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Exact kink-gas phenomenology at low temperatures

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We show that the low-temperature ideal kink-gas phenomenology developed by Currie *et al*. for the classical statistical mechanics of one-dimensional kink-bearing systems is *exact* for all potentials in the nonlinear Klein-Gordon family (e.g., sine-Gordon, ϕ^4, double-sine-Gordon, etc.). A general kink-density formula is presented which does not require explicit knowledge of the kink wave form or its small oscillations.

Much of the recent interest in kink (soliton) excitations in condensed matter[1] has focused on their role in the low-temperature statistical mechanics of quasi-one-dimensional systems. Krumhansl and Schrieffer[2] found that for the "ϕ^4" chain the classical free energy obtained by the transfer-operator method could be nearly reproduced at low temperatures by calculating the free energy of an ideal gas of noninteracting particlelike kinks and phonons. Although this near agreement was quite remarkable, the quantitative disagreement between the ideal-gas phenomenology and the transfer-operator results occurred in both the temperature dependence and numerical factors, and left open the fundamental question of whether the phenomenology could really be trusted and the practical question of how to accurately calculate the density of thermally excited kinks. Recently, Currie, Krumhansl, Bishop, and Trullinger[3] (CKBT) have answered these questions for the ϕ^4 and sine-Gordon (SG) models by correcting the Krumhansl-Schrieffer theory in several respects. In particular, CKBT found that by taking into account the influence of kinks on the phonon density of states,[4] the ideal-gas phenomenology gives low-temperature results in *precise* agreement with improved transfer-operator results.[5,6] Subsequent extensions of the CKBT theory have been made in several directions to include (i) sine-Gordon systems with a "winding-number" density[7] (net imbalance of kink and antikink numbers) where agreement is found with transfer-operator results,[8] (ii) the double-quadratic (DQ) chain[9] whose kinks are nontransparent to phonons, in contrast to the sine-Gordon and ϕ^4 kinks which are transparent (reflectionless), and (iii) systems such as double-sine-Gordon[1,6,10] (DSG) which are capable of supporting more than one type of kink excitation.

The exactness of the low-temperature CKBT phenomenology has up to now been demonstrated only for those special cases [SG (Refs. 3 and 7), ϕ^4 (Ref. 3), DQ (Ref. 9)] where explicit, closed-form expressions for the kink contribution to the free energy could be found and hence compared to transfer-operator results.[5,6,8,9] The derivation of explicit expressions was thought to depend crucially on having explicit knowledge of the "phase shifts" of extended small oscillations in the presence of kinks as well as the frequencies of any localized oscillations (internal modes) of the kinks. Lack of this knowledge prohibited the validation of the phenomenology for more general models (such as DSG) and as a consequence explicit expressions for kink densities could not be found.

In this paper, we report the results of detailed analysis[6] which shows that explicit knowledge of phase shifts and internal-mode frequencies *is not needed* in order to demonstrate the exactness of the kink-gas phenomenology at low temperatures, and indeed, we shall present an explicit formula for low-temperature kink densities for the *entire* class[3] of nonlinear Klein-Gordon kink-bearing systems. All of the quantities entering this formula can be obtainied *directly* from the particular local potential function,[3] $V(\phi)$. This has the practical consequence that *low-temperature kink densities can be obtained without detailed knowledge of the kink waveform (profile) or the small oscillations about the kink*. Thus, we not only place the CKBT phenomenology on a rigorous foundation but also give its simplest and most general expression.

The general class of one-dimensional kink-bearing Hamiltonians considered by CKBT have the form[3]

$$H = A \int_{-\infty}^{+\infty} dx \left[\tfrac{1}{2}\phi_t^2 + \tfrac{1}{2}c_0^2\phi_x^2 + \omega_0^2 V(\phi) \right] , \tag{1}$$

