Variational Approach to Quantum Statistical Mechanics of Nonlinear Systems with Application to Sine-Gordon Chains

Riccardo Giachetti[(a)] and Valerio Tognetti[(b)]
Dipartimento di Fisica, Università di Firenze, 50125 Firenze, Italy

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The path-integral method is used for determination of the quantum corrections to the free energy of nonlinear systems. All quantum effects of the harmonic part of the potential are considered and a variational principle is used to account for the quantum corrections due to the anharmonic part. Correct renormalized frequencies are obtained at any temperature and an effective potential to be inserted in the configurational integral is found. A new general expression for the partition function at any temperature in the low-coupling limit is obtained.

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Methods of reducing quantum statistical calculations to classical ones[1,2] are finding nowadays increasing applications to fluid[3] and solid[4] models. In one-dimensional magnetic chains, classical models are unsatisfactory[5] (see, e.g., the $CsNiF_3$ case) and quantum corrections have been taken into account[6,7] in the low-coupling limit, restricted to the noninteracting soliton approximation, which fails in the range of temperature where the peak of the specific heat occurs.[8] Different expansions have also been proposed.[9,10]

We use here a path-integral approach which improves upon previous variational treatments[11] by considering all the quantum effects of the harmonic part of the potential, while the variational principle, in the first cumulant approximation, is used to account for the renormalized quantum corrections, both of potential and of frequencies, due to the anharmonic part. Besides unifying the previous methods,[6,9,10] our approach gives a correct effective potential for all temperatures in the low-coupling limit and can be applied to systems where the energy scales of linear and nonlinear excitations are well separated. Relegating the mathematical details of the theory to an extended paper, we present in this Letter a brief account of the formalism and a concrete application to the sine-Gordon chain, including a numerical evaluation of the specific heat throughout the temperature range, thus clarifying some controversial issues on soliton behavior in planar magnetic chains.

The path-integral form of the partition function $Z = e^{-\beta F}$ is

$$e^{-\beta F} = \int_{x(0)=x(\beta\hbar)} \mathscr{D}[x(u)] \exp\left[(-1/\hbar)\int_0^{\beta\hbar} du \left((m/2)\sum_{i=1}^{N} \dot{x}_i^2(u) + V(x(u))\right)\right]. \tag{1}$$

The functional integral is evaluated over all the closed paths and the potential V is taken in the discrete form

$$V = (m/2)\sum_{i,j=1}^{N} x_i B_{ij} x_j \; g \sum_{i=1}^{N} U(x_i). \tag{2}$$

We assume that $B_{ij} = B_{i+n,j+n}$ contains all the harmonic interaction $[U''(0)=0]$. The anharmonic part $U(x)$ has been taken to be local for simplicity, since the extension to a general $U(x)$ is straightforward. We define

$$V_0 = W(y) + \sum_{i=1} w_i(y)[x_i(u) - y_i] + (\tfrac{1}{2})\sum_{i,j=1}^{N} [x_i(u) - y_i] w_{ij}(y) [x_j(u) - y_j], \tag{3}$$

with $y = (1/\beta\hbar)\int_0^{\beta\hbar} x(u)\,du$. The functions W, w_i, and w_{ij} must be chosen in order to minimize the right-hand side of the first-order cumulant inequality

$$F \leq F_0 + \langle V - V_0 \rangle_0, \tag{4}$$

where F_0 and the average are defined with use of V_0 instead of V. It is worthwhile to note that $w_{ij}(y)$ are not taken equal to $\partial_{ij}^2 V(y) = mB_{ij} + g\delta_{ij}U''(y)$, but are determined by the variational principle. As will be shown in the following, this is a crucial point to avoid unphysical results at lowest temperatures and just this full application of the variational principle leads to the correct frequency renormalization.

If we denote by Q_{rs} the orthogonal matrix which diagonalizes the symmetric matrix w_{ij} and by $\omega_k(y)$ the corresponding kth eigenfrequency, it can be shown that the search for the extrema with respect to w_{ij} is equivalent to that with respect to $\omega_k(y)$ and Ω_{rs} once the appropriate constraints are inserted.

The evaluation of the functional integral gives

$$e^{-\beta F_0} = (m/2\pi\hbar^2\beta)^{N/2} \int d^N y \exp[-\beta W(y)] \prod\nolimits_k (f_k/\sinh f_k), \tag{5}$$

with $f_k = \hbar\beta\omega_k/2$.

