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TITLE: PHI4 KINKS: STATISTICAL MECHANICS

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Φ^4 Kinks: Statistical Mechanics¹

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Abstract

Some recent investigations of the thermal equilibrium properties of kinks in a 1+1-dimensional, classical ϕ^4 field theory are reviewed. The distribution function, kink density, correlation function, and certain thermodynamic quantities were studied both theoretically and via large scale simulations. A simple double Gaussian variational approach within the transfer operator formalism was shown to give good results in the intermediate temperature range where the dilute gas theory is known to fail.

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1 Introduction

The statistical mechanics of nonlinear coherent structures such as solitons and solitary waves has been a subject of study for quite some time [1]. More recent interest has been fueled by applications not only in condensed matter physics [2][3], but also by potential applications in particle physics (sphalerons) [4] and cosmology (domain walls, baryogenesis) [5].

A particularly simple model that displays behavior representative of a large class of soliton-bearing systems is the “double-well” Φ^4 scalar field theory in 1+1-dimensions. This theory admits exact solitary wave solutions (“kinks”) and our purpose here is to describe the equilibrium statistical mechanics of these objects as studied recently in Refs. [6][7].

The Lagrangian for this theory is

$$L = \frac{1}{2} (\partial_t \Phi)^2 - \frac{1}{2} (\partial_x \Phi)^2 + \frac{1}{2} m^2 \Phi^2 - \frac{1}{4} \Lambda \Phi^4. \quad (1)$$

The equations of motion that follow from (1) admit static kink solutions (centered at $x = x_0$)

$$\Phi_k = \frac{m}{\Lambda} \tanh \left(\frac{m}{\sqrt{2}} (x - x_0) \right). \quad (2)$$

The total energy of an isolated kink is $E_k = \sqrt{8/9} m^3 / \Lambda$ and the negative of a kink, also a solution, is called an antikink.

In numerical work it is customary to use the dimensionless form of this theory, given by the transformations: $\Phi \rightarrow a\phi$, $x \rightarrow x/m$, and $t \rightarrow t/m$, where $a^2 = m^2/\Lambda$. The equation of motion then becomes

$$\partial_{tt}^2 \phi = \partial_{xx}^2 \phi - \phi (\phi^2 - 1). \quad (3)$$

The statistical mechanics of kinks in this system has been studied by two approaches. In the first, and phenomenological, approach one assumes that the kinks and the fluctuations (“phonons”) about the asymptotic field minima may be treated as weakly interacting elementary excitations. Provided the kink density is low, the canonical partition function can then be found by standard methods [1][8][9]. Alternatively, as shown by Krumhansl and Schrieffer (KS) [8], building on earlier work of Sears, Scalapino, and Ferrell [10], it is possible to calculate the partition function, in principle exactly, by exploiting a transfer operator technique. KS showed that in the low temperature (“dilute gas”) limit the partition function naturally factorizes into two contributions both having counterparts in the phenomenological theory; a tunneling term which they were able to identify with the kink contribution, and the

remainder which they identified as linearized phonons. The ideas of KS were further refined and extended to a wider class of systems by Currie *et al* [9]. In particular, interactions of kinks with linearized phonons were considered, leading to substantial corrections to the results of KS.

A key result of these efforts is the prediction that the spatial density of kinks

$$n_k \propto \sqrt{E_k \beta} \exp(-E_k \beta), \quad (4)$$

where E_k is the kink energy ($E_k = \sqrt{8/9}$ for the dimensionless form of the theory) and β , the inverse temperature (for the dimensionless case, $\beta \rightarrow \beta/(a^3 \sqrt{\lambda})$). A related prediction is that at low temperatures the field correlation length λ defined by

$$\langle \phi(0) \phi(x) \rangle \sim \exp(-x/\lambda) \quad (5)$$

has an exponential temperature dependence [9],

$$\lambda = \frac{1}{4} \sqrt{\frac{\pi}{3}} \frac{1}{\sqrt{E_k \beta}} \exp(E_k \beta). \quad (6)$$

Computer simulations to verify these results date back to the work of Koehler *et al* [11] who found only a qualitative agreement. More recent investigations [12][13][14] led to more detailed comparisons; however, significant discrepancies were reported. This led to theoretical speculation [15][16] regarding possible corrections to the dilute gas theory of kinks. It was speculated that these discrepancies could be due to finite size effects and phonon dressing of the bare kink energy (breather contributions to the free energy could also be significant [17]). However, these simulations were not carried out at low enough temperatures and the authors interpreted their results in terms of WKB (dilute gas) formulas that, it turns out, were simply not valid over the range of temperatures studied [6][7]. In Refs. [6][7], by going to low enough temperatures it was shown that the standard dilute gas results were indeed valid. Furthermore, an earlier claim of substantial phonon dressing even at these temperatures [11] was shown not to be correct.

