Dynamic correlations for the Toda lattice in the soliton-gas picture

1982 J. Phys. A: Math. Gen. 15 1831

(http://iopscience.iop.org/0305-4470/15/6/023)

J. Phys. A: Math. Gen. **15** (1982) 1831–1839. Printed in Great Britain

Dynamic correlations for the Toda lattice in the soliton-gas picture

F G Mertens and H Büttner
Physikalisches Institut, Universität Bayreuth, 8580 Bayreuth, West Germany

Received 30 November 1981

Abstract. The static and dynamic force–force correlation function for the one-dimensional Toda lattice is calculated in the soliton-gas approximation. The dispersion and width of the soliton and phonon resonances are discussed in detail. Comparison with other calculations and molecular dynamics results shows that this approximation gives a reasonable description of most of the features in the correlations.

1. Introduction

Since the pioneering work by Toda (1967, 1975) on the linear chain with exponential nearest-neighbour interaction, this lattice has served as an example of a system with anharmonic interactions, where exact results could be compared with various approximation schemes. Furthermore, the integrability of the system makes it interesting for thermodynamical investigations.

In this study certain static and dynamic correlation functions are investigated, using the so-called soliton-gas approximation, where all relevant quantities have, for low temperatures, two independent contributions: one from an ideal gas of solitons on the lattice and the other from quasiharmonic phonons. This approximation has been introduced phenomenologically (Büttner and Mertens 1979, Schneider and Stoll 1980, 1981, Bolterauer and Opper 1981), but certain inaccuracies occurred concerning the momentum or the number of the solitons. Recently a microscopic foundation for the soliton-gas picture has been given (Mertens and Büttner 1981) by using appropriate action-angle variables. Hereby the exact result for the free energy is reproduced and the correct canonical momentum is revealed.

In § 2 the relevant static results for the Toda lattice are reviewed and some new interpretations are given. In § 3 the dynamical correlation function is calculated in the soliton-gas approximation. In § 4 the results are compared with a molecular dynamics simulation (Schneider and Stoll 1980, 1981) and with the results of an approximate analytical method (Diederich 1981a,b); we find that the soliton-gas picture gives a reasonable physical explanation of most of the features in the dynamical correlations.

2. Static properties

Some of the basic results for the Toda lattice are reviewed first. The Hamiltonian for

0305-4470/82/061831+09$02.00

this system with N particles is written as

$$H=\sum_{j=1}^{N}\left[\tfrac{1}{2}p_j^2+V(q_{j+1}-q_j)\right] \tag{1}$$

where

$$V(r_j)=\exp(-r_j)+r_j-1 \tag{2}$$

is the intersite Toda potential. (The Hamiltonian is written in an appropriate scaling, where the length, time and energy units are defined in characteristic parameters of the potential (Toda 1975).) The classical partition function Z at zero pressure is known exactly for this lattice and can be written as

$$(1/N)\ln Z=-\tfrac{1}{2}\ln\beta+\beta(1-\ln\beta)+\ln[\Gamma(\beta)/(2\pi)^{1/2}] \tag{3}$$

with the inverse temperature $\beta=1/T$ and the gamma function $\Gamma(\beta)$. For later comparison the low-temperature expansion is also given:

$$(1/N)\ln Z=\ln T+\tfrac{1}{12}T+\ldots. \tag{4}$$

In order to study the static correlations in this lattice it is quite convenient to use the force–force correlation functions. With the definition

$$e_n=-\partial V/\partial r_n=\exp(-r_n)-1 \tag{5}$$

one calculates the canonical average

$$\langle e_n\rangle=Z^{-1}\int\prod_j \mathrm{d}p_j\,\mathrm{d}q_j\,e_n\exp(-\beta H)=\int \mathrm{d}r\,e_n(r)V(r)\Big/\int \mathrm{d}r\,V(r) \tag{6}$$

and obtains

$$\begin{aligned}&\langle e_n^2\rangle-\langle e_n\rangle^2=\langle(\partial V/\partial r)^2\rangle=\langle(r-V)\,\partial V/\partial r\rangle=\langle r\,\partial V/\partial r\rangle,\\&\langle e_n^2\rangle-\langle e_n\rangle^2=T.\end{aligned} \tag{7}$$

