Variational approach to the thermodynamics of a quantum sine-Gordon field with out-of-plane fluctuations

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The quantum corrections to the partition function of nonlinear systems with a nonlocal kinetic energy are calculated by extending a variational approach based on the path integral and developed in a previous paper, which allows one to take into account in the quantum scheme of the quadratic part of the Hamiltonian. This extension can be useful to study the role of the out-of-plane fluctuations which cause deviations from the sine-Gordon model for some magnetic chains.

I. INTRODUCTION

Theoretical methods giving quantum corrections to classical statistical mechanics have recently raised large interest and found many applications.[1-4] Old approaches were revisited[1] and improved,[5,6] while new theoretical schemes were devised. A new approximate approach based on the path integral[7] was recently proposed and applied to evaluate quantum corrections to the specific heat of a sine-Gordon chain.[8-10] It allows one to construct an effective potential to be inserted in the configurational integral so that quantum fluctuations can be taken into account for low coupling at all temperatures without resorting to the dilute-soliton-gas approximation. The soliton-gas approximation is not valid in the temperature region where the specific heat presents a Schotty-like peak. When the results of these quantum corrections for the sine-Gordon chain were compared with the experimental data of real magnetic chains like $CsNiF_3$ and CHAB $[(C_6H_{11}NH_3)CuBr_3]$, this model appeared to be insufficient because the values of the easy-plane anisotropy are not strong enough to prevent out-of-plane fluctuations.[11,12] On the other hand, the quantum character of these systems has been fully realized.[13] All previous approaches considering the quantum contribution of the out-of-plane fluctuations were always confined to the dilute-soliton-gas approximation.[11,14,15] Although important information about the role of these fluctuations can be inferred in this limit, the soliton-soliton interactions must be taken into account for a realistic comparison.

In this paper we present detailed calculations of thermodynamical quantities for a one-dimensional chain described by the following Hamiltonian depending on canonical coordinates $z=(z_a)$, $a\in[-N,N]$, and conjugate momenta $p=(p_a)$, $a\in[-N,N]$:

$$H(p,z)=T(p)+V(z)\ , \tag{1.1}$$

where the kinetic energy $T(p)$ is a nondiagonal quadratic form

$$T(p)=\tfrac{1}{2}\sum_{a,b=-N}^{N} p_a K_{ab} p_b\ , \tag{1.2}$$

and the potential energy $V(z)$ is given by

$$V(z)=\tfrac{1}{2}\sum_{a,b=-N}^{N} z_a L_{ab} z_b + g\sum_{a=-N}^{Nt} \mathcal{U}(z_a)\ . \tag{1.3}$$

In Eq. (1.3) the symmetric matrices K and L commute and satisfy periodic boundary conditions together with the requirement of translational invariance,[10] and the function $\mathcal{U}(z_a)$ describes a local nonlinear interaction with corresponding coupling constant g.

The nondiagonal form of the kinetic term is able to reproduce the correct dispersion relation of spin waves in real magnetic chains. This is important, in the quantum case, because the contribution of the linear excitations to the renormalization of the Hamiltonian parameters depends upon the functional form of the dispersion curve. Although, at this stage, we neglect nonlinear terms mixing momenta and position coordinates, however, at least one important aspect of the quantum out-of-plane fluctuations can be taken into account, and their relevance can be inferred.

In Sec. II the extension of the theory to the Hamiltonian (1.1) is developed, while in Sec. III its possible application to $CsNiF_3$ is presented.

II. VARIATIONAL APPROACH TO THE PARTITION FUNCTION

We recall the path-integral expression of the partition function,

$$Z=e^{-\beta F}=\int \mathcal{D}[z(u)]\mathcal{D}[p(u)] \times\exp\left\{\frac{1}{\hbar}\int_0^{\beta\hbar} du\,\{p(t)\dot{z}(t) -H[z(t),p(t)]\}_{t=iu}\right\}\ , \tag{2.1}$$

where the Hamiltonian H is given in (1.1). As $[K,L]=0$, there exists an orthogonal transformation which simultaneously diagonalizes the matrices K and L:

