# Quantum corrections to the thermodynamics of nonlinear systems

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The path-integral approach is used for determining quantum corrections to the free energy of nonlinear systems. An effective potential, to be inserted in the configurational integral, is constructed by a new variational scheme which gives the quantum modification of the potential due to the anharmonic part together with the frequency renormalization. The single anharmonic oscillator is studied first. Then the extension to fields is presented and a new general expression for the partition function is given. The method is applied to the sine-Gordon chain and explicit calculations of the specific heat are shown.

## I. INTRODUCTION

Presently, great interest is being devoted to reexamining methods which allow reduction of quantum statistical-mechanical calculations to classical ones.[1-3] Indeed, in the latter case, the few well-known analytical methods for evaluating the phase-space integrals can be implemented by efficient numerical techniques. Following this trend, Monte Carlo simulations have been extended to the quantum case,[2,4,5] using the Trotter formula for spin systems. Also, Wigner expansions find increasing applications to fluid[6] and solid[7] models.

In one-dimensional physics the transfer-matrix approach is also available for the classical equilibrium properties. However, experiments on one-dimensional magnetic chains show that purely classical models are not always satisfactory[8] for interpreting the features of the specific heat in the ferromagnet $CsNiF_3$ (Refs. 9 and 10) and in the antiferromagnets $TMMC[(CH_3)_4NMnCl_3]$ (Ref. 11) and CHAB $[(C_6H_{11}NH_3)CuBr_3]$.[12] Quantum corrections to sine-Gordon and nearly sine-Gordon chains[13,14] were taken into account in the semiclassical (low-coupling) limit, restricted to the noninteracting soliton approximation, which is not valid in the range of temperatures where the peak of the specific heat occurs.[11]

In order to evaluate quantum effects in the high-temperature regime, expansions based on the coherent states[15] and a rearrangement of the Wigner series[16] have been proposed. Similar rearrangements of the Wigner series, by means of an expansion in powers of the interaction potential, have been recently proposed[17] for different applications.

We think that the path-integral approach[18] is the ideal tool for the treatment of quantum fluctuations. Indeed, starting from the classical partition function, this method permits one to construct an "effective" potential to be inserted in a configurational integral.

In preliminary work[19] we have given a brief account of a path-integral approach which improves upon previous variational treatments.[18] All of the quantum effects of the harmonic part of the potential are considered, while the variational principle in the first cumulant approximation is used to account for the quantum corrections due to the anharmonic part. An application to the sine-Gordon chain was given in order to discuss specific-heat measurements on real magnetic chains.[20]

In this paper we explain the method in detail. In Sec. II we present this variational principle applied to a single anharmonic oscillator, directly deriving the frequency renormalization and all limiting cases. An explicit effective potential for all temperatures is calculated for single- and double-well anharmonic potentials. In Sec. III we extend the method to fields. Its application to the sine-Gordon chain is developed in Sec. IV, where explicit calculations of the specific heat are shown and the results for real systems are discussed. In Sec. V we draw some conclusions.

## II. PARTITION FUNCTION FOR AN ANHARMONIC OSCILLATOR

The path-integral form of the partition function of an anharmonic oscillator is[18]

$$Z = e^{-\beta F} = \int_{x(0)=x(\beta\hbar)} \mathscr{D}[x(u)] e^{-\hbar^{-1} S[x(u)]} , \tag{2.1}$$

where $\beta = 1/(k_B T)$, the functional integral is evaluated over all of the closed paths and

$$S[x(u)] = \int_0^{\beta\hbar} du \left[ \frac{m}{2} \dot{x}^2(u) + V(x(u)) \right] . \tag{2.2}$$

Due to the well-known first-order cumulant inequality for the free energy[18]

$$F \le F_0 + \frac{1}{\beta} \langle S - S_0 \rangle_{S_0} \tag{2.3}$$

we shall approximately evaluate (2.1) by calculating

$$e^{-\beta F_0} = \int_{x(0)=x(\beta\hbar)} \mathscr{D}[x(u)] e^{-\hbar^{-1} S_0[x(u)]} , \tag{2.4}$$

where we assume for $S_0$ the functional

$$S_0[x(u)] = \int_0^{\beta\hbar} du \left[ \frac{m}{2} \dot{x}^2 + w(\bar{x}) + b(\bar{x})(x - \bar{x}) + \frac{m}{2} \omega^2(\bar{x})(x - \bar{x})^2 \right] , \tag{2.5}$$

 

with $\bar{x}=\frac{1}{\beta\hbar}\int_0^{\beta\hbar} x\,du$, $x\equiv x(u)$.

The functions $w(\bar{x}),\omega^2(\bar{x})$ will be determined in such a way to minimize the right-hand side (rhs) of Eq. (2.3), while $b(\bar{x})$ turns out to disappear from the final result. In this way, improving previous approaches,[18,21] we consider all of the quantum effects of the harmonic part of the potential, while the variational principle determines the frequency $\omega^2(\bar{x})$ and the quantum spread of the anharmonic part of the potential. It is also convenient to introduce the notation

$$f\equiv f(\bar{x})=\tfrac{1}{2}\beta\hbar\omega(\bar{x}) \tag{2.6}$$

which governs the amount of quantum effects.

The evaluation of the functional integral (2.4) will be performed by summing first over all of the paths with a prescribed average $\bar{x}$ and then integrating over all of the possible values of $\bar{x}$. Introducing the constraint $\bar{x}=\xi$ by the appropriate $\delta$ function and letting $z(u)=x(u)-\xi$, we get

$$e^{-\beta F_0}=\int d\xi\, e^{-\beta w(\xi)}\int\frac{dy}{2\pi}\int_{z(0)=z(\beta\hbar)}\mathscr{D}[z(u)]\exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar}du\left[\frac{m}{2}\dot{z}^2+\frac{m}{2}\omega^2 z^2+i\left[\frac{y}{\beta}-b\right]z\right]\right\}, \tag{2.7}$$

where the result is

$$e^{-\beta F_0}=\left[\frac{m}{2\pi\hbar^2\beta}\right]^{1/2}\int d\xi\frac{f}{\sinh f}e^{-\beta w(\xi)}. \tag{2.8}$$

In order to minimize the inequality (2.3), we must evaluate the term $1/\beta\langle S-S_0\rangle_{S_0}$ which, for the considered action, can prove to be equal to $\langle V-V_0\rangle_{S_0}$.[18] A lengthy but straightforward calculation gives

$$\langle V-V_0\rangle_{S_0}=e^{\beta F_0}\left[\frac{m}{2\pi\hbar^2\beta}\right]^{1/2}\int d\xi\, e^{-\beta w(\xi)}\left[\frac{\hbar^2\beta f^2}{6m\alpha\sinh^2 f}\right]^{1/2}\left[\mathscr{K}(\xi)-\left[\frac{6m\alpha}{\hbar^2\beta}\right]^{1/2}\left[w(\xi)+\frac{m\alpha f^2}{\hbar^2\beta}\right]\right], \tag{2.9}$$

where

$$\mathscr{K}(\xi)=\left[\frac{6m}{\pi\hbar^2\beta}\right]^{1/2}\int d\eta\, V(\xi+\eta)e^{-\eta^2/\alpha}, \tag{2.10}$$

and

$$\alpha\equiv\alpha(\xi)=\frac{\hbar^2\beta}{2mf(\xi)}\left[\coth f(\xi)-\frac{1}{f(\xi)}\right]. \tag{2.11}$$