In the last two equations the special properties of the potential $V(r)$ and the virial theorem have been used. From this result, which is the same for the harmonic lattice if we calculate the corresponding averages of the force, one can determine the static correlation function

$$S_{ee}(q)=\frac{1}{N}\sum_{m,n}\mathrm{e}^{iqa(m-n)}(\langle e_m e_n\rangle-\langle e_m\rangle\langle e_n\rangle). \tag{8}$$

Because all the off-diagonal elements vanish, we arrive at the exact result

$$S_{ee}(q)=T \tag{9}$$

which is independent of q. This is by no means a very astonishing result, because the force is related to the virial and therefore the correlation function only depends on thermodynamic variables. Again the same holds for the harmonic lattice (Büttner 1981).

Another nice feature of the Toda lattice is the fact that for this integrable system one explicitly knows the canonical transformation to action-angle variables (Flaschka 1974, McLaughlin 1975, Eilenberger 1981). The Hamiltonian can be written as the sum of phonon and soliton contributions:

$$H=H_{\mathrm{p}}[J(\phi)]+\sum_{\nu=1}^{N_s}H_s(J_\nu) \tag{10}$$

where the first part depends on the continuous action-variable J for the harmonic phonons, and the second part describes the energy of the various ν-soliton solutions. The partition function can correspondingly be written as a product of two contributions

$$Z = Z_p \cdot Z_s. \tag{11}$$

The harmonic part is (Mertens and Büttner 1981)

$$Z_p = T^N \tag{12}$$

and gives the first term in the low-temperature expansion (4). The soliton part is evaluated here in the soliton-gas approximation (Mertens and Büttner 1981). This is easiest after a canonical transformation to position Q_ν and momentum P_ν variables of a single soliton:

$$Z_s = \sum_{N_s=0}^{\infty} \frac{1}{N_s!} \int \prod_{\nu=1}^{N_s} \frac{dP_\nu \, dQ_\nu}{2\pi^2} \exp\left(-\beta \sum_{\nu=1}^{N_s} H_s(P_\nu)\right) \tag{13}$$

$$= \exp \int \frac{dP\, dQ}{2\pi^2} \ln\{1 + \exp[-\beta H_s(P)]\}. \tag{14}$$

(Since all the variables J_ν or P_ν, respectively, must be distinct (Flaschka 1974), multiple occupancy has to be avoided in (13) and leads to the Fermi factor in (14), instead of the Boltzmann factor.)

A similar calculation has been done by Schneider and Stoll (1980, 1981), who started with the same ansatz, but did not use the correct canonical momentum for the soliton and therefore could not reproduce the low-temperature expansion of the exact result (for discussion see Bolterauer and Opper 1981, Mertens and Büttner 1981).

For an explicit calculation of Z_s one has to substitute P by the parameter α in the one-soliton solution

$$e_n = \sinh^2 \alpha \; \mathrm{sech}^2(\alpha n + t \sinh \alpha). \tag{15}$$

Here α is the only parameter and determines all physical properties of the soliton, like momentum, velocity and energy,

$$P = 4(\alpha \cosh \alpha - \sinh \alpha), \tag{16}$$

$$v = (\sinh \alpha)/\alpha, \tag{17}$$

$$E = \sinh(2\alpha) - 2\alpha. \tag{18}$$

The velocity v has been scaled by the lattice parameter a, which is a second length scale, independent of the length unit defined by the anharmonicity parameter of the Toda potential.

The momentum should not be confused with that of the soliton-bearing chain,

$$P_c = \sum_n p_n = 2 \sinh \alpha, \tag{19}$$

which is not the canonical variable conjugate to the centre of mass of the soliton.

The soliton part of the partition function is then calculated for low temperatures by steepest descent and we find

$$(1/N) \ln Z_s = \tfrac{1}{12} T + \ldots \tag{20}$$

which is identical to the leading anharmonic term in the expansion of the exact partition function (4). In the same way the density of solitons is calculated

$$n(\alpha) = (2/\pi^2)\alpha \sinh \alpha[\exp(\beta E)+1]^{-1} \tag{21}$$

and is shown in figure 1. For $T = 0.25$ one may compare this with the results of a molecular dynamical calculation by Schneider and Stoll (1980, 1981), who identified a large number of single solitons with α in the neighbourhood of 0.7.

