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Thermodynamics of the quantum Toda lattice

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Abstract. A linear chain with exponential plus linear interactions (Toda lattice) can be mapped by the Bethe ansatz to a Fermi gas. The thermodynamics is treated by analogy to the delta-function Bose gas (Yang and Yang). Analytical solutions are given for the strongly anharmonic regime and low temperatures; the general case is treated numerically. For the case of weak anharmonicity the specific heats are compared with earlier approximate calculations. The anharmonic part of the specific heat is shown to be not very different from the corresponding classical result which can be interpreted as the specific heat of an ideal gas of solitons. For the quantum case the soliton-gas picture needs further investigation.

1. Introduction

There are very few quantum gases or liquids, with pairwise interactions among the particles, that have been treated exactly. The first example was a one-dimensional system of bosons with repulsive delta-function interactions which was solved by Lieb and Liniger (1963) using the Bethe ansatz. For this system it is possible to incorporate the interactions into boundary conditions which leads to a formal description of the system as a Fermi gas. Consequently the low-lying excitations are of two kinds: particle and hole excitations (Lieb 1963). The thermodynamics and the finite-temperature excitation spectrum were treated by Yang and Yang (1969).

These methods were generalised by Sutherland (1971, 1972, 1978) to other integrable systems, e.g. with interactions $V(r) \sim r^{-2}$ or $\sinh^{-2} r$, where r is the particle distance. For these systems the Bethe ansatz provides only the asymptotic wavefunctions; however, this is sufficient to obtain the ground state energy, the excitation spectrum and the thermodynamics. For the case of the Calogero model (interaction $V \sim r^{-2}$) these results were shown to be exact (Sutherland 1971) by comparison with other methods (Calogero 1971, Marchioro and Presutti 1970).

Generally an application to lattice models is not possible because bound states are not described by the Bethe ansatz which consists only of scattering states. However, the Toda lattice is an exception. This model (Toda 1967, 1981) is a chain of particles of mass m with nearest-neighbour interactions

$$V(r) = (m\omega^2/\gamma^2)\{\exp[-\gamma(r-r_0)] + \gamma(r-r_0) - 1\}. \quad (1.1)$$

Here the attractive part is linear; for periodic boundary conditions the sum of the linear terms reduces to a constant (§ 2). Thus the remaining problem is essentially that of a gas with exponential repulsive interactions.

Sutherland (1978) showed that the Toda lattice can be considered to be the low density limit of a system with $\sinh^{-2} r$ interactions, which is completely integrable in the classical and the quantum case (Calogero *et al* 1975). The integrability of the

quantum Toda lattice was also proven in the context of Lie algebras for both the periodic and non-periodic case (Olshanetzky and Perelomov 1983).

Sutherland (1978) applied the Bethe ansatz to the $\sinh^{-2} r$ system and performed the classical limit first and the low density limit afterwards. In this case the particle and hole excitations of the quantum problem reduce to the solitons and phonons of the classical Toda lattice.

In order to study the quantum case one can either consider low densities without taking the classical limit or treat the Toda lattice directly. In this way Mertens (1984) obtained analytical results for large γ , which means strong anharmonicity. Here the Toda lattice behaves effectively like a gas of hard spheres with constant attraction, where the radius of the spheres is the scattering length of the exponential part of the potential (1.1); for $\gamma \rightarrow \infty$ the radius of the spheres is r_0 .

For arbitrary γ the problem can be solved numerically (Mertens and Hader 1985). Here the hole excitations can be identified as phonons; for small anharmonicity the particle branch of the spectrum shows nearly the same dispersion as the classical solitons, though the ground state exhibits a large zero-point motion. Therefore it is tempting to interpret the particle excitations as quantum solitons.

The results of the Bethe ansatz can be tested by the quantum transfer-integral method of Mertens (1975, 1976). Assuming a Hartree-Jastrow form for the ground state, the expectation value of the Hamiltonian is calculated exactly and the ground state energy is obtained variationally. For the Toda lattice it agrees within the numerical error of about 0.1% with the Bethe ansatz result (Mertens 1986).

The test is particularly important because a rigorous justification of the Bethe ansatz for the Toda lattice is still missing. In fact, the quantum inverse scattering theory (QIST), which is an algebraisation of the Bethe ansatz technique, has been only partially successful in the case of the Toda lattice (Faddeev 1980, Korepin 1983, Gaudin 1983). On the other hand Sklyanin (1985) has recently combined the QIST with the method of Gutzwiller (1981), which so far could be evaluated only for the case of three or four particles. Sklyanin has reduced the determination of the spectrum to integral equations which are closely related to those of Sutherland (1978) and Mertens (1984).

