, V(U^T\eta+\varphi)\times\exp\left[-\sum_{k=-N}^{N}(\eta_k^2/\alpha_k)\right], \tag{2.10}$$

the potential $V(\varphi)$ being specified in (2.2). The minimization of (1.2) with respect to $w(\varphi)$ yields the vanishing of the average $\langle S-S_0\rangle_0$, so that (2.9) and (2.10) permit a straightforward calculation of $w(\varphi)$. The further minimization with respect to w_{ij} or, equivalently, with respect to ω_k and U_{ki}—once the appropriate orthogonality constraint is introduced for the latter[4]—leads to the following nonlinear self-consistent equation:

$$\sum_{i,j=-N}^{N}U_{ki}(\mathcal{B}_{ij}+P_{ij})U_{lj}=\omega_k^2\delta_{kl}\ , \tag{2.11}$$

where

$$P_{ij}(\varphi)=\delta_{ij}\int d\eta\,\mathcal{U}^{(2)}[(U^T\eta+\varphi)_i]\prod_{k=-N}^{N}\frac{e^{-\eta_k^2/\alpha_k}}{(\pi\alpha_k)^{1/2}}\ . \tag{2.12}$$

Expanding the integral (2.12) in a series of α_k and taking into account (2.2), Eq. (2.11), with $l=k$, gives

$$\omega_k^2=2\Omega_0^2-2\Omega_0^2\sum_{i=-N}^{N}U_{ki}U_{k,i+1}+\Omega_1^2\sum_{i=-N}^{N}U_{ki}^2e^{-D_i/2}\cos(\varphi_i)\ , \tag{2.13}$$

where $D_i=D_i(\beta,\varphi)$ is the temperature-dependent quantum renormalization parameter

$$D_i=\sum_{k=-N}^{N}U_{ki}^2\left[\frac{\alpha_k}{2}\right]\ . \tag{2.14}$$

Differing with previous treatments,[16] $D_i(\beta,\varphi)$ refers only to the quantum part of the fluctuations calculated in self-consistent Gaussian approximation.

Finally, from (2.8), we can write the approximate partition function

$$e^{-\beta F}\simeq e^{-\beta F_0}=\left[\frac{Aa}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\int d\varphi\, e^{-\beta V_{\rm eff}(\varphi)}\ , \tag{2.15}$$

where the effective potential reads

$$V_{\rm eff}(\varphi)=Aa\sum_{i=-N}^{N}\left\{\frac{\Omega_0^2}{2}(\varphi_i-\varphi_{i+1})^2+\Omega_1^2\left[e^{-D_{\rm vac}(0)/2}-e^{-D_i/2}\left[1+\frac{D_i}{2}\right]\cos(\varphi_i)\right]\right\}-\frac{1}{\beta}\sum_{k=-N}^{N}\ln\frac{f_k}{\sinh f_k}\ . \tag{2.16}$$

We want to point out that this effective potential contains the quantum effects calculated in the one-loop approximation, as shown by the presence of the renormalization parameter D. The insertion of $V_{\rm eff}$ in a configurational integral should permit us to use all the classical methods devised for the calculation of the partition function. For vanishing nonlinear interactions we easily get from (2.12) that P_{ij} is proportional to δ_{ij}, and therefore U_{ki} is the orthogonal matrix

$$U_{ki}\mid_{Q=0}\equiv A_{ki}=\begin{cases}\left[\frac{2}{2N+1}\right]^{1/2}\cos\left[\frac{2\pi ki}{2N+1}\right], & -N\le k\le -1\\ (2N+1)^{-1/2}, & k=0\\ \left[\frac{2}{2N+1}\right]^{1/2}\sin\left[\frac{2\pi ki}{2N+1}\right], & 1\le k\le N\ .\end{cases} \tag{2.17}$$

The matrix (2.17) diagonalizes any translational-invariant matrix and, in particular, the symmetric matrix $\mathcal{B}_{ij}$ of nearest-neighbor interaction. By substituting (2.17) in (2.13), we also obtain

$$\omega_k^2\mid_{Q=0}\equiv\Omega_k^2=4\Omega_0^2\sin^2\left[\frac{\pi k}{2N+1}\right]+\Omega_1^2\ , \tag{2.18}$$

i.e., the well-known Klein-Gordon dispersion relation, as obviously was to be expected.