where $\phi(x,t)$ is a dimensionless field, the constants c_0 and ω_0 are characteristic velocity and frequency, respectively, whose ratio $d \equiv c_0/\omega_0$ determines the fundamental length scale (kink width) for variations in ϕ, and the constant A sets the energy scale. The dimensionless, local, nonlinear "potential" function, $V(\phi)$, is assumed to have at least two *degenerate*, absolute minima ($V=0$), say, at $\phi=\phi_1$ and $\phi=\phi_2$ ($\phi_1 < \phi_2$), separated by a barrier which is symmetric about the midpoint $\phi_m = (\phi_1 + \phi_2)/2$. Examples of potentials having only two such minima are the "ϕ^4" (Refs. 2 and 3) $[V(\phi) = \frac{1}{8}(\phi^2 - 1)^2]$ and double quadratic[9] (DQ) $[V(\phi) = \frac{1}{2}(|\phi| - 1)^2]$ double-well potentials. A popular example having an infinite number of degenerate minima is the periodic sine-Gordon (SG) potential $[V(\phi) = 1 - \cos\phi]$. The related doubly periodic double-sine-Gordon[1,6,10] (DSG) potential $(V(\phi) = 2(1-\alpha^2)^{-1} \times [\cos(\frac{1}{2}\phi) - \alpha]^2,\ 0 \leq \alpha < 1)$ has two types of barriers, giving rise to two types of kinks. In order to treat the entire variety of such potentials simultaneously, we shall use ϕ_1 and ϕ_2 to denote any two adjacent absolute minima in $V(\phi)$. We shall assume, as in the above examples, that $V(\phi)$ has been scaled so that it has unit curvature at ϕ_1 and ϕ_2.

Single-kink solutions of the equation of motion $[\phi_{tt} - c_0^2\phi_{xx} + \omega_0^2 V'(\phi) = 0]$ may be obtained by two integrations[3] with appropriate boundary conditions. However, we shall only need to make use of certain general relations involving the static kink waveforms, $\phi_K(x)$, and *not* the full explicit spatial dependence of ϕ_K. For example, the spatial derivative of the static kink (monotonically increasing from ϕ_1 to ϕ_2) profile is related to the local potential by[3] ($z \equiv x/d$)

$$\frac{d\phi_K}{dz} = [2V(\phi_K)]^{1/2}. \tag{2}$$

The rest energy of the kink is given by

$$E_K = A\omega_0 c_0 \int_{-\infty}^{+\infty} dz \left[\frac{1}{2}\left(\frac{d\phi_K}{dz}\right)^2 + V(\phi_K(z))\right]$$
$$= A\omega_0 c_0 \int_{\phi_1}^{\phi_2} d\phi\, [2V(\phi)]^{1/2} \equiv A\omega_0 c_0 \xi\,, \tag{3}$$

where the second equality follows from (2) and shows that the kink rest energy can be obtained *directly* from an integral over the local potential (which we denote by ξ).

The classical free-energy density f can be evaluated exactly using a transfer operator technique[11] as described by CKBT.[3] In the continuum limit (d large compared to the lattice constant l), f can be written at low temperatures as[3]

$$f = f_0 - A\omega_0^2 t_0\,, \tag{4}$$

where f_0 $(= k_B T[l^{-1}\ln(\beta\hbar\omega_0 d/l) + (2d)^{-1}],\ \beta \equiv (k_B T)^{-1})$ is the free-energy density of classical phonons ($\beta\hbar\omega_0 \ll 1$) in the absence of kinks, and t_0 is the "tunnel-splitting" contribution to the lowest eigenvalue ϵ_0 of the pseudo-Schrödinger equation[3,11]

$$\left(-\frac{1}{2m^*}\frac{d^2}{d\phi^2} + V(\phi)\right)\psi_n(\phi) = \epsilon_n \psi_n(\phi)\,, \tag{5}$$

with $m^* \equiv (\beta A\omega_0 c_0)^2$. The "tunneling" free-energy density $f_t = -A\omega_0^2 t_0$ can be evaluated exactly[6] in the low-temperature limit for general $V(\phi)$ using an improved WKB method[5,6] based on the approach employed by Goldstein.[12] As $T \to 0$ ($m^* \to \infty$) we have, for potentials having a single *type* of barrier (e.g., SG, ϕ^4, DQ),

$$f_t = -A\omega_0^2 \frac{\phi_2 - \phi_1}{\sqrt{\pi}B} e^{\eta} m^{*-1/4} \exp(-\xi m^{*1/2})\,, \tag{6}$$

where the temperature-independent quantity η is defined by

$$\eta = \int_{\phi_m}^{\phi_2} d\phi \left(\frac{1}{\sqrt{2V(\phi)}} - \frac{1}{\phi_2 - \phi}\right). \tag{7}$$

For potentials with more than one *type* of barrier (e.g., DSG), there is a contribution to f_t of the form (6) for *each* type.[6,10] The factor B depends only on the *topology* of the potential: $B = 1$ for singly periodic potentials (such as SG), $B = 2$ for double-well potentials (such as ϕ^4 and DQ) and doubly periodic potentials (such as DSG). We emphasize that Eq. (6) contains no reference whatsoever to kink solutions to the equation of motion. Nevertheless, this contribution is reproduced *exactly* by the kink-gas phenomenology. To facilitate comparison of the phenomenological result below to the exact result (6), we first make use of Eq. (2) to reexpress η as

$$\eta = -\ln[(\phi_2 - \phi_1)/2] + \lim_{z\to\infty}\{z + \ln[\phi_2 - \phi_K(z)]\}. \tag{8}$$