The quantity $\alpha$ governs the quantum spread of the potential given by $\mathscr{K}(\xi)$. For real values of $f$ it gives a behavior determined by an harmonic oscillator in the ground state ($\beta\to\infty$) to that of a free particle ($\beta\to 0$). Negative values of $\omega^2(\xi)$ and consequently imaginary values of $f$ can be allowed provided that the temperature is so high that the paths can never go very far from $z(0)$ due to a large kinetic energy ($f=i\nu$, $|\nu|<\pi$). Indeed, as shown in the following, our variational principle prevents this limiting situation and gives always real values of $f$ for lowest temperatures. Taking the minimum of (2.3) with respect to $w(\xi)$, we find

$$w(\xi)=\left[\frac{\hbar^2\beta}{6m\alpha}\right]^{1/2}\mathscr{K}(\xi)-\frac{m\alpha f^2}{\hbar^2\beta^2} \tag{2.12}$$

and the average $\langle V-V_0\rangle_{S_0}$ vanishes. For these reasons, we are allowed to introduce an effective potential $V_{\rm eff}$ in the configurational integral

$$e^{-\beta F}\simeq e^{-\beta F_0}=\left[\frac{m}{2\pi\hbar^2\beta}\right]^{1/2}\int d\xi\, e^{-\beta V_{\rm eff}(\xi)} \tag{2.13}$$

with

$$V_{\rm eff}(\xi)=w(\xi)-\frac{1}{\beta}\ln(f/\sinh f). \tag{2.14}$$

Observing that [the superscript $(2n)$ denotes the $2n$th derivative]

$$(\pi\alpha)^{-1/2}e^{-\eta^2/\alpha}=\sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{\alpha}{4}\right]^n\delta^{(2n)}(\eta) \tag{2.15}$$

we get the following equivalent expression for $w(\xi)$

$$w(\xi)=\sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{\alpha}{4}\right]^n V^{(2n)}(\xi)-\frac{m\alpha f^2}{\hbar^2\beta^2}. \tag{2.16}$$

In order to obtain the best approximation to $F$ we still have to minimize $F_0$ with respect to $\omega$, i.e., with respect to $f$. The equation $\delta F_0/\delta f=0$ reads

$$\omega^2\equiv\omega^2(\xi)=\frac{1}{m}\sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{\alpha}{4}\right]^2 V^{(2n+2)}(\xi)$$
$$=\frac{1}{m}\int d\eta\, V^{(2)}(\xi+\eta)(\pi\alpha)^{-1/2}e^{-\eta^2/\alpha} \tag{2.17}$$

defining the frequency $\omega(\xi)$ of the harmonic part of the approximate functional $S_0$. This self-consistent equation cannot give negative solutions for $\omega^2(\xi)$ such that $f=i\pi$

which would produce unphysical divergences. In particular, for $T=0$, the value of $\omega^2(\xi)$ must always be positive. This can be verified for all physical potentials.

Let us consider the partition function in the two extreme temperature limits, namely very high ($\beta\to 0$) and very low ($\beta\to\infty$) temperatures. The first one corresponds to a quasi-classical situation. From Eqs. (2.14) and (2.17) we have

$$e^{-\beta F}\simeq\left[\frac{m}{2\pi\hbar^2\beta}\right]^{1/2}\int d\xi\exp\left[-\beta\left[V(\xi)+\frac{\hbar^2\beta}{24m}V^{(2)}(\xi)\right]\right], \tag{2.20}$$

which reproduces the first correction in the Wigner expansion.[1,21,22]

In the opposite limit, $\beta\to\infty$, the integral (2.13) can be performed by the saddle-point method. Considering $\xi_m$ as the minimum of $V_{\text{eff}}$, we find for the free energy in the low coupling limit

$$F=\tfrac{1}{2}\hbar\omega(\xi_m)+\frac{1}{\beta}\ln(1-e^{-\beta\hbar\omega(\xi_m)})+g_1+g_2(\beta)\,, \tag{2.21}$$

where $g_1$ is the zero-point correction and $g_2(\beta)$ is a further temperature correction due to the anharmonicity. The main behavior of the system is that of an harmonic oscillator whose frequency is modified by the quantum fluctuations, $\alpha(T=0)=\hbar/(m\omega)$, through Eq. (2.17).

It is worthwhile to note that the one-loop "renormalization" is directly derived by our variational principle, since the self-consistent equation (2.17) does not produce any secular term. The improvement obtained by using variational methods with respect to perturbative ones, where regularization procedures are in order,[17] appears to be evident.

Let us now apply the method to an anharmonic oscillator with an interaction potential

$$V(\xi)=\frac{\lambda}{4}\left[\xi^2\pm\frac{\mu}{\lambda}\right]^2,\quad \lambda>0\,, \tag{2.22}$$

the negative sign corresponding to a double-well potential.

From Eq. (2.12) we have

$$w(\xi)=V(\xi)-3\lambda\left[\frac{\alpha}{4}\right]^2 \tag{2.23}$$

and the self-consistent equation for $f$ reads

$$\frac{3}{f}\left[\coth f-\frac{1}{f}\right]=\left[\frac{4}{Q}\right]^4 t^3f^2-2\left[\frac{4}{Q}\right]^2 t(3y^2\pm 1)\,, \tag{2.24}$$

where we have introduced the dimensionless quantities

$$Q=4\left[\frac{2\hbar^2\lambda^2}{m\mu^3}\right]^{1/2},\quad y=\left[\frac{\lambda}{\mu}\right]^{1/2}\xi,\quad t=\frac{4\lambda}{\mu^2\beta}\,. \tag{2.25}$$

The first one is the "quantum" parameter giving the ratio between the energy of the ground state of the harmonic oscillator and the height ($\mu^2/4\lambda$) of the barrier in the double-well case.

Looking for real solutions of $f$, we observe that the left-hand side (lhs) of (2.24) represents a function taking its maximum value, equal to unity, for $f=0$ and monotonically decreasing when $f$ tends to infinity. The condition for real solutions to exist is therefore

$$\tfrac{1}{2}\left[\frac{Q}{4}\right]^2\frac{1}{t}>\pm 1-3y\,. \tag{2.26}$$

Hence, if the temperature is sufficiently low, we always have real solutions for Eq. (2.24). For a double-well potential at highest temperatures, possible negative values of $\omega^2(\xi)$ can arise, depending on $\xi$, until to the classical value $m\omega^2=V^{(2)}(\xi)$, for $\beta=0$.

In the following we consider the more interesting double-well potential. At increasing temperatures, Eq. (2.25) is not satisfied: we have imaginary $\omega$ and consequently $f=i\nu$ with $-\pi<\nu<\pi$. Equation (2.24) becomes in this case

$$\frac{3}{\nu}\left[\operatorname{cotg}\nu-\frac{1}{\nu}\right]=\left[\frac{4}{Q}\right]^4 t^3\nu^2+2\left[\frac{4}{Q}\right]^2 t(3y^2-1)\,. \tag{2.27}$$

It is important to note that the solution for $\nu$, if any, remains bounded away from $\pm\pi$ at any temperature and depends continuously on $\beta$, having $\nu=0$ for $T\to\infty$ and $1/T=2(4/Q)^2(1-3y^2)$, when, of course, the latter quantity is positive. We stress this point, as it implies that no singularity or unphysical result can arise in the partition function at all temperatures, both for the double-well and single minimum potentials.