In this paper the thermodynamics is treated using the method of Yang and Yang (1969), which is based on the Bethe ansatz (§ 2). Analytical results are given in § 3 for the strongly anharmonic regime and low temperatures; the general case is treated numerically (§ 4). We discuss in detail the high and low temperature regimes. The latter is particularly important when the Toda lattice is used as a model for a solid, but so far most of the literature treats only the classical statistical mechanics. The exceptions are a path-integral approach by Mertens and Büttner (1980) and a semi-classical approximation by Bolterauer and Oppen (1981), which are valid only in the weakly anharmonic regime, however.

A very interesting quantity is the anharmonic part of the specific heat which has been interpreted in a classical phenomenological theory (Mertens and Büttner 1981) as the specific heat of an ideal soliton gas. We show that this anharmonic part is not very different for the quantum and the classical model; this means that solitons also play a role in the quantum Toda lattice.

2. Bethe ansatz and the integral equation of Yang and Yang

After a scaling of all lengths by $1/\gamma$ and energies by $\hbar^2\gamma^2/2m$, the Hamiltonian of the

Toda chain with periodic boundary conditions is

$$H = \sum_n \left(-\frac{\partial^2}{\partial x_n^2} + 2C^2 \exp[-(x_{n+1} - x_n - r_0)] + V_0 \right) \quad (2.1)$$

with the dimensionless coupling constant

$$C = (m\omega / \hbar \gamma^2) \quad (2.2)$$

and $V_0 = 2C^2(a - r_0)$, where a is the lattice parameter. The additive constant V_0 results from the attractive linear term of the potential (1.1) and can be omitted during the calculation; it will be added to the final results for the energies.

Considering large separations the N constants of motion can be identified with the momenta k_n of the particles. When the particles scatter the interactions can produce only rearrangements of the k , since the system is completely integrable. Thus the wavefunctions asymptotically have the Bethe form

$$\psi \sim \sum_P A(P) P \left[\exp \left(i \sum_n^N k_n x_n \right) \right] \quad (2.3)$$

where P denotes one of the $N!$ permutations of the k_n . The amplitudes A depend only on the two-body phase shift $\delta(k_m - k_n)$ which connects two configurations differing by just one permutation (Lieb and Liniger 1963).

$\delta(k)$ is obtained from the solution of the two-body problem (Bruschi *et al* 1982, Mertens 1984), and is essentially the low density limit of Sutherland's (1978) phase shift for the $\sinh^{-2} r$ system. Only the derivative $\delta'(k)$ will be used explicitly in the following:

$$\delta'(k) = r_0 + 2 \ln C - \psi(1 + ik) - \psi(1 - ik) \quad (2.4)$$

where ψ is the digamma function.

In the thermodynamic limit (N and length $L \rightarrow \infty$, with finite density $d = N/L$) $\rho(k)$ is defined as the density of the k , $\rho_h(k)$ as the density of 'holes' and the sum of both is denoted $\rho_{\text{tot}}(k)$. The energy is

$$E/N = \frac{1}{d} \int_{-\infty}^{\infty} dk \rho(k) k^2 + V_0 \quad (2.5)$$

$$d = \int_{-\infty}^{\infty} dk \rho(k). \quad (2.6)$$

ρ_{tot} is related to ρ by

$$2\pi\rho_{\text{tot}}(k) = 1 - \int_{-\infty}^{\infty} dk' \delta'(k - k') \rho(k'). \quad (2.7)$$

In the thermal equilibrium the free energy as a functional of $\rho(k)$ and $\rho_h(k)$ has to be minimised under the constraints (2.6) and (2.7) which leads to the integral equation of Yang and Yang (1969)

$$\varepsilon(k) = k^2 - \mu + \frac{1}{\beta} \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \delta'(k - k') \ln[1 + \exp(-\beta\varepsilon(k'))] - 2C^2 r_0 \quad (2.8)$$

where β is the inverse temperature, μ is the chemical potential and ε is defined by

$$\rho_h / \rho = \exp(\beta\varepsilon). \quad (2.9)$$

The pressure P is obtained from the free energy by $F = N\mu - PL$

$$P = \frac{1}{\beta} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \ln[1 + \exp(-\beta\epsilon(k))] - 2C^2. \quad (2.10)$$

The last terms in the equations (2.5), (2.8) and (2.10) are slight modifications of the original Yang-Yang equations due to the attractive linear part of the Toda potential (see (2.1)).