$$MKM^T=E, \quad MLM^T=F \ , \tag{2.2}$$

with

$$E_{ab}=E_a\delta_{ab} \quad F_{ab}=F_a\delta_{ab} \ . \tag{2.3}$$

Performing the canonical transformation

$$y_a=\sum_b M_{ab}z_b, \quad q_a=\sum_b M_{ab}p_b \ , \tag{2.4}$$

putting the functional integral in a Lagrangian form, and defining

$$x_a=(mE_a)^{-1/2}y_a, \quad N_{ab}=(mE_a)^{1/2}M_{ab} \ , \tag{2.5}$$

where the "mass" m is chosen to be

$$m=\left[\prod_{a=-N}^{N}E_a\right]^{-1/(2N+1)} \tag{2.6}$$

in such a way to preserve the measure of the functional integral, we finally get

$$Z=\int_{x(0)=x(\beta\hbar)}\mathcal{D}[x(u)]e^{-S[x(u)]/\hbar} \ , \tag{2.7}$$

with

$$\begin{aligned}S[x(u)]&=\int_0^{\beta\hbar}du\left[\frac{m}{2}\sum_{a=-N}^{N}\dot{x}_a^2+V(x(u))\right]\\&\equiv\int_0^{\beta\hbar}du\left[\frac{m}{2}\sum_{a=-N}^{N}\dot{x}_a^2+\frac{m}{2}\sum_{a=-N}^{N}E_aF_ax_a^2\right.\\&\quad\left.+g\sum_{a=-N}^{N}\mathcal{U}((N^Tx)_a)\right] \ .\end{aligned} \tag{2.8}$$

According to the general procedure described in Refs. 8 and 10, we consider the first-order cumulant inequality for the free energy F, namely

$$F\le F_0+\frac{1}{\beta\hbar}\langle S-S_0\rangle_0 \ , \tag{2.9}$$

where F_0 is calculated according to (2.1) by inserting an approximate action S_0, while the average $\langle S-S_0\rangle_0$ is performed with $e^{-S_0/\hbar}$ as a weight. The approximate action is chosen to be

$$S_0[x(u)]=\int_0^{\beta\hbar}du\left[\frac{m}{2}\sum_{a=-N}^{N}\dot{x}_a^2+w(\bar{x})+w_a(\bar{x})[x_a(u)-\bar{x}_a]+\frac{1}{2}\sum_{a,b=-N}^{N}[x_a(u)-\bar{x}_a]w_{ab}(\bar{x})[x_b(u)-\bar{x}_b]\right] \ , \tag{2.10}$$

where

$$\bar{x}_a=V(\beta\hbar)^{-1}\int_0^{\beta\hbar}du\,x_a(u), \quad a\in[-N,N] \tag{2.11}$$

and the unknown functions $w(\bar{x})$, $w_a(\bar{x})$, and $w_{ab}(\bar{x})$ are to be determined by the variational principle, i.e., by the minimum condition of the functional (2.9). To this purpose we first substitute S_0 in place of S in Eq. (2.7). The corresponding functional integral can be explicitly calculated by summing first over all the closed paths with a prescribed average $\bar{x}_a=\xi_a$, $a\in[-N,N]$, and then integrating over all the possible values of $\xi\equiv(\xi_a)$, $a\in[-N,N]$. The final result reads

$$\begin{aligned}e^{-\beta F_0}&=\left[\frac{m}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\\&\quad\times\int d\xi\,e^{-\beta w(\bar{x})}\prod_{k=-N}^{N}\frac{f_k(\xi)}{\sinh[f_k(\xi)]} \ ,\end{aligned} \tag{2.12}$$

where, according to Ref. 7, we have set

$$f_k(\xi)=\tfrac{1}{2}\beta\hbar\omega_k(\xi) \ , \tag{2.13}$$

while the "frequency" $\omega_k(\xi)$ is defined together with the orthogonal matrix $U_{ka}(\xi)$ by the diagonalizing relation

$$\sum_{a,b=-N}^{N}U_{ka}w_{ab}U_{jb}=m\omega_k^2\delta_{kj} \ . \tag{2.14}$$

Moreover, the result (2.12) shows that indeed the quantities w_a do not affect the final result, as could be expected by elementary symmetry considerations. Performing the minimization of the right-hand side of (2.9) with respect to w and w_{ab} or, equivalently, with respect to w, f_k, and U_{ka} (see Ref. 10), after the change of variable $\zeta=N^T\xi$, we find that the average $\langle S-S_0\rangle_0$ turns out to be vanishing, so that is possible to define an effective potential to be inserted in the configurational integral (2.15) in order to approximate the free energy F by means of F_0. Equation (2.12) can then be written in the following way:

$$e^{-\beta F_0}=\left[\frac{m}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\int d\zeta\exp[-\beta V_{\text{eff}}(\zeta)] \ , \tag{2.15}$$