As $z \to \infty$, $\phi_K(z)$ approaches ϕ_2 as $\phi_2 - \phi_K(z) \to \phi_0 e^{-z}$, where ϕ_0 is a constant. Thus $\eta = \ln[2\phi_0/(\phi_2 - \phi_1)]$. In addition, we can make use of Eq. (3) and the definition of m^* to rewrite Eq. (6) as

$$f_t = -k_B T \frac{2\phi_0}{\sqrt{\pi}Bd} \xi^{-1/2}(\beta E_K)^{1/2} e^{-\beta E_K}. \tag{9}$$

From a phenomenological point of view CKBT showed[3] that the low-temperature free-energy density of an ideal gas of slowly moving kinks (and antikinks) plus their associated small oscillations (kink-phonons) has the form

$$f = f_0 - k_B T n_K^{\text{tot}}\,, \tag{10}$$

where n_K^{tot} is the total density of kinks plus antikinks [given by Eq. (3.30) of Ref. 3]:

$$n_K^{\text{tot}} = \frac{2E_K}{Bhc_0}\left(\frac{2\pi}{\beta E_K}\right)^{1/2} e^{-\beta(E_K + \Sigma_K)} \quad (\beta E_K \gg 1)\,. \tag{11}$$

Here Σ_K is the self- (free) energy[3] of a static kink, which arises from the influence of the kink on the free energy of extended small oscillations as well as from the free energy of any small oscillations localized about the kink center. In order to show that the phenomenology is exact at low temperatures, we must show that $n_K = \beta|f_t|$, or equivalently upon using Eqs. (9) and (11), we must show that

$$\Sigma_K = -k_B T \ln(\sqrt{2}\,\beta\hbar\omega_0\phi_0\xi^{-1/2}) . \qquad (12)$$

If more than one *type* of kink exists (as in DSG) each type contributes a free-energy density $-k_B T n_{K,i}^{\text{tot}}$, where $n_{K,i}^{\text{tot}}$ is the total density of kinks (plus anti-kinks) of type i. Correspondingly, there is a contribution to f_t of the form (6) from each *type* of barrier in $V(\phi)$. If Eq. (12) can be proved for the kink $\phi_1 \to \phi_2$, it holds true for kinks spanning any other barrier in $V(\phi)$ as well, and thus the phenomenology would be proven exact at low temperatures. We now calculate Σ_K and show that indeed it satisfies Eq. (12).

The spatial and temporal dependence of small oscillations, $\delta\phi(z,t) = \chi(z)\cos\omega t$, about a static kink $\phi_K(z)$ are governed by the eigenvalue equation[3]

$$-\frac{d^2\chi}{dz^2} + U(z)\chi = k^2\chi , \qquad (13)$$

where $U(z) \equiv V''(\phi_K(z)) - 1$ and k is a dimensionless wave vector related to the frequency of oscillation by $k^2 = (\omega/\omega_0)^2 - 1$. Owing to the localized nature of the kink waveform, $\phi_K(z)$, the function $U(z)$ has appreciable value only near the kink center (taken to be $z=0$) and approaches zero as $|z| \to \infty$ since $V''(\phi_{1,2}) = 1$. Moreover, the function $V''(\phi_K(z))$ has a minimum at $z=0$ such that $U(0) < -1$. Thus, there exists a close analogy between Eq. (13) and the Schrödinger equation for a particle moving in a one-dimensional potential well $U(z)$. As discussed by many authors, the spectrum of small oscillations about a single kink must contain a zero-frequency ($\omega = 0$) "translation mode." Thus Eq. (13) *always* possesses a bound-state solution with $\omega_{b,1}^2 = 0$ ($k^2 = -1$), and the corresponding eigenfunction $\chi_{b,1}(z)$ is proportional to the spatial derivative of the kink waveform. Normalizing $\chi_{b,1}(z)$ to unity thus gives

$$\chi_{b,1}(z) = \xi^{-1/2}\frac{d\phi_K}{dz} . \qquad (14)$$

In addition to the translation mode, there may exist additional bound states with frequencies $\omega_{b,n}$ ($n \geq 2$) between 0 and ω_0, corresponding to "internal" (localized) oscillations of the kink waveform. The k values for the N_b bound states are pure imaginary: $k_n = \pm i\kappa_n$ with $\kappa_n = (1 - \omega_{b,n}^2/\omega_0^2)^{1/2}$ ($n = 1, \ldots, N_b$). The spatially extended modes have $\omega^2 = \omega_k^2 = 1 + k^2$ (k real).