With these equations the thermodynamics is complete: the non-linear integral equation (2.8) must be solved for given μ and T . Then $P(\mu, T)$ can be calculated by (2.10); the differential $dG = -S dT + L dP + \mu dN$ of the free enthalpy can be transformed because of $G = \mu N$ into $L dP = N d\mu + S dT$. From here all remaining thermodynamic quantities can be derived.

In the classical limit the integral equation for $\epsilon(k)$ has recently been solved numerically (Theodorakopoulos 1984) and analytically (Oppen 1985). The resulting free energy is identical to the exact classical free energy of Toda (1975). In this paper we give solutions for the quantum mechanical case.

3. Analytical solutions for large anharmonicity and low temperatures

The anharmonicity of the Toda potential (1.1) is controlled by the parameter γ . For $\gamma \rightarrow 0$, (1.1) reduces to a harmonic potential with the eigenfrequency ω . Large γ means large anharmonicity or weak coupling $C = m\omega / \hbar\gamma^2$. For $C \ll 1$ the zero-temperature limit of the central equation of our problem, namely the integral equation (2.8) for $\epsilon(k)$, has been solved (Mertens 1984) by $\epsilon = k^2 - k_F^2$, where $k_F \ll 1$ is the Fermi momentum. Therefore we assume that for sufficiently low temperatures

$$\epsilon(k) = k^2 - k_0^2 \quad (3.1)$$

with $k_0 \ll 1$, where k_0 and thus $\epsilon(k)$ are temperature dependent.

For $|k'| > k_0$ the term $\ln(1 + \exp(-\beta\epsilon))$ in the integrand of (2.8) is exponentially small; therefore the main contribution to the integral comes from $|k'| \leq k_0$. For low temperatures we need to consider only excitations near the Fermi surface which means that $|k|$ is of the order of k_F and k_0 . Because of $k_0 \ll 1$ we have $|k - k'| \ll 1$; thus the kernel $\delta'(k - k')$ can be replaced by a rapidly converging Taylor expansion. If only the first term $\delta'(0) \equiv a_s$ of the expansion is retained we obtain an equation for ϵ in which the integral no longer depends on k

$$\epsilon(k) = k^2 - \mu + a_s \int_{-\infty}^{\infty} \frac{dk'}{2\pi} T \ln[1 + \exp(-\beta\epsilon(k'))] - 2C^2 r_0. \quad (3.2)$$

Thus we see that the ansatz (3.1) is in fact a solution. $k_0(T)$ still has to be determined and we must check for which regime our assumption $k_0 \ll 1$ is fulfilled.

a_s is obtained from the Taylor expansion of the digamma function in (2.4)

$$a_s \equiv \delta'(0) = r_0 + 2 \ln C + 2\gamma_E \quad (3.3)$$

where $\gamma_E = 0.577 \dots$ is Euler's constant. Because of $\delta'(0) = \lim_{k \rightarrow 0} [\delta(k)/k]$ the constant a_s represents the scattering length of the potential in (2.1). As a test we can perform the limit $\gamma \rightarrow \infty$ where the Toda potential reduces to a hard-sphere potential. Returning to the original units we see that in fact $a_s \rightarrow r_0$ for $\gamma \rightarrow \infty$.

Knowing $\varepsilon(k)$, (2.9) gives us

$$\rho(k) = \frac{\rho_{\text{tot}}(k)}{\exp[\beta(k^2 - k_0^2)] + 1}. \quad (3.4)$$

If this is inserted into (2.7) this integral equation can be treated in quite the same manner as that for $\varepsilon(k)$; the result is a constant ρ_{tot}

$$2\pi\rho_{\text{tot}} = 1 - a_s \int_{-\infty}^{\infty} dk' \rho(k') = (a - a_s)/a \quad (3.5)$$

because of (2.6). ρ_{tot} would be $(2\pi)^{-1}$ if a_s were zero. Thus the density $\rho(k)$ in (3.4) is that of free fermions in a volume which is reduced by Na_s . Since the Pauli principle has the same effect on the wavefunctions as a hard sphere with zero radius, we see again (cf § 1) that our system behaves effectively like a gas of hard spheres of radius a_s . An additional constant attraction, resulting from the linear part of the Toda potential, leads to additive constants in the energy, the chemical potential and the pressure (see below).