where the explicit form of the effective potential reads

$$\begin{aligned}V_{\text{eff}}(\zeta)&=V(\zeta)+m\sum_{a,k=-N}^{N}\left[\frac{a_k}{4}\right]U_{ka}^2F_aE_a\\&\quad+g\sum_{n=1}^{\infty}\sum_{a=-N}\left[\frac{D_a}{2}\right]^n\frac{\mathcal{U}^{(2n)}(\zeta a)}{n!}\\&\quad-\sum_{k=-N}^{N}\frac{m\alpha_kf_k^2}{\hbar^2\beta^2}-\frac{1}{\beta}\sum_{k=-N}^{N}\ln\left[\frac{f_k}{\sinh f_k}\right] \ .\end{aligned} \tag{2.16}$$

In (2.16) the parameters

$$\alpha_k=\frac{\hbar^2\beta}{2mf_k^2}(f_k\coth f_k-1) \tag{2.17}$$

give a measure of the influence of the quantum fluctuations, while the quantum renormalization factor

$$D_a=\sum_{k=-N}^{N}\left[\frac{\alpha_k}{2}\right]\left[\sum_{b=-N}^{N}U_{kb}N_{ba}\right]^2 \tag{2.18}$$

differs from the analogous factor obtained in the case of local kinetic energy,[10] since it contains the new dispersion relation. Moreover, the frequencies are determined by the self-consistent equations

$$\sum_{a,b=-N}^{N}U_{ia}\left[F_aE_a\delta_{ab}+\frac{g}{m}P_{ab}\right]U_{kb}=\omega_k^2\delta_{ab}\ ,$$
$$P_{ab}=\sum_{c=-N}^{N}N_{ac}\left[\sum_{n=1}^{\infty}\left[\frac{D_c}{2}\right]^{n-1}\frac{\mathcal{U}^{(2n)}(\zeta_c)}{(n-1)!}\right]N_{bc}\ . \tag{2.19}$$

We shall analyze the free energy in the perturbative case of small anharmonicity.[10]

The frequency ω_k^2 is found to be, up to the first order in g,

$$\omega_k^2=F_kE_k+gE_k\sum_{a=-N}^{N}M_{ka}^2\left[\sum_{n=0}^{\infty}\left[\frac{D}{2}\right]^n\frac{\mathcal{U}^{(2n+2)}(\zeta_a)}{n!}\right], \tag{2.20}$$

exhibiting the modified dispersion relation at the zeroth order. Moreover, the consistent approximation for the renormalization factor D turns out to be independent of the site and is given by the fluctuations around the vacuum, namely

$$D=\frac{1}{2N+1}\sum_{k=-N}^{N}\frac{1}{\beta F_k}\left[\frac{\beta\hbar}{2}\sqrt{E_kF_k}\times\coth\left[\frac{\beta\hbar}{2}\sqrt{E_kF_k}\right]-1\right]. \tag{2.21}$$

The limiting value of D for $T=0$ can be easily calculated by integrating over the Brillouin zone:

$$D(T=0)=\frac{\hbar}{4\pi}\int_{-\pi}^{+\pi}dk(E_k/F_k)^{1/2}\ . \tag{2.22}$$

In the case of nearest-neighbor interactions, the general form of E_k and F_k can be assumed to be

$$E_k=\frac{1}{\mu}[a+b\sin^2(k/2)],$$
$$F_k=\mu[c+d\sin^2(k/2)], \tag{2.23}$$

for positive a,b,c,d and positive mass parameter μ. We get

$$D(T=0)=\frac{\hbar}{\pi\mu}\frac{a+b}{\sqrt{a(c+d)}}\Pi\left[\frac{\pi}{2},-\frac{b}{a},\left[\frac{ad-bc}{a(c+d)}\right]^{1/2}\right], \tag{2.24}$$

where Π denotes the elliptic integral of the third kind. For $b=0$, i.e., for the local kinetic term, Eq. (2.24) reduces to the well-known form

$$D(T=0,b=0)=\frac{\hbar}{\pi\mu}\left[\frac{a}{c+d}\right]^{1/2}K\left[\left[\frac{d}{c+d}\right]^{1/2}\right], \tag{2.25}$$

K being the complete elliptic integral of the first kind. The form (2.25) is used to discuss the sine-Gordon field.[10]

The values of the renormalization factor $D(T)$ for frequencies whose dispersion curve is given in terms of (2.23) can be obtained by calculating the continuum limit of (2.21) with a numerical integration procedure.