The total number of solitons is

$$N_s = N(\ln 2/\pi^2)T \tag{22}$$

for low temperatures.

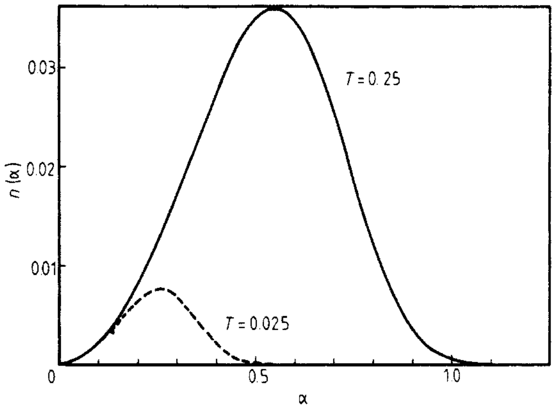

Figure 1. Soliton-number density for two different temperatures.

3. Dynamical properties

The time-dependent force–force correlation is defined by

$$\begin{aligned} S_{ee}(q,t) &= \langle e(-q,t)e(q,0)\rangle, \\ e(q,t) &= \frac{1}{\sqrt{N}}\sum_n e^{iqn}(e_n(t) - \langle e_n\rangle), \end{aligned} \tag{23}$$

where $e_n(t)$ is the general solution of the equation of motion $-\ddot{q}_n = e_n - e_{n-1}$ for the Toda lattice. Since the general solution is not known, only the N_s-soliton solutions $e_n^s(t)$ are considered and thus only the soliton part S_{ee}^s of S_{ee} is calculated. The mean values $\langle e_n^s\rangle$ and $\langle e_m^s(t)e_n^s(0)\rangle$ are defined in this approximation by using the grand canonical ensemble in (13). In the framework of the ideal-gas approximation the N_s-soliton solution can be represented by a sum of N_s single-soliton solutions

$$e_n^s(t) = \sum_{\nu=1}^{N_s} \sinh^2 \alpha_\nu \operatorname{sech}^2 \alpha_\nu(n - Q_\nu + v_\nu t). \tag{24}$$

After a short calculation one finds

$$\langle e_n^s\rangle = \frac{8}{\pi^2}\int_0^\infty d\alpha\, f_\alpha \sinh^3 \alpha \tag{25}$$

where the Fermi factor has been abbreviated by

$$f_\alpha = \ln\{1+\exp[-\beta E(\alpha)]\}. \tag{26}$$

In contrast to the vanishing $\langle e_n\rangle$ in § 2, $\langle e_n^s\rangle$ is positive since the solitons are compressional pulses.

In a similar calculation for the correlation one has

$$\langle e_m^s(t)e_n^s(0)\rangle = \langle e_m^s\rangle\langle e_n^s\rangle + \frac{4}{\pi^2}\int_0^\infty d\alpha\, f_\alpha \alpha \sinh^5\alpha \times \int_{-\infty}^{\infty} dQ\, \operatorname{sech}^2\alpha(m-Q+vt)\operatorname{sech}^2\alpha(n-Q). \tag{27}$$

Though the Q integral could be done at once, it is more convenient first to insert equation (27) into S_{ee}, to replace the Fourier sum by an integral, to substitute $m-Q+vt=y$, and then to perform the y and Q integrations:

$$S_{ee}^s(q,t) = \frac{16}{\pi^2}\int_0^\infty d\alpha\, f_\alpha \frac{\sinh^5\alpha}{\alpha}\frac{(q\pi/2\alpha)^2}{\sinh^2(q\pi/2\alpha)}\exp(-iqvt). \tag{28}$$

At first the static properties are discussed by setting $t=0$. For fixed $q>0$ the asymptotic behaviour for $T\to 0$ is given by

$$S_{ee}^s(q) = S_{ee}^s(q, t=0) \sim \exp(-cq^{3/4}T^{-1/4}) \tag{29}$$

where the unusual exponent is due to the non-analytic behaviour of the integrand for $\alpha\to 0$. This asymptotic region, however, is quite narrow, e.g. for $q=0.1\pi$, T has to be smaller than 0.005. In figure 2 the numerical results for the ratio $S_{ee}^s(q)/S_{ee}(q)$ are shown for two larger temperatures ($T=0.025, 0.25$).