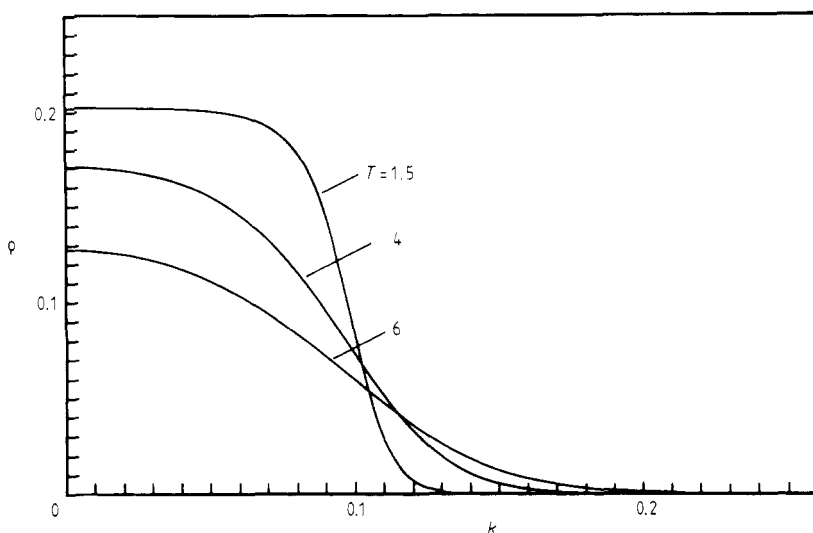


Figure 1. For large anharmonicity the numerically obtained density ρ of occupied k is nearly the same as that of free fermions in a reduced volume, see (3.4), (3.5); temperatures T in 10^{-2} . $P = 0$, $C = 0.01$.

Before we proceed we introduce a more compact notation by the definition of a functional

$$F[f(y)] = \int_0^{\infty} dy \frac{1}{\sqrt{y}} \frac{f(y)}{\exp[\beta(y - y_0)] + 1}. \quad (3.6)$$

With the substitution $k^2 = y$, equation (2.6) together with (3.3) reads $d = \rho_{\text{tot}} F[1]$; using (3.5) we obtain an expression for the lattice constant

$$a = a_s + 2\pi / F[1]. \quad (3.7)$$

The energy (2.5) is

$$E/N = V_0 + F[y]/F[1]. \quad (3.8)$$

After partial integration, (3.2) and (2.10) can be written as

$$\varepsilon(y) = y - \mu + (a_s/\pi)F[y] - 2C^2r_0 \quad (3.9)$$

$$P = F[y]/\pi - 2C^2. \quad (3.10)$$

The chemical potential is obtained by considering $\varepsilon(y_0)$

$$\mu = y_0 + (a_s/\pi)F[y] - 2C^2r_0. \quad (3.11)$$

The elimination of $F[1]$ and $F[y]$ from (3.7), (3.8) and (3.10) yields an equation of state

$$(P + 2C^2)(a - a_s) = 2(E/N - V_0) \quad (3.12)$$

which will be shown together with numerical results in § 4 (figure 4). We note that for fixed length or fixed pressure the temperature dependence of the energy is the same as that of the pressure or the lattice constant, respectively. Therefore we show only $E(T)$ in the following figures and omit $P(T)$ and $a(T)$, respectively. In order to calculate explicitly $E(T)$, $\mu(T)$, etc, we take the two leading terms of the Sommerfeld expansion (see e.g. Ashcroft and Mermin 1976) for the functionals and obtain

$$F[y] = 2k_F^3(\frac{1}{3}g^3(x) + x/g(x)) \quad (3.13)$$

$$F[1] = 2(\partial/\partial y_0)F[y] = 2k_F(g(x) - x/g^3(x)) \quad (3.14)$$

with

$$x = (\pi^2/24k_F^4)T^2 \quad g(x) = (k_0(x)/k_F). \quad (3.15)$$

In the following we consider two special boundary conditions. We start with the pressure $P = 0$, which will be denoted by an index P . Equation (3.10) yields $F_P[y] = 2\pi C^2$ which can be expressed by the Fermi momentum k_F at zero pressure (Mertens 1984)

$$k_P = (3\pi C^2)^{1/3}. \quad (3.16)$$

Together with (3.13) we obtain $g^3 + 3x/g = 1$ which yields $g = 1 - x - 2x^2$ in second order in x . In this way we have eventually determined

$$k_0 = k_P(1 - x - 2x^2) \quad (3.17)$$

and we see that our assumption $k_0 \ll 1$ is indeed fulfilled for $C \ll 1$ and for temperatures which satisfy $x \ll 1$. This means $T \ll 0.02$ for $C = 0.01$, which is the value of C in the figures. Note that T is dimensionless ($k_B T$ is measured in units of $\hbar^2 \gamma^2 / 2m$).