In the general case, the effective potential (2.16) is a rather involved quantity to be calculated. However, the extreme temperature limits, as well as the case of a small coupling constant, can be controlled and we shall show that, even in these circumstances, a lot of information can be obtained. Of all these cases, the simplest and somewhat trivial is the high-temperature limit. From (2.14) and (2.7), for $\beta\to 0$, it is straightforward to find for the effective potential the expression

$$V_{\rm eff}(\varphi)=Aa\sum_{i=-N}^{N}\left\{\frac{\Omega_0^2}{2}(\varphi_i-\varphi_{i+1})^2+\Omega_1^2\left[e^{-D_{\rm vac}(0)/2}-\left[1-\frac{\hbar^2\beta}{24Aa}\right]\cos(\varphi_i)\right]\right\}+(2N+1)\frac{\Omega_0^2\hbar^2\beta}{12}\ , \tag{2.19}$$

which is nothing more than the first Wigner correction.

For large values of R, as it occurs in many physical situations, the convergence of the Wigner series is rather poor, being related to the condition $\Omega_0\hbar\beta \ll 1$, i.e., $t \gg RQ$. In Sec. V we shall present an improvement based on the expansion of the effective potential in terms of Q which justifies previous rearrangements.[19–21]

At low temperatures the main contribution to the partition function arises from the local minima of the effective potential. The general equation for determining these minima is derived in the Appendix, and for the SG it reads

$$\Omega_0^2(2\varphi_i-\varphi_{i+1}-\varphi_{i-1})+\Omega_1^2 e^{-D_i(\varphi)/2}\sin(\varphi_i)=0 . \quad (2.20)$$

In the continuum limit, Eq. (2.20) simply becomes the static SG equation where the frequency Ω_1^2 is affected by the renormalization. We can observe that finite energy kink solutions can be determined also for (2.20). Indeed, in this case, for large values of the continuous-site variable the field must tend to a constant configuration. Therefore, the renormalization factor D also tends to become constant and the usual topological arguments easily apply.

We shall therefore treat separately the vacuum and the one-soliton sectors determining both the renormalization and the contributions to the partition function. Some considerations, however, are in order. Simple quadratic expansions in the neighborhood of local minima are not consistent except for lowest temperatures ($t \ll 2Q$), where the factor D can be calculated at $t=0$, neglecting the classical fluctuations. To take into account both the quantum and classical fluctuations causing temperature-dependent frequency renormalization, we must perform self-consistent Gaussian expansions around the minima. This corresponds to taking into account the interaction among elementary excitations (linear and nonlinear) in the Hartree-Fock (one-loop) approximation going beyond the dilute gas approximation, analogously to the procedure of Ref. 16.

III. THE VACUUM SECTOR

The vacuum of the effective theory is defined to be one of the lowest-energy solutions of Eq. (2.20). These solutions are degenerate and are given by the constant configurations

$$\varphi_i = 2n\pi, \quad n=0,\pm1,\pm2,\ldots . \quad (3.1)$$

In the following it will be useful to consider the case $n=0$, which we shall refer to as the "vacuum sector." In this case the renormalization factor $D_{\rm vac}(T)$ can be consistently calculated on the uniform field configuration and results in being site independent. The diagonalizing matrix U_{ki} is therefore the matrix A_{ki} given in (2.17), so that

$$D_{\rm vac}(T)=\frac{1}{2N+1}\sum_{k=-N}^{N}\frac{\alpha_k}{2} . \quad (3.2)$$

As previously stated, for low but nonvanishing temperatures, the term $D_{\rm vac}(T)$ is obviously a decreasing function, since the quantum character of the system becomes less important while the classical fluctuations cause a further temperature modification of Ω_1 and consequently of ω_k.