For $T=0$ the effective potential reads

$$V_{\text{eff}}=\frac{\lambda}{4}\left[y^2-\frac{\mu}{\lambda}\left[1-3\lambda\frac{\hbar}{\mu m\omega}\right]\right]^2+\frac{\hbar\mu}{m\omega}-27\lambda\left[\frac{\hbar}{4m\omega}\right]^2+O(\lambda^2) \tag{2.28}$$

and the self-consistent equation for the frequency becomes

$$m\omega^2=-\mu+3\lambda y^2+\tfrac{3}{2}\lambda\frac{\hbar}{m\omega}\,. \tag{2.29}$$

From the last two equations the minimum of the poten-

tial is found to be, up to the first order in the coupling constant, at the value

$$\xi_m = \pm \left[ \frac{\mu}{\lambda} \right]^{1/2} \left[ 1 - \tfrac{3}{4}\lambda \frac{\hbar}{\mu m \omega(\xi_m)} \right] , \tag{2.30}$$

where the renormalized frequency at minimum, $\omega(\xi_m)$, is determined by Eq. (2.29) and turns out to be

$$\omega(\xi_m) = \left[ \frac{2\mu}{m} \right]^{1/2} (1 - \tfrac{3}{32} Q) + O(Q^2) . \tag{2.31}$$

This frequency renormalization derives from the quantum effect of the anharmonicity, taken into account in a perturbative way. This would be exhaustive for the single-well potential. In our case, the quantum tunneling is also present and, of course, it cannot be accounted by our first cumulant theory [see Eq. (2.3)]. Therefore our treatment holds whenever the frequency renormalization is much greater than the effects of the quantum tunneling. The latter, in turn, can be easily evaluated and results in

$$\Delta\omega = - \left[ \frac{2\mu}{m} \right]^{1/2} \frac{1}{\pi} e^{-8I(Q)/Q} \tag{2.32}$$

with

$$I(Q) = \tfrac{2}{3}(1+\sqrt{Q})^{1/2} [E(q) - \sqrt{Q} K(q)] , \tag{2.33}$$

where $E$ and $K$ are the complete elliptic integrals of the argument

$$q = \left[ \frac{1-\sqrt{Q}}{1+\sqrt{Q}} \right]^{1/2} . \tag{2.34}$$

The function $I(Q)$ decreases monotonically from its value $\frac{2}{3}$ at $Q=0$ so that we are allowed to neglect the tunneling shift for $Q \lesssim 0.5$, its value being less than 4% of the anharmonic correction. The free energy for $T \to 0$ can be essentially represented by

$$F \simeq \tfrac{1}{2}\hbar\omega(\xi_m) + \tfrac{3}{16}\lambda \frac{\hbar^2}{\mu m} + \frac{1}{\beta} \ln(1 - e^{-\beta\hbar\omega(\xi_m)}) . \tag{2.35}$$

The self-consistent equation (2.24) has been solved for $\omega^2(y)$ for different values of the temperatures at $Q = \frac{1}{4}$. It appears that all of the frequencies tend to become real when the temperature approaches zero (Fig. 1). The effective potential, to be introduced in the configurational integral is plotted in Fig. 2. From its behavior the physical meaning of the quantum effects, according to our treatment, can be easily inferred: the quantum fluctuations make softer the potential, so that the jumps across the barrier activated by the temperature are enhanced.

## III. PARTITION FUNCTION FOR A SELF-INTERACTING SCALAR FIELD

Having discussed the partition function for the single anharmonic oscillator, we now study a system of $(2N+1)$ interaction points $\{x_a\}, |a| \leq N$, which reduces to a scalar field in the limit $N \to \infty$. We shall calculate the partition function

$$Z = e^{-\beta F} = \int_{\{x_a(0)\}=\{x_a(\beta\hbar)\}} \mathcal{D}[x(u)] e^{-\hbar^{-1} S[x(u)]} , \tag{3.1}$$

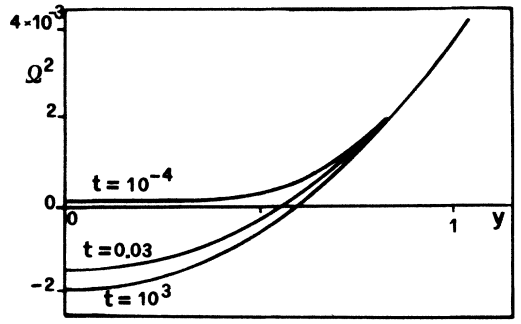


FIG. 1. Dimensionless quantity $\Omega^2 = \hbar^2\omega^2\lambda^2/\mu^4$ vs $y = (\lambda/\mu)^{1/2}\xi$ at different temperatures with $Q = \frac{1}{4}$ for the double-well potential.

where again the functional integral is evaluated over all of the closed paths in the configuration space of the system and where

$$S[x(u)] = \int_0^{\beta\hbar} du \left[ \frac{m}{2} \sum_{a=-N}^{N} \dot{x}_a^2(u) + V(x(u)) \right] . \tag{3.2}$$

Moreover we shall consider potentials of the form

$$V(x) = \frac{m}{2} \sum_{a,b=-N}^{N} x_a B_{ab} x_b + g \sum_{a=-N}^{N} u(x_a) , \tag{3.3}$$

where we assume that the symmetric matrix $B_{ab}$ contains completely the harmonic part of the interaction. These potentials are general enough to cover many models which are frequently met in applications. We also require periodic boundary conditions for our system and translation invariance for the matrix $B$, namely,

$$x_{a \pm (2N+1)} = x_a , \quad B_{a+c,b+c} = B_{ab} . \tag{3.4}$$

The situation is therefore very similar to that of a single oscillator, except for a number of additional technical complications which we must take into account.

According to the procedure developed in Sec. II, we shall calculate the "approximate" free energy $F_0$ determined by the functional

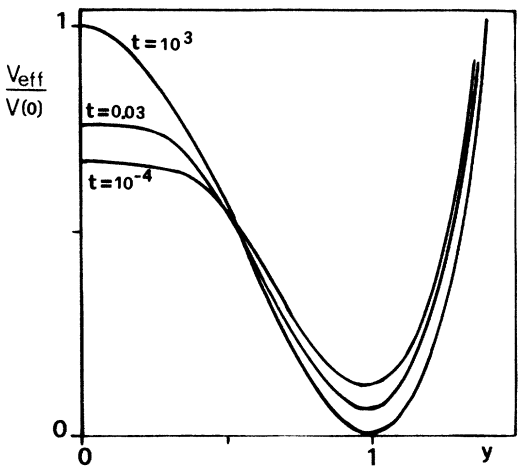


FIG. 2. Effective potential versus $y$ at different temperatures with $Q = \frac{1}{4}$.

$$S_0[x(u)]=\int_0^{\beta\hbar} du\left[\frac{m}{2}\sum_{a=-N}^{N}\dot{x}_a^2+w(\bar{x})+\sum_{a=-N}^{N}w_a(\bar{x})[x_a(u)-\bar{x}_a]+\frac{1}{2}\sum_{a,b=-N}^{N}[x_a(u)-\bar{x}_a]w_{ab}(\bar{x})[x_b(u)-\bar{x}_b]\right], \tag{3.5}$$

where, as in (2.5) $\bar{x}_a$ is the average of $x_a(u)$, and the coefficients $w$, $w_a$, $w_{ab}$ are going to be determined by the minimum problem posed by the inequality (2.3), which keeps holding. As $w_{ab}$ is a symmetric matrix, it can be diagonalized by an orthogonal matrix $U_{ka}$ with determinant equal to unity. We define the eigenfrequencies $\omega_k$ according to

$$\sum_{a,b=-N}^{N}U_{ka}w_{ab}U_{jb}=m\omega_k^2\delta_{jk} \tag{3.6}$$

and, for each $K$, we again introduce the quantities corresponding to (2.6) and (2.10), namely,

$$f_k=\tfrac{1}{2}\beta\hbar\omega_k\ ,$$
$$\alpha_k=\frac{\hbar^2\beta}{2m}\frac{1}{f_k^2}(f_k\coth f_k-1)\ . \tag{3.7}$$

