Finite-Temperature Excitations of the Classical Toda Chain

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The finite-temperature excitation spectrum of the classical Toda lattice is obtained by numerical solution of the Bethe *Ansatz*. Bethe-*Ansatz* thermodynamics agrees exactly with known transfer-integral results. A soliton-phonon phenomenology is developed and its validity assessed with the Bethe-*Ansatz* spectrum as an exact standard. The phenomenology's intrinsic limitations become evident in a transition region, where a distinction between phonon and (nontopological) soliton is impossible.

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Integrable systems are particularly intriguing from the viewpoint of classical statistical mechanics. They provide a testing ground for the conjecture[1] that the thermodynamics of a class of nonlinear systems [calculable by transfer integral (TI) methods] can be exactly described in terms of a phenomenology of ideal gases of solitons and phonons, which interact in a manner reducing available phase space.[2,3] From a practical point of view we would like to know the dispersion relation and the occupation numbers of elementary excitations in order to calculate dynamical structure factors relevant to the observation of solitons in real systems.[4]

Whereas the thermodynamic contributions of harmonic phonons and topological (kink) solitons have been identified,[2] an unequivocal interpretation of anharmonic terms (and hence an exact reconstruction of the *total* free energy) has so far not been possible, either within classical phenomenology[2,3] or via the Bethe *Ansatz* (BA).[5] The exact role of nontopological (breather or pulse) solitons within classical statistical mechanics remains somewhat elusive. It thus seems desirable to circumvent both the necessity of a cutoff and the transition to the classical limit[5] by working out the BA for the simplest discrete integrable system, the Toda lattice,[6] in a form designed for the direct extraction of classical information, i.e., independent of the coupling constant.

In this Letter, I derive the finite-temperature excitation spectrum of the Toda lattice using the semiclassical BA and establish agreeement (within numerical accuracy) between the BA and TI thermodynamics. Furthermore, I develop an improved classical soliton-phonon phenomenology[7] and discuss its validity. It is shown that the exact (BA) excitation spectrum can be described over large regions of phase space using the concepts of thermally renormalized solitons[2] *and phonons.* The transition regime (corresponding to "long-wavelength" excitations), while in fact (BA) smooth, exhibits an apparent singularity within the phenomenological framework. This feature reveals the latter's *intrinsic* limitations and should be generic to nonlinear systems supporting nontopological solitons and acoustic phonons.

The system is defined by the Toda[6] Hamiltonian

$$H=\sum_{n=1}^{N}\left[\frac{p_n^2}{2m}+V(y_n-y_{n-1})\right], \tag{1}$$

where y_n and p_n represent displacement and momentum of the nth atom, $V(r)=(a/b)\times[\exp(-br)+br-1]$, and m is the atomic mass. The free energy of (1) was found to be[6]

$$f=f_0+f'=-T\ln(T/g)-T^2/12+\ldots, \tag{2}$$

for $T<<1$, $g=\hbar\omega_0/(a/b)$, $\omega_0=(ab/m)^{1/2}$. Energies are measured in units of a/b, lengths in units of b^{-1}. Sutherland[8] pointed out the equivalence of $V(r)$ to the $\sinh^{-2}r$ potential[9] in the limit of low densities $d_0<<1$ and succeeded in calculating the zero temperature excitation spectrum (solitons, phonons) within the BA framework in the limit $g\to 0$. In fact all asymptotic phase shifts arising within the inverse scattering theory[10] of the Toda lattice (and hence the complete dynamical information about *interactions* between solitons and or phonons) can be derived[11] from the $\sinh^{-2}r$ potential. The next step is to follow Yang and Yang[12] in their finite-T formulation of the BA. They define admissible values of the single-particle momenta and designate the density of occupied and omitted k values by $\rho(k)$ and $\rho_h(k)$, respectively. The quasiparticle energies and momenta are then given by $\epsilon(k)=-T\ln(\rho/\rho_h)$ and $h(k)=\int_0^k dk'\rho_h(k')$, respectively.

In order to make direct contact to classical "soliton phenomenologies" I take the classical limit of the relevant equations of Ref. 12 *prior to* rather than *after* solving them (semiclassical BA). This manifestly classical approach defines a nonsingular part of ϵ, $\tilde{\epsilon}=\epsilon+f_0$, which then satisfies the integral equation

$$\tilde{\epsilon}(x)=2x^2-\tilde{\mu}(2/\pi)\int_{-\infty}^{\infty}dx'\,K(x-x')\exp[-\beta\tilde{\epsilon}(x')], \tag{3}$$

with $\tilde{\mu}=1+f'=\mu-1/d_0-f_0$, the nonsingular part of the chemical potential, determined by $1=\pi^{-1}\times\int_{-\infty}^{\infty}dx\exp[-\beta\tilde{\epsilon}(x)]$ for conditions of vanishing external pressure; in (3) the kernel $K(x)=\ln|2x|$, $\beta=1/T$, and the momenta are in units of the $T=0$ Fermi momentum $k_F=(8/g)\exp(-\frac{1}{2}d_0)$. The result of the numerical solution of (3) for $T=\frac{1}{2}$ is shown in Fig. 1. Details of the iteration procedure will be published elsewhere.