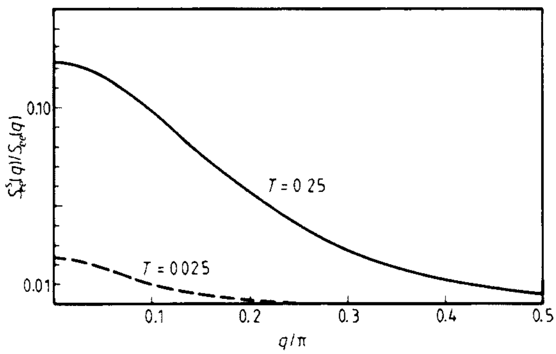

Figure 2. Soliton contribution $S_{ee}^s(q)$ relative to the static correlation function $S_{ee}(q)$.

It is obvious that the soliton contribution to $S_{ee}^s(q)$ is very small for low temperatures. This is in contrast to Schneider and Stoll (1981), who get $S_{ee}^s(q)\sim T$ for $T\to 0$ independent of q, which would mean $S_{ee}^s\sim S_{ee}$ because of (9). But already for the harmonic crystal the force–force correlation is equal to T, and therefore the solitons can produce only small anharmonic effects in the static properties for low temperatures.

The dynamical correlations are described by the Fourier transform of (28)

$$S^{s}_{ee}(q,\omega)=\frac{32}{q\pi}f_{\alpha_0}\frac{\sinh^5\alpha_0}{\alpha_0 v'(\alpha_0)}\frac{(q\pi/2\alpha_0)^2}{\sinh^2(q\pi/2\alpha_0)} \tag{30}$$

where $\alpha_0 \geqslant 0$ is the solution of

$$v(\alpha_0)=\alpha_0^{-1}\sinh\alpha_0=\omega/q. \tag{31}$$

This correlation $S^{s}_{ee}(q,\omega)$ vanishes as a function of ω for $\omega \leqslant q$, increases sharply to a maximum above $\omega = q$, and has an exponential decay for larger ω. In figure 5 on the right the ratio

$$\hat{S}^{s}_{ee}(q,\omega)=S^{s}_{ee}(q,\omega)/S^{s}_{ee}(q) \tag{32}$$

is shown. It is normalised to an area of 2π.

The peak position $\omega_s(q)$ is shown in figure 3 as a function of q. This soliton dispersion is nearly linear and can be very well approximated by

$$\omega_s = q\sinh(\alpha_m)/\alpha_m \tag{33}$$

where α_m is the maximum of the soliton density $n(\alpha)$ in figure 1.

The half-wdith $\Gamma_s(q)$ of S^{s}_{ee} is also linear (see the full line in figure 4).

So far only the soliton part S^{s}_{ee} has been considered. Since the soliton–phonon scattering has been neglected and the phonon part of (10) is harmonic, it is sufficient to treat the phonon contribution S^{p}_{ee} in a quasiharmonic approximation, where the anharmonicities enter only via the temperature-dependent force constant. Using the isothermal sound velocity (Leibfried 1955, Schneider and Stoll 1981) we obtain for

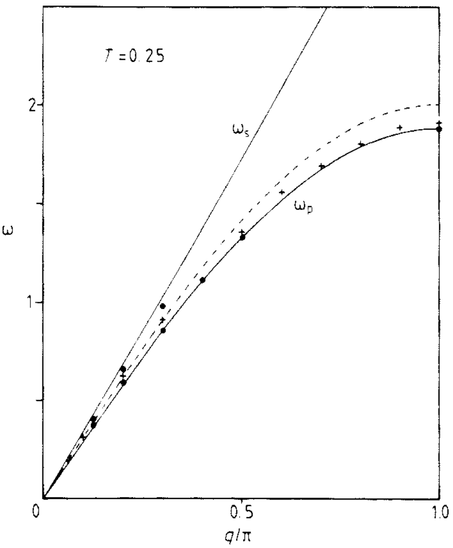

Figure 3. Dispersion of the resonance in $S^{s}_{ee}(q,\omega)$ (full line ω_s); of the quasiharmonic phonons (full line ω_p); of the harmonic phonons (broken line); in $S_{ee}(q,\omega)$ from Diederich (1981b) (full circles); in $S_{ee}(q,\omega)$ from molecular dynamics (crosses) (Schneider and Stoll 1981).