In the next section we report on some results related to real magnetic chains.

III. APPLICATION TO MAGNETIC CHAINS

The one-dimensional ferromagnet $CsNiF_3$ can be described by the following spin Hamiltonian ($S=1$):

$$H=-2J\sum_i(\mathbf{S}_i\cdot\mathbf{S}_{i+1})+A\sum_i(S_i^z)^2-h\sum_i S_i^y\ , \tag{3.1}$$

where $h=g\mu_BH$ is the Zeeman field ($h\sim 1$ K for the usual applied magnetic field). $A=9$ K is the easy-plane-anisotropy parameter and $J=11.8$ K is the exchange integral. Assuming an unitary lattice spacing, the dispersion relation for the spin waves reads

$$\omega^2(k)=4\Omega_0\left[\frac{1}{4R^2}+\sin^2\left[\frac{k}{2}\right]\right]\times\left[1+\frac{b}{4R^2}+b\sin^2\left[\frac{k}{2}\right]\right], \tag{3.2}$$

where $\Omega_0^2=4S^2J\tilde{A}$, $R^2=2JS/h$, and $b=4J/\tilde{A}$, with $\tilde{A}=A[1-1/(2S)]$.

The Hamiltonian (3.1) can be mapped into the sine-Gordon field for harmonic exchange and for very high anisotropy,[16] yielding

$$H=2JS^2\sum_i\left[\frac{\tilde{A}}{2JS^2}P_i^2+\tfrac{1}{2}(\phi_i-\phi_{i+1})^2+\frac{1}{R^2}(1-\cos\phi_i)\right], \tag{3.3}$$

the angles $\{\phi_i\}$ being the canonical coordinates and $\{P_i\}$ the corresponding conjugate momenta. In this limit, the energy of the static classical kink is $E_{\text{kink}}=8S\sqrt{2hJS}$. This kink soliton is also a nonlinear solution in a system where the out-of-plane fluctuations are considered.[15] The parameter R measures the length of the kink (in lattice units), while the quantum character of the system is ruled by the coupling parameter $Q=\hbar\Omega_0/RE_{\text{kink}}$.

The insufficiency of a perfect planar model was proved by several authors,[10,12] and additional terms which take into account the deviations from the sine-Gordon model have been considered for the spin Hamiltonian (3.1). This can be done by using an approximate Villain transformation mapping (3.1) into a Bose-operator Hamiltonian[15] in the low-coupling limit. The dispersion relation of the linear oscillations around the vacuum is given by (3.2). If we disregard nonlinear terms mixing kinetic and configurational variables, we can use the model (1.1)–(1.3), where the diagonal values E_k and F_k of the matrices K and L, respectively, are given by (2.23) with the following identification of the parameters:

$$a=1+\frac{b}{4R^2},\quad c=\frac{\Omega_0^2}{R^2},$$
$$d=4\Omega_0^2,\quad g=\mu=\frac{1}{2\tilde{A}}. \tag{3.4}$$

The partition function of this model is then calculated as a function of Q, R, and b. The anharmonic part of the potential is taken again as sine Gordon, so that the total Hamiltonian (3.3) reads

$$H=2JS^2\sum_i\left[\frac{\tilde{A}}{2JS^2}\left[1+\frac{b}{4R^2}\right]P_i^2+\frac{\tilde{A}}{2JS^2}\frac{b}{4}(P_i-P_{i+1})^2+\tfrac{1}{2}(\phi_i-\phi_{i+1})^2+\frac{1}{R^2}(1-\cos\phi_i)\right]. \tag{3.5}$$

Some considerations are in order. The classical contribution to the specific heat is, of course, the same for the discrete sine-Gordon system as well as for the system described by the Hamiltonian (3.5) because of the classical equipartition theorem. On the contrary, in the quantum case, the modified dispersion relation changes the linear contribution, together with the renormalization factor $D(T)$, which also causes a different nonlinear contribution.