The function W which minimizes the inequality (4) reads

$$W(y) = \int d^N\eta\, V(Q^T\eta + y) \prod_k \frac{\exp(-\eta_k^2/\alpha_k)}{(\pi\alpha_k)^{1/2}} - m \sum_k \frac{\alpha_k f_k}{\hbar^2\beta^2}, \tag{6}$$

where the parameter

$$\alpha_k = (\hbar^2\beta/2mf_k^2)(f_k \coth f_k - 1) \tag{7}$$

is twice the difference between quantum and mean square displacements of the kth oscillator of frequency $\omega_k(y)$. These quantities give the behavior of the Gaussian quantum spread from the harmonic oscillator in the ground state ($\beta \rightarrow \infty$) to the free particle at high temperatures. Moreover, $W(y)$ is such that $\langle V - V_0 \rangle_0$ vanishes, allowing the definition of an effective potential V_{eff} to be inserted in the configurational integral, giving an equivalent "classical" free energy F_0 which accounts for the quantum corrections in the one-loop approximation. Explicitly, denoting by $U^{(n)}$ the nth derivative of U, from Eqs. (5) and (6), we get

$$V_{\text{eff}} = V(y) - \beta^{-1} \sum_k (\ln f_k - \ln \sinh f_k) - g \sum_r \sum_{n=2}^{\infty} \frac{(n-1)}{n!} U^{(2n)}(y_r)(\tfrac{1}{2}D)^n, \tag{8}$$

with the quantum renormalization factor

$$D = \sum\nolimits_k Q_{kr}^2 (\alpha_k/2). \tag{9}$$

The variational principle for $\omega_k(y)$ and $Q_{rs}(y)$ leads to the following self-consistent equations:

$$\sum\nolimits_{r,s} Q_{ir}[B_{rs} + (g/m)P_{rs}(y)]Q_{ks} = \omega_k^2(y)\delta_{ik}, \tag{10}$$

$$P_{rs}(y) = \delta_{rs} \int d^N\eta\, U^{(2)}((Q^T\eta + y)_r) \prod_k \frac{\exp(-\eta_k^2/\alpha_k)}{(\pi\alpha_k)^{1/2}}. \tag{11}$$

In Eq. (8), the logarithmic terms represent the difference between the quantum and classical free energy of harmonic oscillators whose frequencies are renormalized, through Eqs. (10) and (11), by the quantum fluctuations. The spread of the anharmonic part is also present in V_{eff}. This approximate treatment of the quantum effects does not require the knowledge of the classical "trajectory" and the problem is now referred to the evaluation of the configurational integral with an effective potential. In a different context, effective potentials, at finite temperatures, were introduced in field theories[12] without any variational principle for determination of the frequencies.

The self-consistent equations (10) and (11), although easily solvable for a single anharmonic oscillator, look formidable for interacting fields and their solution involves a self-consistent diagonalization of a matrix which, in the general case, can be done by numerical iterative methods. However, some properties of the frequencies $\omega_k(y)$ can be inferred from the structure itself. In particular, it is worthwhile to note that Eqs. (10) and (11) prevent us from having imaginary $\omega_k(y)$ with $f_k = i\pi$, which would cause unphysical divergences in the effective potential, and that all frequencies are real in the limit $\beta \rightarrow \infty$, while $\omega_k^2(y) = (1/m)\partial_{ij}^2 V(y)$ only for $\beta = 0$.

We finally note that in some range of temperatures V_{eff} can be easily evaluated. At highest temperatures or for small quantum effects, we have $\alpha_k \simeq \hbar^2\beta/(6m)$ and the effective potential reads

$$V_{\text{eff}} = V(y) + (\hbar^2\beta/24m) \sum\nolimits_j \partial_{jj}^2 V(y) \tag{12}$$

in agreement with Ref. 11 and reproducing the first term of the Wigner approach.[1]

At lowest temperatures, the evaluation of the configurational integral can be performed around the local minima with steepest descent procedure. In this, ω_k's are calculated at these minima and represent the renormalized frequencies of the oscillations around vacuum and soliton solutions. However, for a consistent full treatment of finite-temperature effects in the mean-field approximation, the classical renormalizations of the frequencies turn out to be included also.