In order to better understand the spirit of the approximation, we find it useful to split $D_{\rm vac}(T)$ into its two component parts,

$$D_{\rm vac}(T)=D(T)-D_{\rm cl}(T) , \quad (3.3)$$

where

$$\begin{aligned} D(T)&=\frac{1}{2N+1}\sum_{k=-N}^{N}\frac{\hbar^2\beta}{4Aaf_k}\coth f_k , \\ D_{\rm cl}(T)&=\frac{1}{2N+1}\sum_{k=-N}^{N}\frac{\hbar^2\beta}{4Aaf_k^2} , \end{aligned} \quad (3.4)$$

respectively, represent the total and the classical fluctuation of the field.[22]

For vanishing temperature, we have

$$D(0)=D_{\rm vac}(0), \quad D_{\rm cl}(0)=0 . \quad (3.5)$$

Hence, the evaluation of the partition function within a simple Gaussian approximation around the vacuum turns out to be inconsistent for increasing temperatures. To perform the meaningful self-consistent Gaussian approximation, we apply the standard decoupling procedure to the $\cos(\varphi_i)$ term, extracting all possible pair averages, namely,

$$\begin{aligned} \cos(\varphi_i)\simeq 1&+\sum_{n=1}^{\infty}\frac{(-1)^n}{(n-1)!}\left[\frac{D_{\rm cl}}{2}\right]^{n-1}\frac{\varphi_i^2}{2} \\ &-\sum_{n=1}^{\infty}\frac{(-1)^n(n-1)}{n!}\left[\frac{D_{\rm cl}}{2}\right]^{n} . \end{aligned} \quad (3.6)$$

The subtraction of the last term is necessary to restore the correct average of $\cos(\varphi_i)$ so that

$$\langle\cos(\varphi_i)\rangle_{\rm cl}=e^{-D_{\rm cl}/2} . \quad (3.7)$$

In this way, we get

$$\cos(\varphi_i)\simeq e^{-D_{\rm cl}/2}\left[1-\tfrac{1}{2}(\varphi_i^2-D_{\rm cl})\right] . \quad (3.8)$$

By substituting (3.8) into the expression (2.16) of the effective potential and performing the appropriate expansions, we obtain

$$\begin{aligned} V_{\rm eff}(\varphi)=&\frac{Aa}{2}\sum_{i=-N}^{N}[\Omega_0^2(\varphi_i-\varphi_{i+1})^2+\Omega_1^2e^{-D/2}\varphi_i^2]+Aa\Omega_1^2(2N+1)\left[e^{-D_{\rm vac}(0)/2}-e^{-D/2}\left[1+\frac{D}{2}\right]\right] \\ &-\frac{1}{\beta}\sum_{k=-N}^{N}\ln\frac{f_k^{(0)}}{\sinh f_k^{(0)}} , \end{aligned} \quad (3.9)$$

where $f_k^{(0)}$ is calculated using

$$(\omega_k^{(0)})^2=4\Omega_0^2\sin^2\left[\frac{\pi k}{2N+1}\right]+\Omega_1^2 e^{-D/2} . \tag{3.10}$$

As the frequencies are configuration independent, the partition function reads

$$Z_{\rm vac}(T)=\left[\frac{Aa}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\prod_{k=-N}^{N}\left[\frac{f_k^{(0)}}{\sinh f_k^{(0)}}\right]\exp\left\{-\beta Aa\Omega_1^2(2N+1)\left[e^{-D_{\rm vac}(0)/2}-e^{-D/2}\left[1+\frac{D}{2}\right]\right]\right\}$$
$$\times\int d\varphi\exp\left[-\frac{\beta Aa}{2}\sum_{k=-N}^{N}(\omega_k^{(0)})^2\varphi_k^2\right] . \tag{3.11}$$

Performing the $(2N+1)$-independent Gaussian integrations, we then obtain the vacuum contribution at finite temperatures to the free energy per site

$$\frac{F_{\rm vac}}{2N+1}=\frac{1}{\beta(2N+1)}\sum_{k=-N}^{N}\ln(2\sinh f_k^{(0)})+Aa\Omega_1^2\left[e^{-D_{\rm vac}(0)/2}-e^{-D/2}\left[1+\frac{D}{2}\right]\right] . \tag{3.12}$$