The calculation of the partition function $e^{-\beta F_0}$ is done by first diagonalizing the matrix $w_{ab}$ and then proceeding as in Sec. II. The result is the expected one, i.e.,

$$e^{-\beta F_0}=\left[\frac{m}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\int d\xi\, e^{-\beta w(\xi)}\prod_{k=-N}^{N}\frac{f_k(\xi)}{\sinh f_k(\xi)}\ . \tag{3.8}$$

In a similar way

$$\langle V-V_0\rangle_{S_0}=e^{\beta F_0}\left[\frac{m}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\int d\xi\, e^{-\beta w(\xi)}\prod_{k=-N}^{N}\left[\left[\frac{\hbar^2\beta}{6m\alpha_k}\right]^{1/2}\frac{f_k}{\sinh f_k}\right]$$
$$\times\left\{\mathcal{K}(\xi)-\left[\prod_{k=-N}^{N}\left[\frac{6m\alpha_k}{\hbar^2\beta}\right]^{1/2}\right]\left[w(\xi)+\sum_{k=-N}^{N}\frac{m\alpha_k f_k^2}{\hbar^2\beta^2}\right]\right\} \tag{3.9}$$

with

$$\mathcal{K}(\xi)=\left[\frac{6m}{\pi\hbar^2\beta}\right]^{(2N+1)/2}\int d\eta\, V(U^T\eta+\xi)\exp\left[-\sum_{k=-N}^{N}(\eta_k^2/\alpha_k)\right]. \tag{3.10}$$

Minimizing (2.3) with respect to $w$ we get

$$w(\xi)=\int d\eta\, V(U^T\eta+\xi)\prod_{k=-N}^{N}\frac{e^{-\eta_k^2/\alpha_k}}{(\pi\alpha_k)^{1/2}}-\sum_{k=-N}^{N}\frac{m\alpha_k f_k^2}{\hbar^2\beta^2} \tag{3.11}$$

and again $\langle V-V_0\rangle_{S_0}=0$. Therefore, using the expansion (2.16) for each $k$ we define an effective potential $V_{\text{eff}}(\xi)$ which accounts for the self-consistent one-loop corrections

$$V_{\text{eff}}(\xi)=V(\xi)+\sum_{k=-N}^{N}\left[\frac{\alpha_k}{4}\right](UBU^T)_{kk}+g\sum_{n=1}^{\infty}\sum_{a=-N}^{N}\left[\sum_{k=-N}^{N}\left[\frac{\alpha_k}{4}\right]U_{ka}^2\right]^n\frac{u^{(2n)}(\xi_a)}{n!}$$
$$-\sum_{k=-N}^{N}\frac{m\alpha_k f_k^2}{\hbar^2\beta^2}-\frac{1}{\beta}\sum_{k=-N}^{N}\ln\left[\frac{f_k}{\sinh f_k}\right]. \tag{3.12}$$

Using (3.12) we can write

$$e^{-\beta F}\simeq e^{-\beta F_0}=\left[\frac{m}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\int d\xi\, e^{-\beta V_{\text{eff}}(\xi)}\ . \tag{3.13}$$

We now consider the minimum of $F_0$ with respect to $w_{ab}$. It is shown in Appendix A that the search for the extrema with respect to $w_{ab}$ is equivalent to that with respect to $\omega_k(\xi)$ and to the elements of the diagonalizing matrix $U_{ka}(\xi)$, once the appropriate constraints are imposed. The variational principle for these quantities leads to the following self-consistent equations:

$$\sum_{a,b=-N}^{N} U_{ia}\left[B_{ab}+\frac{g}{m}P_{ab}(\xi)\right]U_{kb}=\omega_k^2\delta_{ik} \tag{3.14}$$

with

$$P_{ab}(\xi)=\delta_{ab}\int d\eta\, u^{(2)}[(U^T\eta+\xi)_a]\prod_{k=-N}^{N}\frac{e^{-\eta_k^2/\alpha_k}}{(\pi\alpha_k)^{1/2}}$$

$$=\delta_{ab}\sum_{n=0}^{\infty}\frac{1}{n!}u^{(2n+2)}(\xi_a)\left[\frac{D_a}{2}\right]^n, \tag{3.15}$$

where we have defined the quantum renormalization factor

$$D_a(\xi)=\sum_{k=-N}^{N}U_{ka}^2(\xi)\left[\frac{\alpha_k}{2}\right]. \tag{3.16}$$

Moreover, using Eqs. (3.14) and (3.15), the expression of the effective potential can be recast in the more compact form

$$V_{\rm eff}(\xi)=V(\xi)-\frac{1}{\beta}\sum_{k=-N}^{N}\ln\left[\frac{f_k}{\sinh f_k}\right]$$

$$-g\sum_{a=-N}^{N}\sum_{n=2}^{\infty}\frac{(n-1)}{n!}u^{(2n)}(\xi_a)\left[\frac{D_a}{2}\right]^n. \tag{3.17}$$

The self-consistent equations (3.14) and (3.15), although easily solvable for a single anharmonic oscillator, become formidable for interacting fields and their solution could be obtained by a numerical procedure. However, the *a priori* knowledge of the classical "trajectory" is not in principle required.

The expression (3.17) for the effective potential holds at any value of $\beta$. However, as it occurs in the case of the anharmonic oscillator, the high- and low-temperature limits produce a simpler expression for $V_{\rm eff}$, which allow a better understanding of its physical content. The high-temperature limit is easy to calculate. From the definitions (3.7) we have $\alpha_k\to\hbar^2\beta/6m+O(\beta^2)$ as $\beta\to 0$, so that $\alpha_k$ is actually independent of $k$ up to terms of the second order in $\beta$. But in this case

$$\sum_{k=-N}^{N}\left[\frac{\alpha_k}{4}\right]U_{ka}^2=\frac{\hbar^2\beta}{24m}\sum_{k=-N}^{N}U_{ka}^2=\frac{\hbar^2\beta}{24m} \tag{3.18}$$

by the orthogonality of $U$ and

$$\sum_{k=-N}^{N}\left[\frac{\alpha_k}{4}\right](UBU^T)_{kk}=\frac{\hbar^2\beta}{24m}\sum_{a=-N}^{N}B_{aa} \tag{3.19}$$

by the properties of the trace. Finally, since

$$\sum_{k=-N}^{N}\frac{m\alpha_k f_k^2}{\hbar^2\beta^2}+\frac{1}{\beta}\sum_{k=-N}^{N}\ln\left[\frac{f_k}{\sinh f_k}\right] \tag{3.20}$$

is vanishing up to terms of the second order in $\beta$, so that from (3.12) we find

$$V_{\rm eff}(\xi)\simeq V(\xi)+\frac{\hbar^2\beta}{24m}\sum_{a=-N}^{N}[B_{aa}+gu^{(2)}(\xi_a)]$$

$$=V(\xi)+\frac{\hbar^2\beta}{24m}\sum_{a=-N}^{N}\frac{\partial^2}{\partial\xi_a^2}V(\xi),\quad \beta\to 0. \tag{3.21}$$

We thus recognize that the correction to the classical potential is just the first term of the Wigner expansion, as found in Ref. 18: indeed this limit is not sensitive of the quantum properties of the harmonic oscillators that have been completely accounted for in the functional $S_0$.