We now apply our theory to the sine-Gordon (SG) chain. We have

$$\begin{aligned} B_{rs} &= \Omega_0^2(2\delta_{rs} - \delta_{r,s-1} - \delta_{r,s+1}) + \Omega_1^2\delta_{rs}, \\ U(y) &= \sum\nolimits_r (m\Omega_1^2/g^3)[1 - (g^2y_r^2/2) - \cos(gy_r)], \end{aligned} \tag{13}$$

so that, with neglect of zero-point constants,

$$V_{\rm eff}=(m\,\Omega_0^2/2)\,\textstyle\sum_r (y_r-y_{r+1})^2-\beta^{-1}\sum_k \ln(f_k/\sinh f_k)-(m\,\Omega_1^2/g^2)\sum_r \cos(gy_r)e^{-g^2D/2}(1+g^2D/2), \tag{14}$$

and

$$P_{rs}=\delta_{rs}(m\,\Omega_1^2/g)[\cos(gy_r)e^{-g^2D/2}-1]. \tag{15}$$

It is straightforward to see that Eq. (10) cannot give negative values for any $\omega_k^2(y)$ for lower and lower temperatures, where the main contribution to the partition function arises from the local minima of $V_{\rm eff}$. These can be determined, for low coupling, by the following equation:

$$\Omega_0^2(2y_r-y_{r-1}-y_{r+1})+(\Omega_1^2e^{-g^2D/2}/g)\sin(gy_r)=0, \tag{16}$$

which, in the continuum limit, becomes the sine-Gordon equation with the renormalized frequency $\Omega_1\exp(-g^2D/4)$. For $\beta\to\infty$ the only contribution comes from the vacuum sector $y_r=0$. Taking into account that Q_{kr} is now the matrix which diagonalizes B_{rs}, we obtain the self-consistent equation

$$\omega_k^2=4\Omega_0^2\sin^2(k/2)+\Omega_1^2\exp(-g^2D_0/2), \tag{17}$$

with $D_0=(1/N)\sum_k\hbar/2m\omega_k$. When the temperature increases the variation of D can be calculated according to Eq. (9); the classical Gaussian (Hartree-Fock) approximation, holding at low temperatures, gives a further renormalization to Ω_1 represented by the replacement of α_k with $\alpha_k'=(\hbar/m\omega_k)\coth(\hbar\beta\omega_k/2)$. The new renormalization factor $\hat{D}$ contains both quantum and classical temperature effects.[6] The contribution of the local minimum, corresponding to a static solution $y=y^{(S)}$, must also be included. By substituting the solution $y^{(S)}$ in Eq. (10), we get the new spectrum of the small oscillations and the results of Ref. 6 are recovered.

At highest temperatures, or for small quantum effects, Eq. (12) gives the following effective potential:

$$V_{\rm eff}=N\hbar^2\beta 2\Omega_0^2/24+\textstyle\sum_r\{(m\,\Omega_0^2/2)(y_r-y_{r+1})^2-(m/g^2)\Omega_1^2[1-g^2\hbar^2\beta/(24m)]\cos(gy_r)\}. \tag{18}$$

The first term is the quantum correction[11] of the oscillators, of frequency $\Omega_k=2\Omega_0\sin(k/2)$, related with the nearest-neighbor interaction: At this level they are equivalent to N Einstein oscillators with frequency $\overline{\Omega}=\sqrt{2}\Omega_0$. On the other hand, the quantum effects related to the SG potential can be taken into account by simple renormalization of the frequency Ω_1.

Let E_S be the classical soliton energy and let us consider the low-coupling ($Q=\hbar\Omega_1/E_S\ll 1$) displacive limit [$\epsilon=(\Omega_1/2\Omega_0)^2\ll 1$]: The point of view of Eq. (18) can be extended to lower temperatures by use of the our effective potential. Indeed, under these conditions, the contribution of the logarithmic term to $V_{\rm eff}$ in Eq. (8) mainly comes from oscillators with higher k's, so that this term, containing only quantum corrections, can be safely expanded in terms of Ω_1. Of course, any modification of the radiation due to nonlinearity is included in the configurational integral which is not necessarily bound to the dilute-gas approximation.