The expression is in perfect agreement with the results of Refs. 14 and 16 if the continuum limit is taken. The latter can be done by taking into account the expression of $D(0)$, namely,

$$D(0)=\frac{1}{2N+1}\sum_{k=-N}^{N}\frac{\hbar}{2Aa\omega_k^{(0)}} . \tag{3.13}$$

It can be seen that (3.13), stemming only from our variational principle, reproduces the well-known results of semiclassical renormalization.[14,15] At the lowest order, we have

$$D(0)=\frac{8QR}{\pi\sqrt{1+4R^2}}K\left[\frac{2R}{\sqrt{1+4R^2}}\right] , \tag{3.14}$$

with K being the complete elliptic integral of the first kind and reproducing the well-known logarithmic divergence in the continuum limit. A mass renormalization

$$m\rightarrow m\exp[-D(0)/4]$$

is thus required and the further procedure of Ref. 16 is straightforward.

IV. THE ONE-SOLITON SECTOR

To apply the same self-consistent scheme for the expansions around nonuniform minima, as given by Eq. (2.20), we have to take into account that the classical fluctuations will now modify the mass of the static kinks as we are now going to show.

We assume that $\varphi_i^{(S)}$ is the kink configuration which minimizes the effective potential in the Gaussian self-consistent approximation. Let

$$\varphi_i=\varphi_i^{(S)}+\theta_i . \tag{4.1}$$

Using (3.8) for approximating $\cos\theta_i$ and the analogous equation

$$\sin\theta_i\simeq e^{-D_{\rm cl}/2}\theta_i , \tag{4.2}$$

with a $D_{\rm cl}$ generally different from that introduced in the vacuum sector, we obtain an effective potential

$$V_{\rm eff}=Aa\sum_{i=-N}^{N}\left\{\frac{\Omega_0^2}{2}[(\varphi_i^{(S)}-\varphi_{i+1}^{(S)})^2+(\theta_i-\theta_{i+1})^2+\theta_i(2\varphi_i^{(S)}-\varphi_{i+1}^{(S)}-\varphi_{i-1}^{(S)})]\right.$$
$$\left.+\Omega_1^2\left\{e^{-D_{\rm vac}(0)/2}-e^{-D/2}\left[\cos(\varphi_i^{(S)})\left[1-\frac{\theta_i^2-D}{2}\right]-\theta_i\sin(\varphi_i^{(S)})\right]\right\}\right]-\frac{1}{\beta}\sum_{k=-N}^{N}\ln(f_k^{(S)}/\sinh f_k^{(S)}) , \tag{4.3}$$

where the $f_k^{(S)}$ of the one-soliton sector are determined by solving the eigenvalue equation

$$\sum_{i,j=-N}^{N}U_{ki}[\mathcal{B}_{ij}+\delta_{ij}\Omega_1^2 e^{-D/2}\cos(\varphi_i^{(S)})]U_{lj}=(\omega_k^{(S)})^2\delta_{kl} . \tag{4.4}$$

Minimizing Eq. (4.3) with respect to θ_i we obtain that the soliton configuration is again determined by Eq. (2.20), where the purely quantum factor $D_i(\varphi)$ must be substituted by the total renormalization factor $D(\varphi^{(S)})$.

A particular care must be used to deal with the zero-frequency translation mode, which is a solution of Eq. (4.4) when $\varphi_i^{(S)}$ is a soliton configuration in the continuum

limit. Indeed, in this case, the correct way of approaching the problem is that of promoting the center of the soliton to a collective coordinate, while keeping all the other $\omega_k^{(S)} \neq 0$ modes. The center of the soliton, related to the translation invariance, is therefore a classical coordinate and consequently the $\omega_k^{(S)}=0$ fluctuations are to be omitted in evaluating the renormalization factor.