Inserting $g(x)$ into (3.14) we obtain

$$F_P[1] = 2k_P(1 - 2x - 5x^2) \quad (3.18)$$

and finally

$$\begin{aligned} a &= a_0 + (\pi/k_P)(2x + 9x^2) \\ \mu &= \mu_0 - k_P^2(2x + 3x^2) \\ E/N &= E_0/N + k_P^2(2x + 9x^2). \end{aligned} \quad (3.19)$$

a_0 , μ_0 and E_0 are the zero-temperature values of Mertens (1984). The specific heat per particle

$$C_P = (\pi^2/6k_P^2)T + (\pi^4/16k_P^6)T^3 \quad (3.20)$$

is shown in figure 6 in § 4 together with results for higher temperatures.

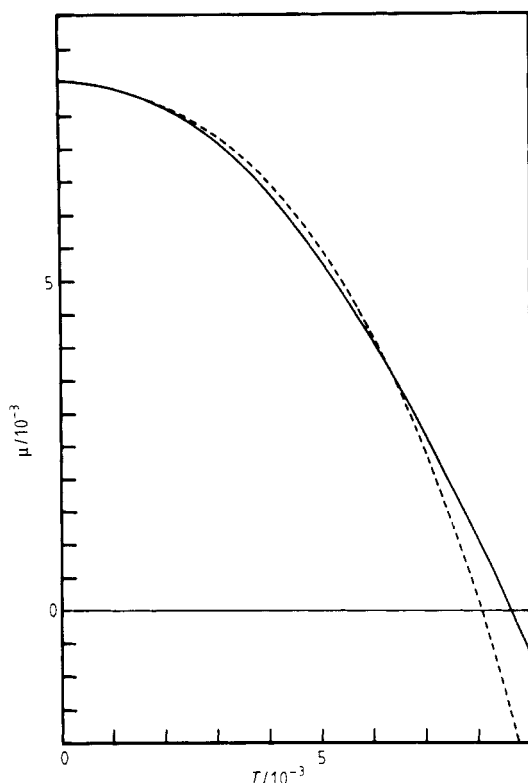


Figure 2. Chemical potential against temperature. Broken curve: analytical result (3.19); full curve: numerical result (§ 4). $C = 0.01$, $P = 0$.

The second boundary condition, fixed length $L = Nr_0$, is treated in quite the same way. The results are

$$\begin{aligned} P &= (2/3\pi)k_L^3(1+6x-9x^2) \\ E/N &= \frac{1}{3}k_L^2(1+6x-9x^2) \\ C_L &= (\pi^2/6k_L^2)T + (\pi^4/48k_L^6)T^3 \end{aligned} \quad (3.21)$$

where $k_L = \pi/(-2 \ln C - 2\gamma_E)$ is the Fermi momentum for fixed length. For $C = 0.01$ the condition $k_0 \ll 1$ is fulfilled if $T \ll 0.3$.

4. Numerical results for the general case and discussion

The central equation is the non-linear integral equation (2.8) for $\varepsilon(k)$. An iterative solution converges after a slight modification, namely the subtraction of $\varepsilon(0)$ which also eliminates the constants

$$\varepsilon(k) = \varepsilon_0 + k^2 + \int_{-\infty}^{\infty} \frac{dk'}{2\pi} K(k, k') T \ln[1 + \exp(-\beta\varepsilon(k'))] \quad (4.1)$$

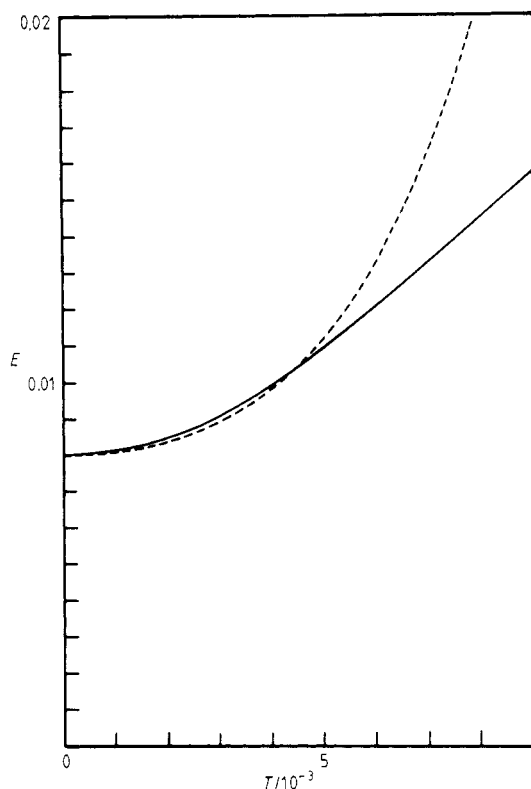


Figure 3. Energy against temperature. Broken curve: analytical result (3.19); full curve: numerical result (§ 4). $C = 0.01$, $P = 0$.

with $K = 2 \operatorname{Re}\{\psi(1 - ik') - \psi[1 + i(k - k')]\}$. Apart from the temperature, $\varepsilon(0) = \varepsilon_0$ is the only parameter in (4.1). It has to be varied until the chosen boundary condition is satisfied. For constant pressure (2.10) must be fulfilled; for the case of constant length the linear integral equation (2.7) for $\rho(k)$ must be solved first in order to obtain the lattice constant by (2.6)[†]. After having fixed ε_0 , all thermodynamic quantities can be calculated from $\varepsilon(k)$ and $\rho(k)$, e.g. energy and entropy.