In the low-coupling limit we obtain

$$e^{-\beta F_0}=(m/2\pi\hbar^2\beta)^{N/2}\textstyle\prod_k(f_k^0/\sinh f_k^0)$$
$$\times\int d^Ny\,\exp\{-\beta(m/2)\textstyle\sum_r[\Omega_0^2(y_r-y_{r+1})^2-(2\Omega_1^2e^{-g^2D/2}/g^2)\cos(gy_r)]\}, \tag{19}$$

where $f_k^0=\hbar\beta\Omega_0\sin(k/2)$. The quantum renormalization factor can be calculated at all temperatures with use of the frequency spectrum of the oscillations around the vacuum solution within an approximation consistent with the displacive limit. One obtains

$$D=\frac{4Q^2R}{t}\sum_{n=1}^{\infty}\left[(n\pi)^4+\frac{QR}{\xi t}\left(\frac{1+\xi^2}{16R^2}\right)(n\pi)^2+\left(\frac{Q^2R}{2\xi t^2}\right)^2\right]^{-1/2}, \tag{20}$$

with $t=k_{\rm B}T/E_S$, $R=\Omega_0/\Omega_1$, and $\xi=(1+\epsilon)^{-1/2}$. From the behavior of $D(T)$, plotted in the inset of Fig. 1, one can see that its value, at the temperatures where the peak of the specific heat for the classical system occurs, is only 30% of the value at $T=0$.

The equivalent free energy F_0 as given by Eq. (19) presents some interesting aspects and constitutes an important improvement over previous theories. In the high-temperature limit $V_{\rm eff}$, as given by Eq. (18), is recovered. For decreasing temperatures, the free energy presents a Debye behavior with an added contribution due to a classical SG potential in which Ω_1 is replaced by its quantum renormalized counterpart.

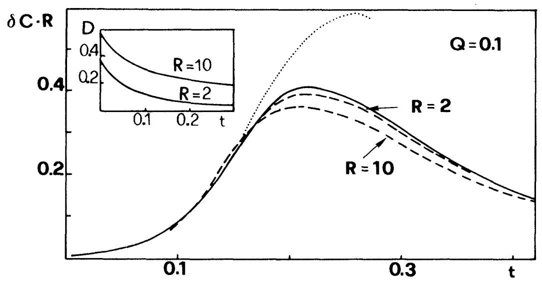

FIG. 1. Nonlinear contribution to specific heat $C = C^{nl}/(4\epsilon)^{1/2}$ vs t. Full line: classical result. Dotted line: classical result without soliton-soliton interaction (Ref. 13). Dashed lines: quantum results for $Q = 0.1$ and $R = 2$, 10. Inset: quantum renormalization factor D vs t for $R = 2$, 10.

Thus the contribution of all nonlinear excitations to free energy can be reduced to the calculation of a classical configurational integral where all the well-known classical techniques, such as interacting-soliton models,[13] high-temperature expansions, and, eventually, transfer matrix numerical calculations, can be used.

The nonlinear contribution to the specific heat versus the temperature is shown in Fig. 1 together with the classical result. For the range in which Q and R are considered, the quantum corrections are important for the harmonic part, while they do not much affect the anharmonic contribution. The large difference with respect to the classical dilute-gas approximation is mainly due to the soliton-soliton interaction which can be considered nearly classical. If the one-dimensional ferromagnet $CsNiF_3$ could be thought of as a sine-Gordon system, the appropriate values of its parameters would be $Q \simeq 0.11$, $R \simeq 5$. Hence, the quantum corrections would not sensibly modify the behavior of the classical specific heat obtained by the exact transfer-matrix approach.[14] The mismatch with experiments must be attributed to the inadequacy of the planar model and to the great influence of the out-of-plane quantum fluctuations.

We finally observe that our general results support the numerical conclusions of Ref. 10, which hold in a limited range of temperature only. The discrepancy already noted in Ref. 10 with respect to Ref. 9 is confirmed. Although Eq. (19) could lead to qualitative conclusions similar to those of Ref. 9, the correct renormalization factor is quite different, so that the quantum corrections are, in fact, much smaller than those predicted in Ref. 9, raising some doubts on the validity of that approach, which does not reproduce even the high-temperature results given by our Eq. (18).

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[a] Also at Istituto Nazionale di Fisica Nucleare, Sezione di Firenze, Firenze, Italy.

[b] Also at Centro Interuniversitario Struttura della Materia, Unità di Firenze, Firenze, Italy.

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