We now consider the limit of low temperatures, $\beta\to\infty$. From (3.13) it appears that in this case the most appropriate way to calculate the partition function is by using the saddle-point method. Its application requires the knowledge of the minima of the effective potential: we suppose that the absolute minima of $V_{\rm eff}$, i.e., the vacua, are represented by constant configurations, $\xi_a=$const, and we are going to study the contribution to the partition function of any vacuum sector. The contribution from solitons, whenever such solutions are allowed, can be handled along the same pattern: a detailed calculation will be worked out in the next section for the sine-Gordon case.

Let us consider the case $\xi_a=$const. From (3.15) it can be seen that the elements $P_{aa}$ are constant and independent of the index $a$: hence the matrix $P$ is a constant multiple of the identity matrix and $U$ is just the matrix which diagonalizes $B$. Due to the condition (3.4) of translation invariance for $B$, the matrix $U$ can be explicitly calculated and reads

$$A_{ka}\equiv U_{ka}(\xi_a=\text{const})=\begin{cases}\left[\dfrac{2}{2N+1}\right]^{1/2}\cos\left[\dfrac{2\pi ka}{2N+1}\right], & -N\le k\le -1\\ (2N+1)^{-1/2}, & k=0\\ \left[\dfrac{2}{2N+1}\right]^{1/2}\sin\left[\dfrac{2\pi ka}{2N+1}\right], & 1\le k\le N.\end{cases} \tag{3.22}$$

At low temperatures equation (3.7) gives

$$\alpha_k\to\frac{\hbar}{m\omega_k}\quad\text{as }\beta\to\infty. \tag{3.23}$$

Observing that $\alpha_k=\alpha_{-k}$ and using the explicit form (3.22) for $U_{ka}$, the quantum renormalization factor (3.16) reads

$$D=\sum_{k=-N}^{N}\left[\frac{\alpha_k}{2}\right]\to\sum_{k=-N}^{N}\frac{\hbar}{2m\omega_k}\quad\text{as }\beta\to\infty \tag{3.24}$$

recovering a previous result.[13,23] This expression can be inserted in Eq. (3.14) and, through Eq. (3.15), we obtain the usual self-consistent equation for the renormalized frequencies of the small oscillations around the vacuum. Note that in this case $P_{ab}$ and $U_{ka}=A_{ka}$ are constant with $\xi$.

Another important limiting situation occurs when the coupling $g$ is low. We consider, as unperturbed frequencies $\Omega_k$ the square roots of the eigenfunctions of the matrix $B$ or

$$\sum_{a,b=-N}^{N} A_{ia}B_{ab}A_{kb}=\Omega_k^2\delta_{ik} . \tag{3.25}$$

We can now expand the matrix $U_{ia}(\xi)$ defined in Eq. (3.14) according to

$$U_{ia}=A_{ia}+gA_{ia}^{(1)} . \tag{3.26}$$

Following the procedure explained in Appendix B we obtain

$$\omega_k^2\simeq\Omega_k^2+\frac{g}{m}\sum_{a=-N}^{N}A_{ka}^2P_{aa}\equiv\Omega_k^2+\omega_k^{(1)^2} . \tag{3.27}$$

Letting $f_k^{(0)}=(\beta\hbar\Omega_k/2)$ and $f_k^{(1)}=(\beta\hbar\omega_k^{(1)}/2)$, the logarithmic term in the effective potential (3.17) can be given by the form

$$-\frac{1}{\beta}\sum_{k=-N}^{N}\ln\left[\frac{f_k^{(0)}}{\sinh f_k^{(0)}}\right] -\frac{1}{\beta}\sum_{k=-N}^{N}\left[\frac{1}{f_k^{(0)}}-\coth f_k^{(0)}\right]\frac{f_k^{(1)^2}}{2f_k^{(0)}} . \tag{3.28}$$

Some explanations are in order about the validity and the meaning of this expansion. Note first that even if $\Omega_k$ vanishes for some value of $k$, Eq. (3.28) is valid provided that the temperature is not too low, so to have $f_k^{(1)}\ll 1$; in this condition the main contribution to (3.28) comes from terms with high $\Omega_k$. Moreover, the perturbative expansion (3.26) apparently fails when $\Omega_k$ goes to zero, where a low coupling can completely modify the spectrum of the small oscillations. (Typical instances occur when nonconstant minima like solitons or solitary waves are considered.) However, for $f_k^{(1)}\ll 1$, the error deriving from the use of (3.28) is again very small. On the other hand, the nonperturbative effects, as the presence of translation modes, are correctly included in the configurational integral.

Eventually, after some algebra, we can write the expression of the effective potential for low values of $g$ as

$$V_{\rm eff}(\xi)=V(\xi)-\frac{1}{\beta}\sum_{k=-N}^{N}\ln\left[\frac{f_k^{(0)}}{\sinh f_k^{(0)}}\right] +g\sum_{a=-N}^{N}\sum_{n=1}^{\infty}\frac{1}{n!}u^{(2n)}(\xi_a)\left[\frac{D}{2}\right]^n . \tag{3.29}$$

As shown in Eq. (3.28), the quantities $\alpha_k$ in Eq. (3.29) can be approximately evaluated using $f_k^{(0)}$, so that the quantum renormalization factor $D$ turns out to be independent of $\xi$ and the calculation of $V_{\rm eff}$ becomes straightforward. The equivalent free energy $F_0$ describes a system of quantum harmonic oscillators with an added contribution due to nonlinearity calculated by a configurational integral in which the parameters of the potential are modified by the quantum fluctuations.

## IV. SINE-GORDON CHAIN

In order to show in detail the applicability of our method, we consider the discrete sine-Gordon chain with lattice constant $a$. We have

$$V(\varphi)=ma^2\sum_b\left[\tfrac{1}{2}\Omega_0^2(\varphi_b-\varphi_{b+1})^2-\Omega_1^2\cos\varphi_b\right] , \tag{4.1}$$

so that

$$B_{ab}=\Omega_0^2(2\delta_{ab}-\delta_{a,b-1}-\delta_{a,b+1})+\Omega_1^2\delta_{ab} ,$$
$$u(\varphi)=m\Omega_1^2\sum_b\left[1-\frac{\varphi_b^2}{2}-\cos\varphi_b\right] . \tag{4.2}$$

In the continuum limit this system exhibits kink solitons with classical energy $E_S=8ma^2\Omega_0\Omega_1$. The quantum behavior of the system is ruled by the parameter

$$Q=\hbar\Omega_1/E_s \tag{4.3}$$

generally known as the "coupling parameter"[15] (the coupling parameter of Ref. 13 is 8 times larger). The strength of the anharmonicity of the system (4.1) is measured by

$$\epsilon=1/(4R^2)=(\Omega_1/2\Omega_0)^2 , \tag{4.4}$$

where $R$ represents the length of the kink in lattice units.[13] For largest values of $R$ (displacive limit[15]), the discrete chain is well described by a continuum model.

The frequency of the radiation in the classical case is given by

$$\Omega_k^2=\Omega_1^2+4\Omega_0^2\sin^2(ka/2) . \tag{4.5}$$

Up to some inessential additive constants, the effective potential of Eq. (3.17) specifies to

$$V_{\rm eff}(\varphi)=\tfrac{1}{2}ma^2\Omega_0^2\sum_b(\varphi_b-\varphi_{b+1})^2-\frac{1}{\beta}\sum_k\ln\left[\frac{f_k}{\sinh f_k}\right] -ma^2\Omega_1^2\sum_b e^{-D/2}\left[1+\frac{D}{2}\right]\cos\varphi_b , \tag{4.6}$$

while from Eq. (3.15) we have

$$P_{ab}=\delta_{ab}ma^2\Omega_1^2(e^{-D/2}\cos\varphi_b-1) . \tag{4.7}$$

On this particular case it can be explicitly checked by the use of Eq. (3.16) that (3.14) cannot produce negative values of $\omega_k^2$ for lower and lower temperatures.