We begin the discussion of the results with the strongly anharmonic case $C = 0.01$ in order to compare with the analytical results of § 3. Figures 2 and 3 show the energy $E(T)$ and the chemical potential $\mu(T)$ for zero pressure. The analytical approximations turn out to be valid for $T \leq 0.005$, which agrees with the estimate $T \ll 0.02$ below (3.17). The results for constant length are not shown because the qualitative behaviour of the T dependence is the same; here the range of validity of the analytical calculation is one order of magnitude larger, in accordance with the estimate $T \ll 0.3$ (see (3.21)). In the PV diagrams of figure 4 the isotherms for the two lowest temperatures agree well with the analytical results from the equation of state (3.12). Finally the specific heats are shown in figure 5; for the discussion see below.

[†] The numerical procedure is described here only in principle. In order to avoid a need for the integral equations to be solved many times, the procedure must be modified in practice, depending on the particular boundary condition.

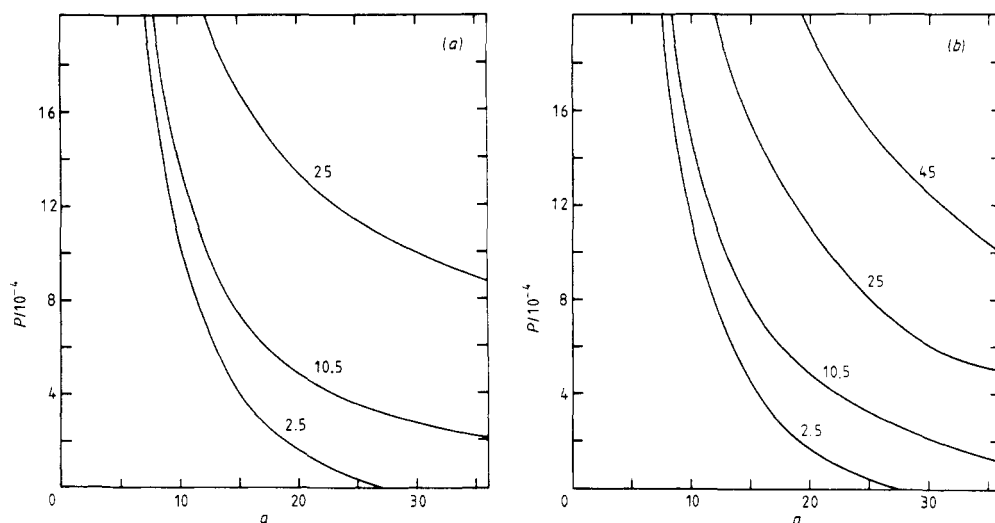


Figure 4. Isotherms in the PV diagram; a is the lattice parameter, temperatures in 10^{-2} ; (a) from the equation of state (3.12), (b) numerical (§ 4) $C = 0.01$.

Let us consider now the case of the coupling constant $C = 1$ which is accessible only numerically. In figure 6 we see that the densities $\rho(k)$ and $\rho_{\text{tot}}(k)$ are completely different from those of a free fermion system, in contrast to the case $C = 0.01$. We note that $\rho_{\text{tot}}(k)$ is generally temperature dependent; in fact $\rho_{\text{tot}}(k)$ is not the density of states, since the k_n in (2.3) are not the quantum numbers. Thus we see that the Fermi system to which our problem has been mapped by the Bethe ansatz generally gives only a formal description. Therefore $\rho(k)$ and $\rho_{\text{tot}}(k)$ do not have a direct physical meaning but only the integrals which contain them, e.g. the energy, the entropy and