The equilibrium statistical mechanics of kinks in the ϕ^4 model (1) was investigated by implementing a Langevin code on a massively parallel computer [6]. The key idea is to supplement the equation of motion (3) with noise and viscosity terms obeying an appropriate fluctuation-dissipation theorem so that the system is driven to thermal equilibrium at the desired temperature [18]. To understand the numerical results in the high and intermediate temperature region not susceptible to a dilute gas analysis, a double Gaussian wave function approximation for the quantum mechanical problem which results from applying the transfer operator method was used. Not only is this

method accurate but it also suggests a natural decomposition of nonlinear phonon and kink degrees of freedom in the intermediate temperature regime [7].

The main results of these investigations are: (1) the dilute gas predictions for the kink density and the correlation length are in good agreement with the simulations below a certain (theoretically estimable) temperature, (2) above this temperature the double Gaussian results for the kink number and the correlation length agree with the simulations, (3) kinks are found to “disappear” into the thermal phonon background above a characteristic temperature, in good agreement with theoretical prediction, (4) the double Gaussian approximation accurately describes the classical single point field distribution function at high and intermediate temperatures where the dilute gas (WKB) approximation breaks down, and (5) the internal energy and the specific heat calculated in the double Gaussian approximation show an interesting energy sharing process between kinks and nonlinear phonons in an intermediate-temperature range below the characteristic temperature at which kinks appear: a peak in the specific heat in this temperature range is shown to be due essentially to kinks.

2 Numerical Results

The Langevin equation for the dimensionless theory is

$$\partial_{tt}^2\phi = \partial_{xx}^2\phi - \eta\partial_t\phi - \phi(1 - \phi^2) + F(x, t). \quad (7)$$

To guarantee an approach to equilibrium, the Gaussian, white noise F and the viscosity η are related via the fluctuation-dissipation theorem:

$$\langle F(x, t)F(x', t') \rangle = 2\eta\bar{\beta}^{-1}\delta(x - x')\delta(t - t'). \quad (8)$$

Numerical simulations were performed on lattices with 16384 sites and the Langevin equation was solved numerically using standard methods [6]. The system size was 1 to 2 orders of magnitude larger than that in most previous simulations. Large system sizes are necessary to get acceptable statistics at low temperatures and to avoid finite size effects. Systems were evolved from a random initial condition to equilibrium.

To compute the kink number an operational way to identify kinks is needed even though the exact kink solution is available theoretically. Several possible definitions were examined, all of which relied on a knowledge of the kink size. From the classical solution for a kink centered at x_0 , $\phi = \tanh((x - x_0)/\sqrt{2})$, the kink scale L_k was approximately 8 lattice units in the simulations. Raw kink configurations are shown in Fig. 1. At low temperatures ($\bar{\beta} > 5$), kinks may be identified easily, however at higher temperatures this is clearly not the case.

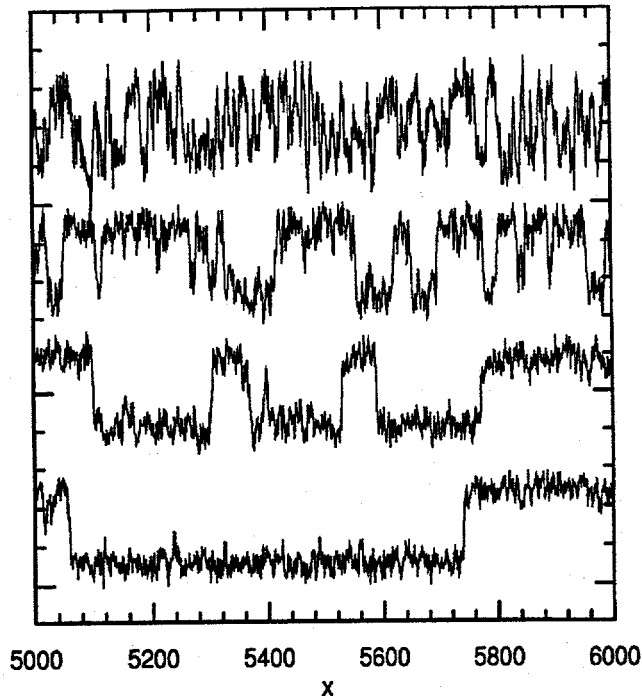


Figure 1: Sample field configurations, from top to bottom, at $\bar{\beta} = 2, 4, 5.5, 8$. Only a 1000 lattice unit sample of the total lattice size of 16384 is shown.