However, we can also observe that the nonuniformity of $D(\varphi^{(S)})$ is confined to the region where the kink has a sensible variation, so that in the infinite length limit, the contribution of the nonuniformity tends to zero[16,23] and therefore we can consistently assume the vacuum expression for D. The final expression of the effective potential reads

$$V_{\rm eff}=E_S(T)+\frac{Aa}{2}\sum_{k=-N}^{N}(\omega_k^{(0)})^2\theta_k^2 + Aa\Omega_1^2\sum_{i=-N}^{N}\left[e^{-D_{\rm vac}(0)/2} - e^{-D/2}\left[1+\frac{D}{2}\cos(\varphi_i^{(S)})\right]\right] - \frac{1}{\beta}\sum_{k=-N}^{N}\ln\frac{f_k^{(S)}}{\sinh f_k^{(S)}} , \tag{4.5}$$

where $E_S(T)$ represents the renormalized kink energy

$$E_S(T)=Aa\sum_{i=-N}^{N}\left[\frac{\Omega_0^2}{2}(\varphi_i^{(S)}-\varphi_{i+1}^{(S)})^2 + \Omega_1^2 e^{-D/2}[1-\cos(\varphi_i^{(S)})]\right] , \tag{4.6}$$

reproducing the value $e^{-D/4}E_S$ in the continuum limit.

From (4.3) we can derive the free energy F_S of the one-soliton sector,

$$F_S-F_{\rm vac}=E_S(T)+\frac{1}{\beta}\sum_{k=-N}^{N}\ln\left[\frac{\sinh f_k^{(S)}}{\sinh f_k^{(0)}}\right] + Aa\Omega_1^2 e^{-D/2}\frac{D}{2}\sum_{i=-N}^{N}[1-\cos(\varphi_i^{(S)})] . \tag{4.7}$$

This is exactly the same expression derived in Ref. 16 in the continuum limit. From here on, therefore, one could repeat the procedure developed in Refs. 14 and 16 in order to calculate the effective coupling constant and the finite-temperature correction to the free energy,

$$-\beta\Delta F=\exp[-\beta(F_S-F_{\rm vac})] , \tag{4.8}$$

due to the presence of solitons in the dilute gas approximation.

V. LOW-COUPLING EXPANSION

In the above-developed framework, we treated a one-loop (Hartree-Fock) self-consistent theory in order to take into account the soliton interactions. However, this approach is known to give worse and worse results for increasing temperatures and eventually leads to a first-order phase transition at the "critical" reduced temperature $t \simeq 1/e$ (Ref. 16) when the self-consistent equations (3.4) and (3.10) have no more solutions. On the other hand, even in the classical case the two-soliton interaction must be eventually included[7] in order to reproduce, up to $t \simeq 0.22$, the correct behavior of the nonlinear contribution to the specific heat, as computed in Ref. 9. Therefore, it turns out to be more useful to consider an expansion around the local minima and to derive an appropriate effective potential as a series in the anharmonicity.

In the low-coupling limit we can expand the frequencies (2.13) in powers of Q. Recalling that D_i is proportional to Q and setting $U=A+O(Q)$, from (2.13) we get

$$\omega_k^2=\Omega_k^2+\Omega_1^2\sum_{i=-N}^{N}A_{ki}^2[e^{-D/2}\cos(\varphi_i)-1]+O(Q^2) , \tag{5.1}$$

where Ω_k is given by (2.18) and $D=D(T)$ is the quantum renormalization parameter, consistently calculated to order Q using Ω_k in (2.7) and (2.14). For $\beta\hbar\Omega_1 D/8 \ll 1$ it makes sense[4] to expand the logarithmic term in the effective potential (2.16), eventually obtaining

$$V_{\rm eff}(\varphi)=Aa\sum_{i=-N}^{N}\left[\frac{\Omega_0^2}{2}(\varphi_i-\varphi_{i+1})^2+\Omega_1^2[e^{-D_{\rm vac}(0)/2}-e^{-D/2}\cos(\varphi_i)]\right]-Aa\Omega_1^2(2N+1)\frac{D}{2}-\frac{1}{\beta}\sum_{k=-N}^{N}\ln\frac{F_k}{\sinh F_k} , \tag{5.2}$$

where $F_k=\beta\hbar\Omega_k/2$. The partition function is therefore given by

$$Z(T)=\left[\frac{Aa}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\prod_{k=-N}^{N}\left[\frac{F_k}{\sinh F_k}\right]\exp\left[-\beta Aa\Omega_1^2(2N+1)\frac{D}{2}\right]\int d\varphi\exp\left[-\beta Aa\sum_{i=-N}^{N}\left[\frac{\Omega_0^2}{2}(\varphi_i-\varphi_{i+1})^2 + \Omega_1^2[e^{-D_{\rm vac}(0)/2}-e^{-D/2}\cos(\varphi_i)]\right]\right] . \tag{5.3}$$