In this temperature range the main contribution to the partition function arises from local minima. These are given by the following equation:

$$\Omega_0^2(2\varphi_b-\varphi_{b+1}-\varphi_{b-1})+\Omega_1^2e^{-D/2}\sin\varphi_b +\sum_{k,a}\left[\frac{\alpha_k}{4}\right]P_{aa}\frac{\partial U_{ka}^2}{\partial\varphi_b}=0 . \tag{4.8}$$

For low coupling we observe that the third term is of higher order in $\Omega_1^2$ so that in the continuum limit Eq. (4.8) becomes the well-known sine-Gordon equation with the renormalized frequency $\bar{\Omega}_1=\Omega_1\exp(-D/4)$.

For $\beta\to\infty$ the only contribution derives from the vacuum sector $\varphi_b=0$. Taking into account that $U_{ka}$ is independent of $\varphi$, being the matrix that diagonalizes $B_{ab}$ [see Eq. (3.22)] we obtain from (3.14) the self-consistent equation

$$\omega_k^2=4\Omega_0^2\sin^2(ka/2)+\Omega_1^2\exp[-D_0(T=0)/2]\ , \qquad D_0(T=0)=\frac{1}{2N+1}\sum_k\frac{\hbar}{2ma^2\omega_k}\ . \tag{4.9a}$$

At lowest order, $D_0(T=0)$ turns out to be

$$D_0(T=0)=\frac{8QR}{\pi(1+4R^2)^{1/2}}K\left[\frac{2R}{(1+4R^2)^{1/2}}\right] \tag{4.9b}$$

in agreement with previous results.[13]

When the temperature increases, the quantum renormalization factor $D_0(T)$ decreases, indicating that the system becomes more and more classical. According to Eq. (3.16) for the case $\varphi_b=0$, we find at lowest order in terms of the reduced temperature $t=k_BT/E_S$, with $\rho=(1+\epsilon)^{1/2}$,

$$D_0(t)=\frac{4Q^2R}{t}\sum_{m=1}^{\infty}\left[(n\pi)^4+\frac{QR}{\rho t}\left[\frac{1+\rho^2}{16R^2}\right](n\pi)^2+\left[\frac{Q^2R}{2\rho t^2}\right]^2\right]^{-1/2}\ , \tag{4.10}$$

The behavior of $D_0(t)$ is plotted in Fig. 3 for $Q=0.1$ and $R=2$ and 10. (See Appendix C for details.)

For nonvanishing $T$ the contribution of other local minima (i.e., static solitons) $\varphi=\varphi^{(S)}$ must be included. The diagonalizing matrix $U_{ka}$ is now space dependent, representing the new density of states caused by the modification of the spectrum of small oscillations by the presence of the soliton in the dilute-gas approximation.[24] However, it has been shown[13,25] that the corrections to the factor $D$ are vanishing for infinite length of the system. Therefore, the $\varphi$ dependent $U_{ka}$, which takes into account the phase shift of the radiation,[24,26] must be inserted only to evaluate the logarithmic term.

As mentioned in the Introduction, some magnetic chains[27] present some interesting features of the specific heat[9,11,12] which seem to be caused by sine-Gordon solitons. However, the peak of the specific heat occurs in a range of temperatures ($t\sim0.2$) where the dilute-gas approximation is no more valid and the contribution of soliton-soliton interactions must be taken into account yet in the classical case.[28,29] On the other hand, the quantum renormalization factor $D_0(t)$ is only 30% of the value at $T=0$ in this range of temperatures (see Fig. 3), signalizing that, at least for low coupling, the quantum fluctuations should not affect too much the nonlinear contribution. It is instead essential to entirely consider the quantum character of the harmonic oscillators.[11]

The expansion (3.29), valid in the displacive limit ($\epsilon\ll1$) appears to be promising in these conditions, extending the results obtained by a Wigner-type expansion.[16] Using the equation (3.29) we obtain

$$e^{-\beta F_0}=\left[\frac{ma^2}{2\pi\hbar^2\beta}\right]^{(2N+1)/2}\prod_k\frac{\hbar\beta\Omega_0\sin(ka/2)}{\sinh[\hbar\beta\Omega_0\sin(ka/2)]}\int d\varphi\exp\left[-\beta\frac{ma^2}{2}\sum_b[\Omega_0^2(\varphi_b-\varphi_{b+1})^2-2\Omega_1^2e^{-D_0/2}\cos\varphi_b]\right]\ . \tag{4.11}$$

This expression for the free energy, valid for $t>Q/2$, constitutes an important improvement with respect to previous theories. In order to give a physical meaning to (4.11) we first consider the high-temperature limit. In this case we recover from (4.11) the first Wigner correction (3.21):

$$V_{\rm eff}=\frac{(2N+1)\hbar^2\beta2\Omega_0^2}{24}+\sum_b\left[\frac{ma^2\Omega_0^2}{2}(\varphi_b-\varphi_{b+1})^2-ma^2\Omega_1^2\left[1-\frac{\hbar^2\beta}{24ma^2}\right]\cos\varphi_b\right]\ . \tag{4.12}$$

The first term represents the quantum correction[18] of the oscillators of frequency $2\Omega_0\sin(ka/2)$ due to the interaction of nearest neighbors. At this order they are equivalent to $(2N+1)$ Einstein oscillators with frequency $\sqrt{2}\Omega_0$. The quantum effects related to the sine-Gordon cosine potential are accounted by a simple renormalization of the frequency $\Omega_1$.

For decreasing temperatures, the quantum effects must be completely considered for the aforementioned harmonic oscillators, while the renormalization of the frequency $\Omega_1$, with the appropriate $D$ factor, is again consistent. Therefore the free energy (4.11) presents a Debye behavior with an added renormalized contribution due to the nonlinearity, in agreement with the fully quantum results based on the massive Thirring model.[30,31]

Summing up, the nonlinear quantum contribution to the free energy can be reduced to the calculation of a classical configurational integral where all modifications of the radiation due to nonlinearity are included. We are thus able to overcome the dilute-gas approximation and use the well-known classical techniques, as the interacting-soliton model,[28] high-temperature expansions, and eventually transfer-matrix numerical calculations.