Owing to the symmetry of $U(z)$ $[U(-z) = U(z)]$ we can take the eigenfunctions $\chi(z)$ to have definite parity [even (+) or odd (−)]:

$$\chi_+(k,z) = \tfrac{1}{2}[f_+(-k)g(k,z) + f_+(k)g(-k,z)] , \qquad (15a)$$

$$\chi_-(k,z) = \frac{i}{2k}[f_-(-k)g(k,z) - f_-(k)g(-k,z)] , \qquad (15b)$$

where $f_\pm(k)$ are Jost functions.[13] The function $g(k,z)$ contains the spatial dependence of the small oscillations and has the asymptotic form $g(k,z) \to \exp(-ikz)$ as $z \to +\infty$ ($\text{Im}k \leq 0$). The Jost functions can be used to define "phase-shift" functions $\Delta_\pm(k)$ for real k via

$$f_\pm(k) = |f_\pm(k)| \exp[(i/2)\Delta_\pm(k)] . \qquad (16)$$

The kink self- (free) energy has the form[3]

$$\Sigma_K = \Delta F + k_B T \sum_{n=2}^{N_b} \ln(\beta\hbar\omega_{b,n}) , \qquad (17)$$

where ΔF is the change in the free energy of spatially extended small oscillations due to the presence of the kink and the second term is the classical free energy of small oscillations (if any) localized about the center of the kink.

The change in the densities of states, $\Delta\rho_\pm(k)$, for the extended oscillations can be expressed[3] in terms of the phase-shift functions, $\Delta_\pm(k)$, with the result[6] that

$$\Delta F = -k_B T N_b \ln(\beta\hbar\omega_0) - \frac{k_B T}{4\pi}\int_{-\infty}^{+\infty}\frac{dk}{k+i}[\Delta_+(k) + \Delta_-(k)] . \qquad (18)$$

Using the fact[6] that the Jost functions, $f_\pm(k)$, have simple zeros at the k values $-i\kappa_{n,\pm}$ corresponding to the bound states of even or odd parity, respectively, we have managed to perform the integration in (18) without the need for explicit knowledge of $\Delta_\pm(k)$. We find that the internal mode frequencies $\omega_{b,n}$ drop out of (17), leaving

$$\Sigma_K = k_B T\left\{-\ln 2\beta\hbar\omega_0 + \tfrac{1}{2}\left[\ln f_-(-i) + \lim_{k\to -i}\ln\left(\frac{-2if_+(k)}{k+i}\right)\right]\right\} . \qquad (19)$$

The value of $f_-(-i)$ can be obtained by comparing the asymptotic ($z \to \infty$) dependence of $\chi_+(k=-i,z)$ with that of the normalized translation mode $\chi_{b,1}(z)$ [using (14) and discussion after (8)]:

$$\chi_{b,1}(z) \underset{z\to\infty}{\sim} \phi_0\xi^{-1/2}e^{-z} . \qquad (20)$$

This yields

$$f_-(-i) = \chi_{b,1}(z=0)\xi^{1/2}/\phi_0 . \qquad (21)$$

The last term in (19) can be evaluated, following Newton,[13] as

$$\lim_{k\to -i}\ln\left(\frac{-2if_+(k)}{k+i}\right) = \ln\left(\frac{2\xi^{1/2}}{\phi_0\chi_{b,1}(z=0)}\right) . \qquad (22)$$

Substituting (21) and (22) into (19), $\chi_{b,1}(z=0)$ drops out and we obtain Eq. (12). Thus the phenomenology is proven exact at low temperatures.

Substitution of (12) into (11) and elimination of ϕ_0 in favor of η [see (7)] yields a *general* formula for the low-temperature density of kinks (plus antikinks) of a given type:

$$n_K^{\text{tot}} = \frac{\phi_2 - \phi_1}{\sqrt{\pi}\, Bd}\, e^{\eta} (\beta A \omega_0 c_0)^{1/2} e^{-\beta E_K}. \tag{23}$$

Since η is given by (7) and E_K by (3), we see that n_K^{tot} can be obtained *directly* from simple integrals over the potential $V(\phi)$. Explicit knowledge of the kink waveform or its small oscillations is not needed.

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