The simplest thing to do is to count the number of zero-crossings of the field, since one may argue that these are the “tunneling events” which correspond to kinks. However, at higher temperatures there are zero-crossings due to thermal noise (phonons), and counting all zero-crossings would lead to a gross overestimation of the number of kinks. At high temperatures it is not possible to distinguish unambiguously between kinks and nonlinear phonons (the overcounting problem occurs even at intermediate temperatures where the kinks are more or less distinct). A possible solution is to use a smoothed field by either averaging or block-spinning the actual field configuration over a length of the order of the kink scale. The latter approach was taken in previous simulations [12][13][14]. This solution is not without flaws either, as rapid fluctuations can still appear as kinks. In Refs. [6][7] the following method was used: at a particular time find all zero-crossings. To test the legitimacy of a given zero-crossing check for zero-crossings one kink scale (8 lattice units) to its right and to its left. If no zero-crossings are found, count it as a kink; otherwise not.

The number of kinks is plotted against $\bar{\beta}$ in Fig. 2. Above $\bar{\beta} \sim 6$, the two methods for counting kinks agree. Moreover, in this (low temperature) range, the dilute gas expression for the kink number (4) is in excellent agreement with the data. At elevated temperatures, there is a clear disagreement between the two methods of counting kinks. In this temperature regime the number of kinks computed with the

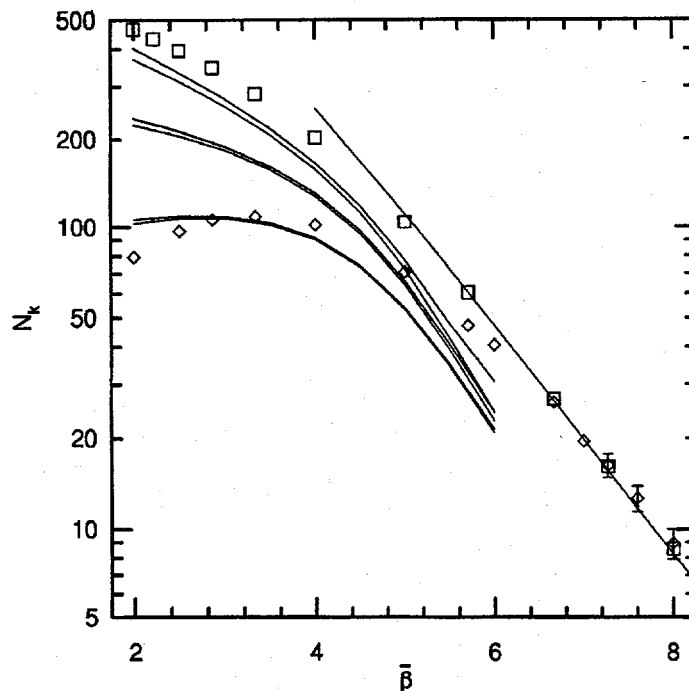


Figure 2: Total number of kinks as a function of $\bar{\beta}$. Squares denote counts with a smoothed field (averaging length of 8 lattice units) definition of kinks, diamonds for the zero-crossing counting method discussed in Sec. 2, and the solid beginning at $\bar{\beta} = 4$ is a fit to the WKB prediction (4). Also shown are three predictions from the double Gaussian theory (for details, see Ref. [7]).