In order to write the second Yang and Yang[12] equation we have used the transformation $\rho(x)=(2\beta/\pi)(1-d/d_0)\exp(-\beta\tilde{\epsilon})r(x)$, which in the limit $g\rightarrow 0$ yields the linear integral equation

$$r(x)=1+(2\beta/\pi)\int_{-\infty}^{\infty}dx'\,K(x-x')\exp[-\beta\tilde{\epsilon}(x')]r(x'), \tag{4}$$

solvable either by iteration or by discretization and matrix inversion; the relevant thermodynamical quantity here is thermal expansion. The normalization condition $\int_{-\infty}^{\infty}dx\,\rho(x)=d$ leads to $\Delta l=d^{-1}-d_0^{-1}=\pi T/2I$, where $I=\int dx\exp(-\beta\tilde{\epsilon})r$. The agreement between Toda's direct classical (TI) results[6] and our integrated quantities (Table I) presents conclusive evidence that the semiclassical BA and, in particular, Sutherland's kernel[8] remain valid for finite temperatures and can be relied upon to yield the correct excitation spectrum.

The form of the excitation spectrum derived by Eqs. (3) and (4) is shown in Fig. 1 and 2 for $\beta=2$. There is no trace of a singularity in the quasiparticle energies and only a broad maximum of the particle density at $k_m\simeq 0.85\,k_F$. Excitations are clearly of particle character since the ratio of occupied to omitted k values is of order $\hbar$ for all k, unlike the case for $T=0$ with its well defined Fermi sea. It follows that an *exact* "reconstruction of the statistics" of classical soliton bearing systems[1,2] can be achieved trivially[12] for any finite T in terms of the numerical solution of (3) and (4) . *The number of particles and the entropy contribution from any interval dk coincide with those of a classical gas of noninteracting particles with energies* ϵ *and momenta* h $(2\pi\rho_h=dh/dk)$ *in an interval* $dh/2\pi$.

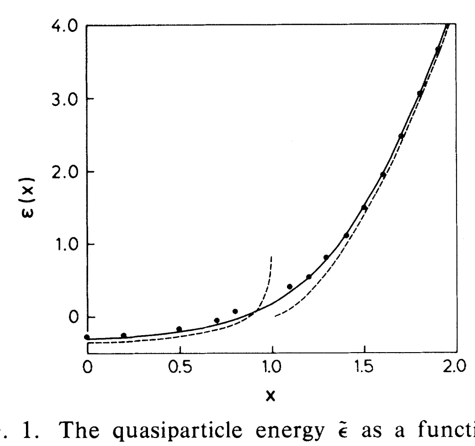

FIG. 1. The quasiparticle energy $\tilde{\epsilon}$ as a function of k/k_F, for $T=0.5$. The solid line is the result of the numerical solution, the dashed line describes $\epsilon_0(k)$, and the points are thermally renormalized energies.

However self-contained the above treatment may be, it seems hard to believe that the system can lose *all* memory of its solitons and phonons even at a relatively low temperature. It is therefore of considerable interest to relate the exact results derived above with a consistent soliton/phonon phenomenology.[7] This is a point that has led to some controversies over the last few years, in particular with reference to "breathers" of the sine-Gordon equation.[2,3,5]

To lowest order in the temperature, we may view the energies of the quasiparticles with $|k|<k_F$ as (minus) the free energy of the corresponding phonon mode, i.e., $\epsilon_0(k)=-T\ln(2\beta g\sin\theta)$, $k/k_F=\cos\theta$; the Boltzmann factor $\exp(\beta\epsilon)$ describes the classical limit of the Bose-Einstein distribution for the population of a particular phonon mode. For $|k|>k_F$ the result of Ref. 8 holds, $\epsilon_0(\phi)=\sinh 2\phi-2\phi$, $k/k_F=\cosh\phi$, corresponding to the energy of a free soliton (Fig. 1). Corrections

TABLE I. Classical thermodynamics from Eqs. (3) and (4). The free energy $1+f'$ and the thermal expansion are given for two different temperatures; the exact results (Ref. 6) are in parentheses. The numerical results involve 17 and 25 iterations of (3) and (4), respectively. The integrations were performed for 25 points in the interval $0\leqslant x\leqslant 2.2$ $(T=0.5)$ and $0\leqslant x\leqslant 3$ $(T=2)$; note that both ϵ and ρ are even functions of x.