In the classical case the full nonlinear contribution to the specific heat, $\delta C$,[32] is much lower than the first-order transfer-matrix result.[24] The latter coincides with the dilute-soliton gas approximation.[24] The quantity $R\delta C$ is a universal function of the reduced temperature $t$. It has

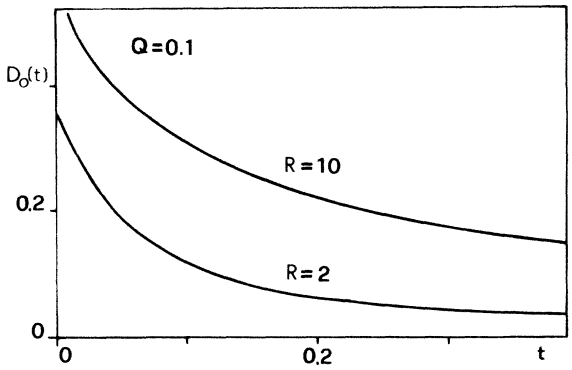


FIG. 3. Quantum renormalization factor $D_0(t)$ versus the reduced temperature $t=k_BT/E_S$ of a sine-Gordon chain for different $R$ with $Q=0.1$.

been shown[29] that the large difference with respect to the classical dilute-soliton gas approximation is mainly due to the soliton-soliton interaction (see Fig. 4 and Appendix D). Therefore it is evident that the quantum correction must be superimposed to the interacting system rather than to the dilute-gas results. In this framework, for evaluating the quantum $\delta C$ in the region of the peak through Eq. (4.11), we can simply replace $\Omega_1$ with $\Omega_1\exp(-D/4)$ in the classical expansions given in Appendix D. The results are given in Figs. 4 and 5. For the considered range of $R$ and $Q$, the quantum corrections, which are indeed important for the harmonic part, do not much affect the anharmonic contribution in quantitative agreement with the results of the quantum sine-Gordon model.[30,31,33]

If the one-dimensional ferromagnetic $CsNiF_3$ could be thought as a fully easy-magnetization-plane system and consequently as a sine-Gordon system, the appropriate parameters would be $Q\simeq 0.11$ and $R\simeq 5$ for a magnetic field of about 5 kG. Hence, as shown in Fig. 5, the quantum effects on the nonlinear contribution to the specific heat would be small, not overcoming 10%. However, the experimental data are much lower than this prediction, showing the already observed inadequacy of the easy-magnetization-plane model. A theory which could take

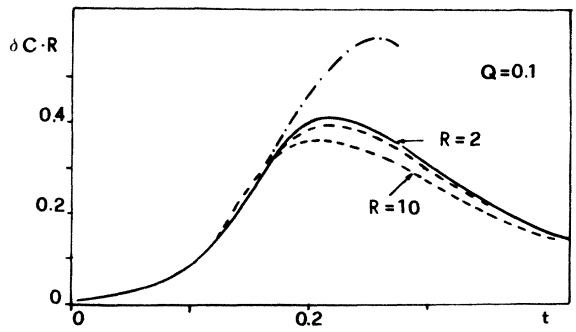


FIG. 4. Nonlinear contribution to specific heat of a sine-Gordon chain versus $t$. Solid line represents the classical result. Dotted line represents the classical result without soliton-soliton interaction. Dashed lines represent quantum results for $Q=0.1$, $R=2$ and 10.

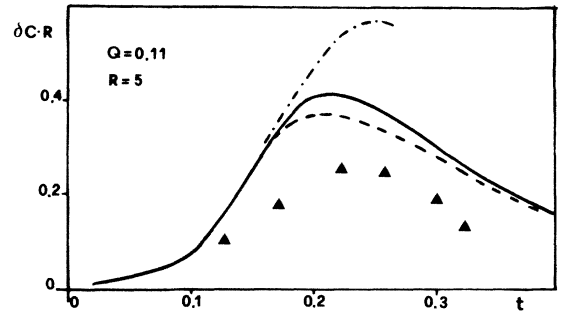


FIG. 5. Nonlinear contribution to the specific heat versus $t$ at $Q=0.11$ and $R=5$ (dashed line). The solid line is the classical result. Triangles are experimental data from Ref. 9 as presented in Ref. 33. Dotted line as in Fig. 4.

into account the out-of-plane fluctuations is essential, but it cannot be limited to the dilute-soliton gas approximation.[14]

## V. CONCLUSIONS

The new variational approach, developed here, seems to offer a useful tool for calculating the quantum corrections to the classical free energy. Our theory unifies the methods described in Refs. 5, 13, and 16 giving a correct effective potential to be inserted in the configuration integral, at any temperature, in the low-coupling limit. Moreover, the frequency renormalization is a direct consequence of our variational principle.

The expansion for small anharmonicity [Eq. (3.29)] has been applied to the sine-Gordon chain the displactive limit showing, as a new result, that the specific heat can be calculated by the previous classical expression with a simple renormalization of the frequency. Moreover, in this limit, the quantum renormalization factor is approximately evaluated using the spectrum of the small oscillations around the vacuum.

The method appears to be very general and can be simply extended to the calculation of static correlation functions. Work is in progress in this direction, together with its application to other nonlinear models which could better describe some real system.

## APPENDIX A

We present here the explicit evaluation of the minimum of $F_0$ with respect to $w_{ab}$. Since the matrix $w_{ab}$ is symmetric it can be diagonalized by an orthogonal matrix $U_{ka}$. We therefore split the problem in two steps: First we calculate the minimum of $F_0$ with respect to the eigenfrequencies of $w_{ab}$, i.e., equivalently, with respect to $f_k$. Secondly, we minimize with respect to $U_{ka}$. Of course some care is due in this second step, and we have to use Lagrange multipliers to account for the orthogonality constraints on the matrix $U_{ka}$. We have

$$\frac{\partial V_{\rm eff}}{\partial f_k}=\frac{1}{4}\left\{(UBU^T)_{kk}+g\sum_{a=-N}^{N}\sum_{n=1}^{\infty}U_{ka}^2\left[\sum_{l=-N}^{N}\left[\frac{\alpha_e}{4}\right]U_{la}^2\right]^{n-1}\frac{u^{(2n)}(\xi_a)}{(n-1)!}-\frac{4f_k^2}{\hbar^2\beta^2}\right\}\frac{\partial\alpha_k}{\partial f_k} \tag{A1}$$

so that the equation $\delta F_0/\delta f_k=0$ gives

$$f_k^2=\frac{\hbar^2\beta^2}{4}\sum_{a,b=-N}^{N}U_{ka}[B_{ab}+gP_{ab}(\xi)]U_{kb}\ , \tag{A2}$$

where $P_b$ is given one of the following two expressions:

$$P_{ab}=\delta_{ab}\sum_{n=0}^{\infty}\left[\sum_{l=-N}^{N}\left[\frac{\alpha_l}{4}\right]U_{la}^2\right]^n\frac{u^{(2n+1)}(\xi_a)}{n!}$$

$$=\delta_{ab}\int d\eta\, u^{(2)}[(U^T\eta+\xi)_a]\prod_{k=-N}^{N}\frac{e^{-\eta_k^2/\alpha_k}}{(\pi\alpha_k)^{1/2}}\ . \tag{A3}$$

Equation (A2) shows that the quantities $m\omega_k^2$ are the diagonal elements of the symmetric matrix $U(B+gP)U^T$. Actually we shall prove that the latter matrix can be supposed diagonal, so that $m\omega_k^2$ are just its eigenvalues.

The minimum with respect to $U$ must be evaluated under the orthogonality constraint

$$UU^T-I=0 \tag{A4}$$

so that, letting

$$M(\xi)=V_{\rm eff}(\xi)+{\rm Tr}[(UU^T-I)\lambda]\ , \tag{A5}$$

where $\lambda$ is the matrix of the Lagrange multipliers, we have to solve the system

$$\frac{\partial M(\xi)}{\partial U_{ka}}=\frac{\partial M(\xi)}{\partial\lambda_{kl}}=0\ . \tag{A6}$$