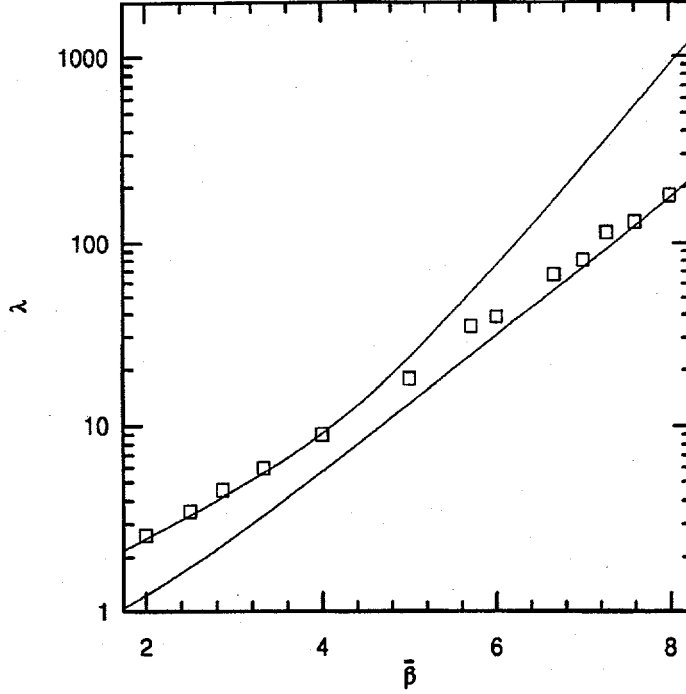


Figure 3: The correlation length λ as a function of $\bar{\beta}$. The two solid lines are the theoretical predictions (top, double Gaussian and bottom, WKB). The crossover of the ranges of validity of the two theories occurs at $\bar{\beta} \sim 5$.

smoothing method depends strongly on the smoothing scale. For $\bar{\beta} < 6$, the number of kinks cannot be extracted with any confidence from the smoothing method.

The correlation length λ is plotted against $\bar{\beta}$ in Fig. 3. For $\bar{\beta} > 6$, the WKB prediction (5) holds, whereas for $\bar{\beta} < 5$, where the wave function overlaps are not negligible, the double Gaussian approximation is valid. (Fortunately, there are no ambiguities here with regard to measurements at higher temperatures.)

3 Transfer Operator and Double Gaussian Approximation

The canonical partition function for the Lagrangian (1) is given by the functional integral

$$Z = \int D\phi D\pi \exp(-\beta H(\phi, \pi)) \quad (9)$$

where π is the canonical momentum of the field and H , the field Hamiltonian. The transfer operator technique [10] reduces the calculation of the partition function in the thermodynamic limit to simply finding the ground state energy of the double well

quantum Hamiltonian (here written for the dimensionless case),

$$H_Q = \frac{1}{2}p^2 - \frac{1}{2\beta^2}\bar{\phi}^2 + \frac{1}{4\beta^4}\bar{\phi}^4 \quad (10)$$

where $\bar{\phi} = \beta\phi$. At low temperatures the two wells are widely separated and the ground state energy is given by the oscillator ground state energy for one of the wells minus the tunnel-splitting term, usually calculated by WKB methods. The dilute gas or WKB approximation for the kink number is valid when the tunnel-splitting is small enough such that only the first two energy eigenstates are necessary to estimate the ground state energy of the Hamiltonian (10)[19]. At higher temperatures where kinks still exist, higher energy states cannot be ignored. Since kinks are associated with tunneling, one expects them to vanish when the ground state energy is higher than the classical barrier height: this intuition is confirmed by the simulations [6][7].

One can compare the simulations of the kink system with numerical solutions for the energy eigenvalues of the Hamiltonian H_Q . Instead, a different approach may be taken by implementing a double Gaussian variational method (see [7] for details) which is an order of magnitude more accurate than the simple Gaussian approximation [20] for this problem and correctly accounts for the reduction of energy due to overlap terms in the wave functions of the two wells, at least for moderate to large overlaps. Three qualitatively different regimes exist: (1) all the energy eigenvalues lie above the classical barrier, (2) the ground state energy lies below the classical barrier height, and (3) the energy difference between the ground and first excited state becomes negligible in comparison with the energy difference between the ground and the second excited state (this occurs for $\beta > 6$). The simulations [6] confirm the theoretical expectations that there are no kinks in region (1), that there are kinks, but that the dilute gas approximation is invalid in region (2), and finally, that the dilute gas approximation is accurate in region (3) (a regime unexplored in detail by previous simulations).