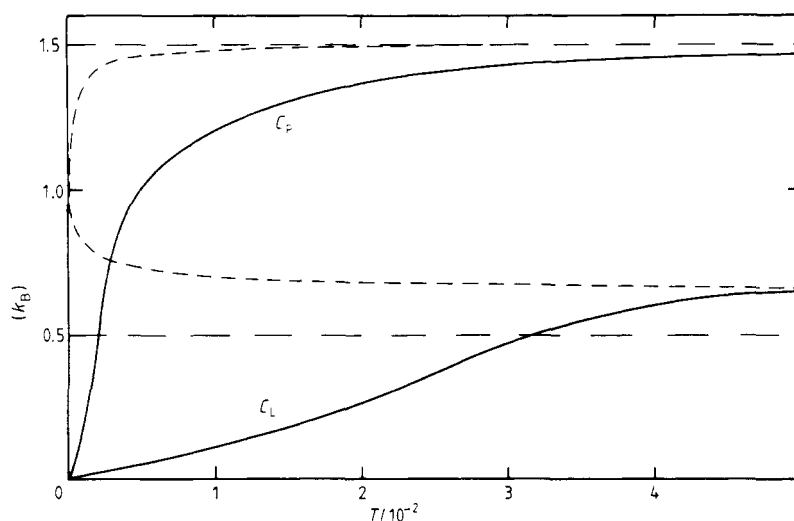


Figure 5. Specific heats at zero pressure and constant length in the case of large anharmonicity. Broken curves: classical results; chain curves: asymptotics for $T \rightarrow \infty$. $C = 0.01$.

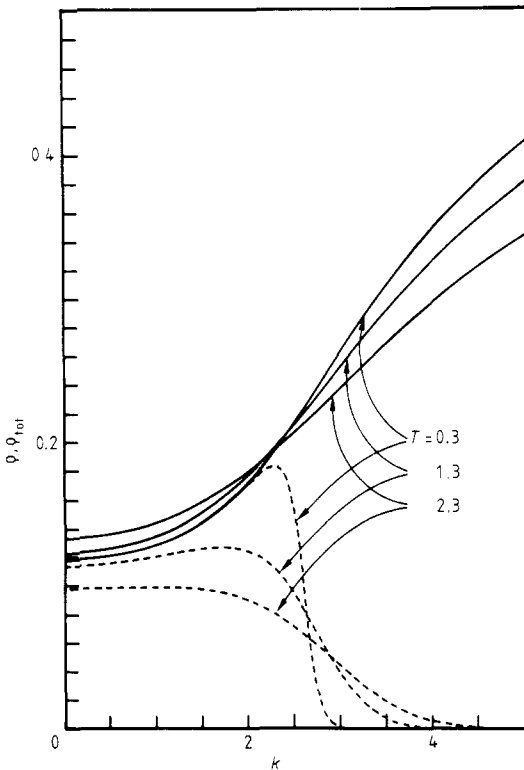


Figure 6. Total density ρ_{tot} (full curves) and density ρ of the occupied k (broken) for the coupling $C = 1$ at three different temperatures. $P = 0$.

the pressure. (For the excitation spectrum the situation is similar: the energy and momentum of the excitations are obtained as functions of k ; the elimination of k finally yields the dispersion relation.)

The temperature dependences of energy, pressure, lattice constant and chemical potential turn out to be qualitatively similar to those of the case $C = 0.01$ and therefore they are not displayed here. Instead we concentrate on the derivatives of E , namely the specific heats for constant length $L = Nr_0$ and zero pressure (figure 7):

$$C_L = \left(\frac{\partial E}{\partial T} \right)_L \quad C_P = \left(\frac{\partial E}{\partial T} \right)_{P=0}. \quad (4.2)$$

For high temperatures the specific heats approach the results of Toda and Saitoh (1983) for the classical model. For $T \rightarrow \infty$, $C_P \rightarrow \frac{3}{2}$ and $C_L \rightarrow \frac{1}{2}$ which are the values for a classical gas of hard spheres. $C_L(T)$ has a maximum in contrast to the monotonic classical curve.

When the results for two different systems with the coupling constants C_1 and C_2 are compared it should be noted that the temperatures T_1 and T_2 of the systems are comparable if $T_1/C_1 = T_2/C_2$. Therefore the units for the abscissae in figures 5 and 7 have been chosen such that the figures can be compared directly. It can be seen that the system with $C = 1$ with increasing temperature approaches the classical results more rapidly than the system with $C = 0.01$. In this context we mention that the