Equation (5.3) looks very useful. Nonlinear contributions to the free energy are contained in the configurational integral, which corresponds to a classical SG chain with Ω_1 replaced by its quantum renormalized counterpart $\Omega_1(T)=\Omega_1 e^{-D(T)/4}$. Therefore, in order to compute this integral, all classical methods can be used, as, e.g., temperature expansions[7,8] or numerical transfer-operator techniques.[9,10] Moreover, it appears that the free energy contains a Debye-like contribution by harmonic oscillators with frequencies Ω_k: hence, this contribution is included in a fully quantum way.

The modifications introduced by the presence of solitons are still contained in the configurational integral: For instance, the phase shifts of the frequencies are con-

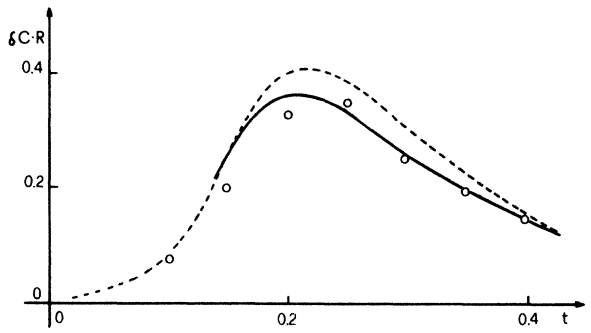

FIG. 1. Nonlinear contribution to the specific heat vs reduced temperature t for $Q=0.1$ and $R=10$ (solid line). The dashed line is the classical result (Ref. 9). The circles are quantum Monte Carlo data from Ref. 18.

sidered "classically," but this is correct within the low-coupling approximation and the translation mode has surely a classical behavior.

The condition of validity of (5.3), $\beta\hbar\Omega_1 D/8 \ll 1$, also reads $t \gg (2\pi)^{-1}Q^2\ln(8R)$ and has to be compared with the condition $t \gg RQ/2$, under which the Wigner expansion (2.19) holds. Hence, (5.3) is a great improvement in the displacive limit $R \gg 1$, as it occurs in many experimental situations concerning one-dimensional ferromagnets.[24] The quantum temperature-dependent renormalization parameter $D(T)$ can be computed using the relation

$$\coth x - \frac{1}{x} = 2\sum_{n=1}^{+\infty} \frac{x}{x^2+n^2\pi^2} \ . \tag{5.4}$$

At the lowest order we obtain the following expression for D:[25]

$$D(t) = \frac{4Q^2R}{t} \sum_{n=1}^{+\infty} \left\{ \left[(n\pi)^2 + (1+4R^2) \left[\frac{Q}{2t} \right]^2 \right] \times \left[(n\pi)^2 + \left[\frac{Q}{2t} \right]^2 \right] \right\}^{-1/2} \ . \tag{5.5}$$

One could get a straightforward improvement by including in Ω_k the renormalization of Ω_1 and performing the calculation self-consistently.

In Fig. 1 we reported the full nonlinear contribution to the specific heat δC obtained by (5.3) using the classical expansions for the free energy from Refs. 7 and 8, for $Q=0.1$ and $R=10$. It follows that the quantum effects on δC are rather small, but essential, for having a satisfactory fit with the results of a quantum Monte Carlo simulation.[18]

Finally, it is worthwhile noting that the above Monte Carlo simulation has been done after separating the harmonic and anharmonic parts of the Hamiltonian and using the knowledge of the exact free energy corresponding to the former, in close analogy with the full treatment of the quadratic contributions yielded by the use of the trial action (2.4). The accuracy of the numerical method has been checked with the exact results of quantum SG obtained by applying the Bethe ansatz.[26]

VI. CONCLUSIONS

Our improved version of the variational approach to the Feynman path-integral formulation of the statistical mechanics has been applied for calculating the temperature-dependent renormalization of the SG field. This method is essentially based on the idea of taking into account in a fully quantum way the quadratic part of the Hamiltonian along the path and applying the variational principle for evaluating both the frequency renormalization and the quantum anharmonic effects by means of an effective potential. The latter has been calculated at all temperatures for the SG field.