The classical single point field distribution function $P[\phi]$ was measured directly in the simulations. For the analogous quantum mechanical problem this is just the square of the ground state wave function Ψ_0 . Results from the simulations and the double Gaussian approximation are compared in Fig. 4. The presence of kinks implies a double peak in $P[\phi]$ [21] (the converse is false) while a single peak at the origin means that kinks and thermal phonons can no longer be distinguished. From the simulations such a transition occurs at $\beta \simeq 1.7$, in agreement with the theoretical calculation of when Ψ_0^2 goes over from a double to single peaked distribution. As expected, this is also the temperature ($\beta = 1.734$) where the ground state energy crosses the classical barrier height (a discussion of various methods to determine the characteristic

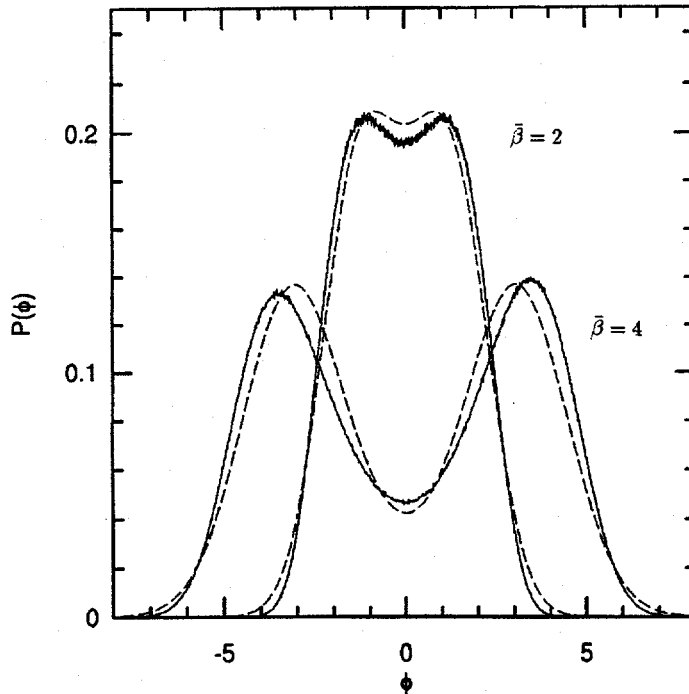


Figure 4: The classical distribution function $P[\phi]$ from the simulation compared with the distribution Ψ^2 from the double Gaussian approximation (dashed lines). The underestimation of the wave function overlap in this approximation is already visible at $\bar{\beta} = 4$.

temperature is given in Ref. [22]). The double peaks in the distribution function move inward from the classical minimum as the temperature increases (this is clearly seen in Fig. 4). Physically this can be understood as nonlinear phonon corrections due to the fact that near each minimum, the potential is not symmetric under reflection around the minimum. The double Gaussian approximation underestimates the tunneling or overlap contribution at low temperatures ($\sim \exp(-\sqrt{2\bar{\beta}})$ for double Gaussian versus $\sim \exp(-\sqrt{8/9\bar{\beta}})$ for WKB). This can be seen already at $\bar{\beta} = 4$ in Fig. 4.

The equilibrium kink number has traditionally been calculated only in the phenomenological approach. In Ref. [7] an effective kink number was defined starting from the transfer operator formalism. In the WKB limit the formula agrees with the standard result up to a prefactor (which is actually not known explicitly in the standard calculation). At intermediate temperatures the double Gaussian approximation can be used to estimate the kink number expected in the simulations. The results are consistent with the simulations but show a dependence on an averaging length which again points to the problem of defining precisely what is a kink at elevated temperatures (Fig. 2).

The correlation length as computed in the double Gaussian approximation is in excellent agreement with the simulations for $\bar{\beta} < 5$. There is a smooth crossover in