The second of these equations gives the constraint (A4). To write the explicit form of the first equation, we calculate the variation of $M$, $\Delta M$, under a variation $\Delta U$. After some lengthy algebra, we get

$$\Delta M=2\sum_{k=-N}^{N}\left[\frac{\alpha_k}{4}\right][(\Delta U)BU^T]_{kk}+2g\sum_{a,k=-N}^{N}\left[\frac{\alpha_k}{4}\right]\frac{u^{(2n)}(\xi_a)}{(n-1)!}$$
$$\times(\Delta U_{ka})U_{ka}\left[\sum_{l=-N}^{N}\left[\frac{\alpha_l}{4}\right]U_{la}^2\right]^{n-1}+\sum_{k=-N}^{N}[(\Delta U)U^T(\lambda+\lambda^T)]_{kk} \tag{A7}$$

from which it is straightforward to compute the derivative of $M$ with respect to $U_{ka}$. As $U$ is nonsingular, the first of equations (A6) is equivalent to

$$\sum_{a=-N}^{N}U_{ia}\frac{\partial M}{\partial U_{ka}}=0 \tag{A8}$$

whose explicit form reads

$$\left[\frac{\alpha_k}{4}\right][U(B+gP)U^T]_{ik}+\tfrac{1}{2}(\lambda+\lambda^T)_{ik}=0\ . \tag{A9}$$

But $(\lambda+\lambda^T)$ is symmetric, so that, defining the diagonal matrix

$$A_{ik}=\alpha_k\delta_{ik} \tag{A10}$$

from Eq. (A9) we get the commutation relation

$$[A,U(B+gP)U^T]=0\ . \tag{A11}$$

Therefore, there exists an orthogonal matrix $\tilde{U}$ determining a similarity transformation which simultaneously diagonalizes both $U(B+gP)U^T$ and $A$. Since $A$ is already diagonal, we can suppose, without loss of generality, that $\tilde{U}$ commutes with $A$. By substituting $U$ with $\tilde{U}U$ we conclude that, up to an inessential redefinition of $U$, the matrix $U(B+gP)U^T$ is diagonal. Equation (A2) is then written in the general form given by Eq. (3.14).

## APPENDIX B

We present the detailed derivation of (3.27). Observing that, up to the first order in $g$ we have (in matrix notation)

$$U^{-1}=(A+gA^{(1)})^{-1}=(I-gA^{-1}A^{(1)})A^{-1} \tag{B1}$$

equation (3.14) gives

$$\omega_k^2=[ABA^{-1}+g(A^{(1)}BA^{-1}-ABA^{-1}A^{(1)}A^{-1}) +gAPA^{-1}]_{kk} . \quad \text{(B2)}$$

However,

$$(A^{(1)}BA^{-1}-ABA^{-1}A^{(1)}A^{-1})_{kk} =[A^{(1)}A^{-1},ABA^{-1}]_{kk} \quad \text{(B3)}$$

and from (3.25) we note that $(ABA^{-1})_{ik}=\Omega_i^2\delta_{ik}$ is a diagonal matrix. Therefore, the evaluation of the $(k,k)$ matrix element of the commutator (B3) gives a vanishing result and Eq. (B2) reduces to

$$\omega_k^2=\Omega_k^2+g(APA^{-1})_{kk} , \quad \text{(B4)}$$

i.e., to (3.27).

## APPENDIX C

The quantum renormalization factor $D_0$ for the vacuum sector has the general expression (3.24). Under the usual conditions we shall replace the sum by an integral. Recalling the explicit form (3.7) for $\alpha_k$ and using the notations introduced in Sec. IV, we find that a convenient expression for calculating $D_0$ at low temperatures is

$$D_0(t)=8QR\int_1^{\Lambda}dx\frac{\coth\frac{Qx}{2t}-\frac{2t}{Qx}}{[(x^2-1)(\Lambda^2-x^2)]^{1/2}} \quad \text{(C1)}$$

$[\Lambda=(1+4R^2)^{1/2}]$ which gives immediately (4.9) for $T=0$.

To evaluate $D_0$ at high temperature, instead, the following form turns out to be more convenient:

$$D_0(t)=\frac{4Q^2R}{t}\int_{\Lambda_1}^{\Lambda_2}dx\frac{\coth x-\frac{1}{x}}{[(x^2-\Lambda_1^2)(\Lambda_2^2-x^2)]^{1/2}} , \quad \text{(C2)}$$

where $\Lambda_1=Q/2t$ and $\Lambda_2=(Q/2t)\Lambda$. By using the well-known expansion

$$\coth x-\frac{1}{x}=2\sum_{n=1}^{\infty}\frac{x}{x^2+n^2\pi^2} \quad \text{(C3)}$$

and performing the change of variable $x\to x^2$, we get

$$D_0(t)=\frac{4Q^2R}{t}\sum_{n=1}^{\infty}\int_{\Lambda_1^2}^{\Lambda_2^2}\frac{dx}{(x+n^2\pi^2)[(x-\Lambda_1^2)(\Lambda_2^2-x)]^{1/2}} \quad \text{(C4)}$$

whose evaluation is elementary and gives (4.10). For very high temperatures the series (4.10) gives

$$D_0=\frac{2Q^2R}{t}+0(1/t^2) \quad \text{(C5)}$$

describing the asymptotic vanishing of the renormalization factor when the system approaches the classical regime.

## APPENDIX D

The well-known formula which allows the calculation of the specific heat from the free energy is

$$C=-T\frac{\partial^2F}{\partial T^2}=-\left[2k_B\beta^2\frac{\partial F}{\partial\beta}+k_B\beta^3\frac{\partial^2F}{\partial\beta^2}\right] . \quad \text{(D1)}$$

In the classical case the free energy $F_{\rm cl}$ is expressed in terms of high- and low-temperature approximations. A standard high-temperature expansion gives

$$F_{\rm cl}=(2N+1)\frac{E_S}{8R}\left[1+\sum_{n=1}^{\infty}A_{2n-1}q^{2n-1}\right] \quad \text{(D2)}$$

with $q=(4t)^{-2}=(\beta E_S/2)^2$. At low temperature an expansion for the classical free energy has been found by using an accurate transfer equation approach and reads

$$F_{\rm cl}=(2N+1)\frac{E_S}{8R}\left[\sum_{n=1}^{\infty}a_nt^n-\tau_s(t)-\tau_{ss}(t)\right] , \quad \text{(D3)}$$

where

$$\begin{aligned}\tau_s(t)&=16\sqrt{2t/\pi}e^{-1/t}\sum_{n=0}^{\infty}b_nt^n ,\\ \tau_{ss}(t)&=\frac{64}{\pi}e^{-2/t}\left[\ln\frac{4\gamma}{t}-\tfrac{5}{4}t\left[1+\ln\frac{4\gamma}{t}\right]-\tfrac{1}{8}t^2\left[1+\tfrac{13}{4}\ln\frac{4\gamma}{t}\right]\right] ,\end{aligned} \quad \text{(D4)}$$

and $\gamma\simeq0.5772$ denotes the Euler-Mascheroni constant. The explicit values of the coefficients $A_n$ of Eq. (D2) as well as $a_n$ and $b_n$ of Eqs. (D3) and (D4) can be found in Refs. 5 and 27. It must be observed that the low-temperature expansion (D3) has a transparent physical interpretation in the framework of an interacting-soliton theory.[27,34] Indeed the first series in (D3) gives the contribution of radiation and radiation-radiation interaction; the function $\tau_S$ accounts for the one-soliton and radiation-soliton interaction and, finally, $\tau_{SS}$ contains two solitons interacting both between themselves and with radiation.

According to what we have developed in Sec. IV, the free-energy including the quantum corrections in the low-coupling approximation is obtained from (D2) and (D3) by replacing the soliton energy $E_S$ with its renormalized counterpart

$$E_S^{(q)}=E_S\exp(-D/4) . \quad \text{(D5)}$$

Consequently, also the reduced temperature $t$ must be substituted by $t_q=t\exp(D/4)$. As the renormalization factor is $t$ dependent [see, e.g. (4.10)], the appropriate caution is needed to evaluate the derivatives giving the specific heat (D1).

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