In this unified scheme the temperature renormalization of the vacuum and the one-soliton sector is easily recovered at low temperature in a total one-loop (Hartree-Fock) approximation. Furthermore, and this is a new improvement, our effective potential can give, in a wider range of temperatures with respect to previous treatments, useful recipe for reducing quantum statistical-mechanics calculations to classical ones. The explicit results for the nonlinear contribution to the specific heat of SG chains give very good agreement with Monte Carlo simulations. In a forthcoming paper, we shall present an application to nonintegrable potentials, such as φ^4 and double SG, for which quantum inverse scattering results are not available.

APPENDIX

In this appendix we derive the minimum equation (2.20) for the effective potential. By direct differentiation of (2.16) we find

$$\frac{\partial V_{\rm eff}}{\partial \varphi_i} = Aa \left[\Omega_0^2(2\varphi_i - \varphi_{i+1} - \varphi_{i-1}) + \Omega_1^2 e^{-D_i/2} \left[1 + \frac{D_i}{2} \right] \sin(\varphi_i) \right] + Aa\Omega_1^2 \sum_{j=-N}^{N} \cos(\varphi_j) \frac{D_j}{2} e^{-D_j/2} \frac{\partial}{\partial \varphi_i} \left[\frac{D_j}{2} \right] + \frac{\partial}{\partial \varphi_i} \left[-\frac{1}{\beta} \sum_{k=-N}^{N} \ln \frac{f_k}{\sinh f_k} \right] \ . \tag{A1}$$

From (2.7) and the definition of f_k we find the identity

$$\frac{\partial}{\partial \varphi_i} \left[-\frac{1}{\beta} \sum_{k=-N}^{N} \ln \frac{f_k}{\sinh f_k} \right] = \frac{1}{\beta} \sum_{k=-N}^{N} \left[\coth f_k - \frac{1}{f_k} \right] \frac{\partial f_k}{\partial \varphi_i} = Aa \sum_{k=-N}^{N} \frac{\alpha_k}{4} \frac{\partial \omega_k^2}{\partial \varphi_i} \ . \tag{A2}$$

By means of the identity

$$\frac{\partial}{\partial\varphi_i}U^{-1}=-U^{-1}\left[\frac{\partial}{\partial\varphi_i}U\right]U^{-1} \tag{A3}$$

and using (2.11) and (2.13), we easily get

$$\frac{\partial\omega_k^2}{\partial\varphi_i}=\left[\frac{\partial U}{\partial\varphi_i}U^{-1},U(\mathcal{B}+P)U^{-1}\right]_{kk}+\left[U\frac{\partial P}{\partial\varphi_i}U^{-1}\right]_{kk}=\Omega_1^2\sum_{j=N}^{N}U_{kj}^2\frac{\partial}{\partial\varphi_i}[e^{-D_j/2}\cos(\varphi_j)]\ . \tag{A4}$$

Here the diagonal elements of the commutator are vanishing, due to the fact that the matrix $U(\mathcal{B}+P)U^{-1}$ is diagonal. Inserting (A4) into (A2) gives

$$\begin{aligned}\frac{\partial}{\partial\varphi_i}\left[-\frac{1}{\beta}\sum_{k=-N}^{N}\ln\frac{f_k}{\sinh f_k}\right]&=Aa\Omega_1^2\sum_{j=-N}^{N}\frac{D_j}{2}\frac{\partial}{\partial\varphi_i}[e^{-D_j/2}\cos(\varphi_j)]\\&=-Aa\Omega_1^2\sum_{j=-N}^{N}\frac{D_j}{2}e^{-D_j/2}\frac{\partial}{\partial\varphi_i}\left[\frac{D_j}{2}\right]\cos(\varphi_j)-Aa\Omega_1^2\frac{D_i}{2}e^{-D_i/2}\sin(\varphi_i)\ ,\end{aligned} \tag{A5}$$

where use has been made of the definition (2.14). From (A1) we eventually obtain Eq. (20).

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