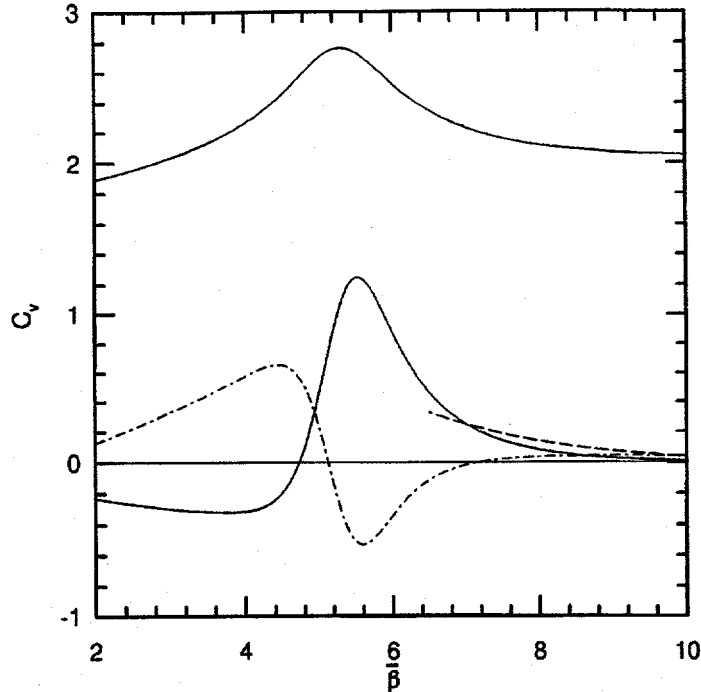


Figure 5: The specific heat C_v from the double Gaussian approximation (top curve). The peak in C_v is at $\bar{\beta} \simeq 5.4$. The contribution of the linear phonons is a constant (here, this value = 2). Individual contributions from kinks (solid line) and nonlinear phonons (dot-dashed line) are shown below. The WKB calculation for the kink contribution is shown from $\bar{\beta} = 6.5$ onwards.

the numerical results to the exponential dependence on $\bar{\beta}$ predicted by the dilute gas theory from $\bar{\beta} \sim 6$ onwards. Thus the two theories agree with the simulations in the appropriate temperature ranges.

Finally, in the double Gaussian approximation one can compute the internal energy and the specific heat [7]. The Schottky anomaly in the specific heat is clearly seen at $\bar{\beta} \simeq 5.4$. Disentangling the overlap contribution from the diagonal contribution allows one to associate the peak in C_v with the overlap contribution, *i.e.*, with the kinks (Fig. 5). A similar computation for the internal energy shows that in this temperature range the kink contribution dominates over both linear and nonlinear phonons (Fig. 6). Thus the kinks are indeed relevant to the thermodynamics of the system at least over some finite range of temperatures (at low temperatures the thermodynamics is dominated by linear phonons).

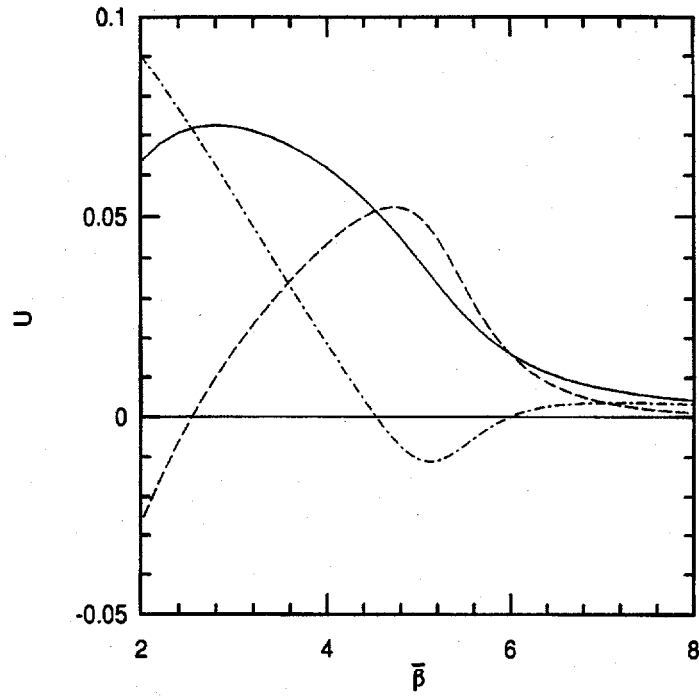


Figure 6: Internal energy against $\bar{\beta}$ using the double Gaussian approximation. Kink (dashed line) and nonlinear phonon (dot-dashed line) contributions are shown separately (modulo an irrelevant constant energy shift). Note that the kink contribution is dominant in the region where the specific heat has a maximum.

4 Conclusions

As a consequence of the above results, we conclude that the dilute gas/WKB approximation is excellent for $\beta > 6$ with no further phonon dressing of the bare kink energy beyond that already included in (4) and (6) at these low temperatures. At higher temperatures, the WKB analysis fails, though theoretical progress is possible with the double Gaussian technique. Using this technique we can analytically calculate the temperature range where kinks dominate the thermodynamics.

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