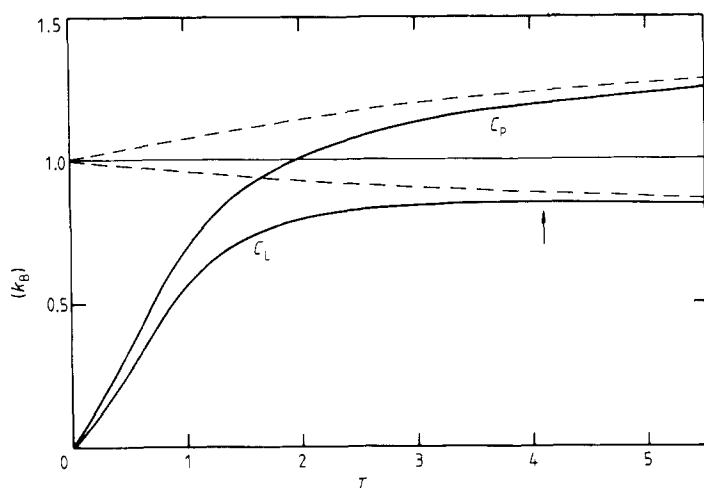


Figure 7. Specific heats at zero pressure and constant length for the coupling $C = 1$. The arrow indicates the maximum of C_L ; the asymptotic values for $T \rightarrow \infty$ are $\frac{3}{2}$ and $\frac{1}{2}$. The broken curves are the classical results.

excitation spectrum at zero temperature exhibits dispersion relations which become more and more classical the larger C is (Mertens and Hader 1985). In the classical limit $C \rightarrow \infty$ the dispersion is that of solitons and phonons (Sutherland 1978, Mertens 1984).

The weakly anharmonic regime $C \geq 1$ is particularly interesting for low temperatures. Here the specific heat C_P naturally is completely different from the corresponding classical quantity C_P^{Cl} (figure 7). However, if the specific heat of a harmonic lattice (C_H or C_H^{Cl} , respectively) is subtracted, the anharmonic parts $C_P - C_H$ and $C_P^{\text{Cl}} - C_H^{\text{Cl}}$ are no longer very different; only for very low temperatures are there certain deviations (figure 8)[†] which are qualitatively similar for the whole regime $0.5 < C < \infty$. This confirms earlier approximate results from a path-integral approach (Mertens and Büttner 1980) and a semiclassical calculation (Bolterauer and Oppen 1981).

As $C_P^{\text{Cl}} - C_H^{\text{Cl}}$ in the phenomenological theory of Mertens and Büttner (1981) can be calculated as the specific heat of an ideal soliton gas, these authors have interpreted the resemblance of $C_P - C_H$ as a first hint that solitons play a role also in the quantum Toda lattice.

However, since $C_P - C_H$ is not identical to $C_P^{\text{Cl}} - C_H^{\text{Cl}}$ but differs in a characteristic way (figure 8), we are presently investigating the soliton-gas picture for the quantum case. For this purpose the finite-temperature excitation spectrum must be calculated. The particle and hole excitations are understood as soliton and phonon quasiparticles (in contrast to the zero-temperature case where these excitations are eigenstates). Finally the thermal behaviour of the quasiparticle ensembles has to be compared with $C_P - C_H$.

[†] For $T < 0.2$ we have checked our numerical results by an anharmonic perturbation theory (Leibfried and Ludwig 1961) where the Toda potential is expanded up to the fourth order. The result is $C_P - C_H = \pi^2 T / (12 \times 16 \times C^2)$, and the same with a negative sign for $C_L - C_H$; here $C_H = \pi T / 6C$ is the Debye approximation for the harmonic lattice.

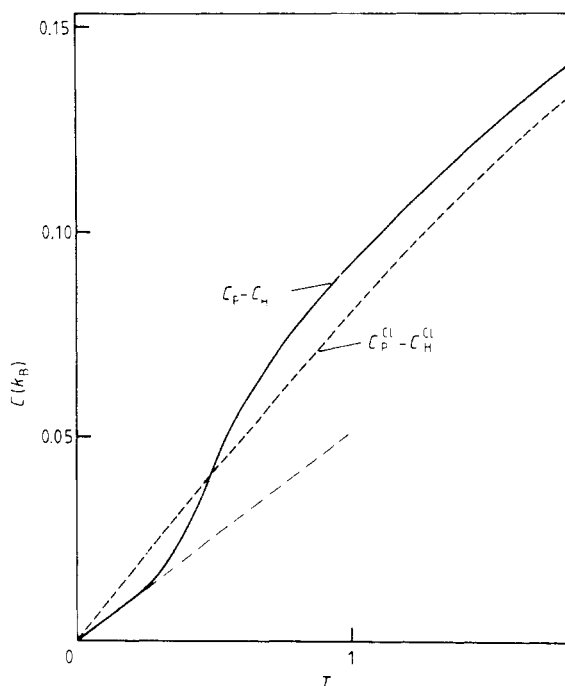


Figure 8. Anharmonic part of the specific heat at zero pressure for the coupling $C = 1$; the corresponding classical result is broken. The chain curve is the result of a perturbation theory; see second footnote. $P = 0$.

Acknowledgment

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