T	$1+f'$	Δl
0.5	0.9797 (0.9793)	0.270 (0.270)
2.0	0.6941 (0.6931)	1.270 (1.270)

due to finite T can be included either via the phase shifts of the purely classical theory or via the BA at $T=0$. Both approaches lead to the same result if correctly interpreted. We may describe either the rearrangement that takes place in $\rho(k)$ for $k/k_F<1$ as a particle is created at q outside the Fermi sea (phonon phase shift due to a soliton) *or* the change in $\rho_h(k)$ for $k/k_F>1$ due to the creation of a hole at q inside the Fermi sea (soliton spatial shift due to a phonon[3]) by the same function $\Delta(k,q)$.[11] Similar expressions govern the rearrangement of particles within the Fermi sea due to the excitation of a hole (phonon-phonon interaction) and the rearrangement of holes outside due to the excitement of a particle (soliton-soliton interaction). Whereas the latter might be neglected at low temperatures (low soliton densities), the former, although of order g, will lead to finite effects in the presence of a thermal ensemble, i.e., $O(T/g)$ phonons.

As the temperature rises the following picture emerges: (a) There is an extra entropy produced inside the Fermi sea by the "backflow" associated with the excitation of each hole. This leads to a change in the quasiparticle energy

$$\Delta\epsilon(k)=(T^2/4)[1-(k/k_F)^2]^{-1}. \tag{5}$$

The beginnings of an asymptotic expansion in $1/\beta$ become apparent. Agreement is excellent for $k<<k_F$ (cf. Fig. 1) but the correction term (5) becomes singular as $k\rightarrow k_F$. In the region of its validity, however, (5) is equivalent to renormalization of k_F to a value $k_m=(1-T/4)k_F$; for the case of Fig. 2 this yields $k_m/k_F=0.875$, remarkably close to the position of the broad maximum of ρ. If we adopt this new "Fermi momentum" and *assume* that no particles have been lost from $|k|<k_m$ we may compute the free energy of the phonon sector[13]:

$$f_{ph}=f_0-T^2/8. \tag{6}$$

(b) The creation of a soliton consists of a particle at $k>k_F$ plus the backflow of the Fermi sea; at finite T the latter produces an additional entropy, which may be interpreted as a change in the free energy needed to create a solition (thermal renormalization of the soliton mass[2]). It amounts to $\Delta\epsilon(k)=-T\ln(2\beta g\sinh\phi e^{-\phi})$ and describes correctly deviations from ϵ_0 for $k/k_F>1.1$ (Fig. 1). Furthermore, the appearance of the singular term $-f_0$ in $\epsilon(k)$ for all k now guarantees correct phase-space counting—and, ultimately, classical statistics.

(c) At this stage we fill up the system with solitons until thermal equilibrium has been attained.

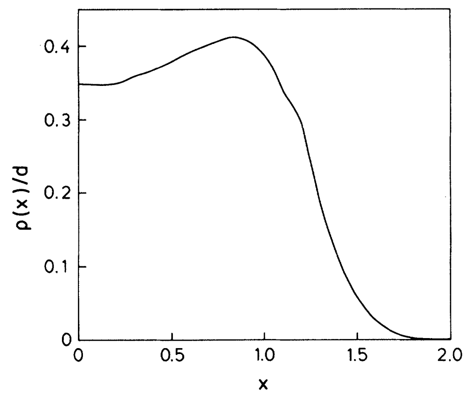

FIG. 2. The density of particles vs k/k_F for $T=0.5$. The square-root singularity of $T=0$ has given way to a broad maximum.

The free energy of the soliton sector will now be given by

$$f_s=-T\int_{|k|>k_m}dk\,\rho_h(k)\exp[-\beta\epsilon(k)], \tag{7}$$

with an important proviso: As the phonon gas evolves by the successive buildup of holes, the density of holes outside the Fermi sea—and thus the available phase space for solitons—is reduced. The corrected density of states

$$\rho_h(k)=(d/2\pi)\phi[1-(T/4\phi)\sinh^{-2}\phi], \tag{8}$$

should again be understood as the beginning of an asymptotic expansion in $1/\beta$ [cf. (5) above]. Nevertheless, if used in (7) [cf. our discussion following (5)], it reveals a remarkable degree of self-consistency. Both leading terms in (7), of order $T^{4/3}$[14] and T^2, respectively, vanish as a result of exact cancellations, leaving (6) as the simplest phenomenological reconstruction of the total free energy.

The heuristic soliton-phonon scheme I have presented is successful in a *quantitative* sense in interpreting the exact excitation spectrum of an exemplary classical nonlinear system *away* from the transition region. Its weakness lies in its structure as an asymptotic series in $1/\beta$ and the concomitant overemphasis on a singularity that does not exist for $T>0$. The analogy with the Bethe-*Ansatz* description is in fact deeper. Equations (3) and (4) cannot be solved by asymptotic methods either.

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