We want to study now the influence of the modified dispersion relation on the quantum corrections. Our calculation will be confined to the case of small Q (low coupling) and large R (displacive limit) where some expansions are performed according to the procedure described in Refs. 8–10. The final result for the nonlinear contribution to the free energy, at not too low temperatures, $k_BT>QE_{\rm kink}/2$, reads

$$e^{-\beta F_0}=\left[\frac{m}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}e^{(2N+1)/\beta u(\Omega_0/R)^2D/2}\left[\prod_k\frac{f_k}{\sinh f_k}\right]\int d\phi\exp\left[-\frac{\beta\mu}{2}\sum_a\left[\Omega_0^2(\phi_a-\phi_{a+1})^2-\frac{2\Omega_0^2}{R^2}e^{-D/2}\cos\phi_a\right]\right]. \tag{3.6}$$

The factor D is determined by the linear fluctuations around the vacuum and is given in (2.21). In this way the linear part is calculated in a complete quantum scheme, while the nonlinear contribution is given in a semiclassical (first-cumulant) approximation. The values of $D(T)$ are plotted in Fig. 1 versus the reduced temperature $t=k_BT/E_{\rm kink}$ at fixed Q and R, for different values of b. The selected values, $Q=0.11$ and $R=5$, refer to typical parameters for $CsNiF_3$. The presence of the out-of-plane fluctuations increases the values of $D(T)$ at all temperatures, giving substantial corrections for $b\simeq 10$, as for the $CsNiF_3$ case.

Starting from Eq. (3.6) we can calculate the nonlinear contribution to the specific heat by means of the modification of the classical free-energy expansion.[4,17] The final result is presented in Fig. 2. The quantum corrections increase for increasing values of b and the position of the peak is shifted at lower temperatures with decreasing height of the maximum. This trend has been observed in Ref. 11, where the dilute-soliton-gas approximation is used, but the phase shift is that of the the nonlinear out-of-plane terms. The latter are not considered in our framework; however, the influence of the linear part of the out-of-plane fluctuations is evaluated in the interacting-soliton regime, showing the relevance of the use of the modified dispersion relation to determine the correct re-

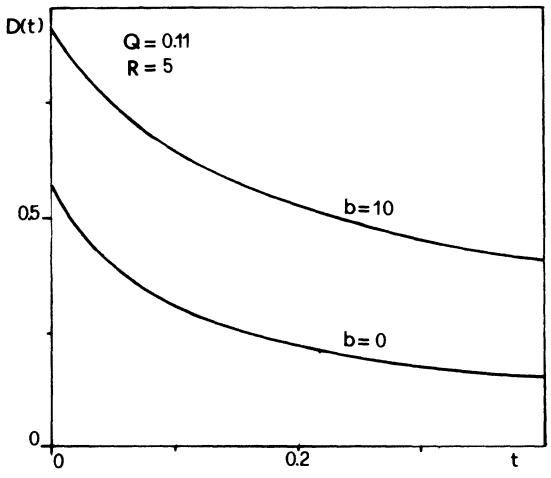

FIG. 1. Quantum renormalization parameter $D(T)$ vs reduced temperature t for $Q=0.11$, $R=5$, and $b=0,10$.

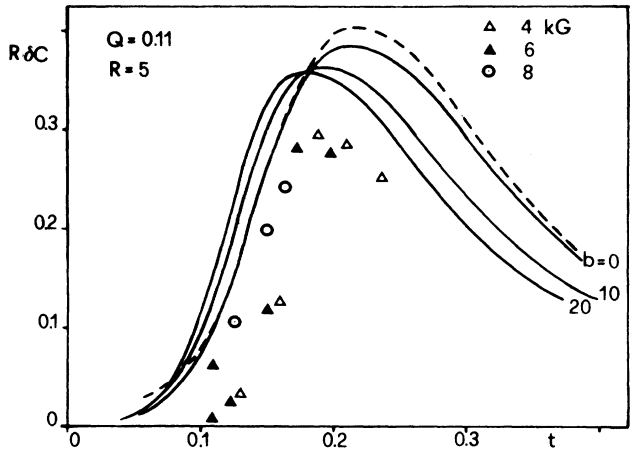

FIG. 2. Nonlinear contribution to the specific heat vs reduced temperature for $Q=0.11$ and $R=5$. Dashed curve: classical sine-Gordon result. Solid curves: quantum results at different values of b. Experimental data from Ref. 18.

normalization factor, which clearly affects the quantum behavior. The agreement with the experimental data[18] apparently improves. However, it must be noted that classical-transfer-matrix calculations for the ferromagnet Hamiltonian (3.1) (Ref. 13) give much higher peaks, showing, at least for the classical case, the importance of nonlinear out-of-plane terms. Recent quantum calculations[19,20] seem to be in agreement with the experiments, and much higher corrections should be required to describe the quantum behavior starting from the classical spin Hamiltonian. In this case some doubts arise about the possibility of using a semiclassical approach.

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