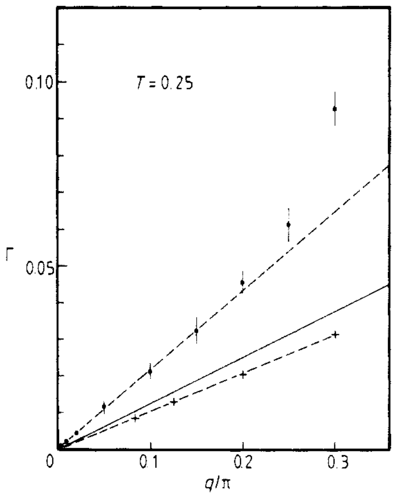

Figure 4. Half-width of the resonance in $S^{s}_{ee}(q,\omega)$ (full line); in the high-frequency part of Diederich's (1981b) $S_{ee}(q,\omega)$ (crosses); in the molecular dynamics results of Schneider and Stoll (1981) for $S_{ee}(q,\omega)$ (circles; the error bars result from our estimating the widths by means of the published drawings).

the dispersion of the peak position (figure 3)

$$\omega_p^2 = (1 - \tfrac{1}{2}T + \ldots)2(1 - \cos q). \tag{34}$$

In a one-dimensional system there is a width of certain dynamical form factors due to multi-phonon processes even in the harmonic approximation. Mikeska (1973) has shown that the density–density correlation function approximately has a Lorentzian shape with a width

$$\Gamma_p = \tfrac{1}{4}Tq^2. \tag{35}$$

As a very rough estimate we have taken this width for S_{ee}^p in figure 5.

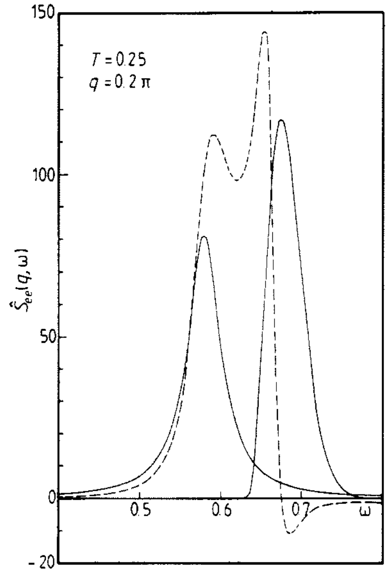

Figure 5. Dynamic correlation function: soliton part $S_{ee}^s(q, \omega)$ on the right and phonon part $S_{ee}^p(q, \omega)$ on the left; the broken line is Diederich's (1981b) total $S_{ee}(q, \omega)$.

4. Discussion

We now want to compare our results with those of related calculations in the literature. Diederich (1981a, b) applies a new approximation scheme to the dynamical equations for the response functions in q space, which are solved numerically. The resulting displacement–displacement correlation function S_{xx} is connected to the force–force correlation S_{ee} by the exact relation (Schneider and Stoll 1981)

$$\omega^4 S_{xx}(q, \omega) = S_{ee}(q, \omega)2(1 - \cos q). \tag{36}$$

For not too low temperatures (e.g. $T = 0.25$) $S_{ee}(q, \omega)$ shows the following structure. For small q there is a single resonance. At somewhat larger q values ($q = 0.1\pi$) a second peak appears on the low-frequency side and becomes more pronounced with increasing q. At still higher q ($q = 0.4\pi$) the high-frequency peak vanishes and only one peak remains. The dispersion of the high-frequency peak is linear (see the circles in figure 3) and follows our soliton dispersion with a deviation of only 4%. The half-wdith of the normalised peak also grows linearly with q (see the crosses in figure 4) and is about 15% smaller than our soliton width $\Gamma_s(q)$. We therefore conclude that the high-frequency peak in S_{ee} is a soliton resonance. (The 15% difference in the width may result from uncertainties in S_{ee} which are indicated e.g. by an overshooting to negative values, see figure 5.) The dispersion of the low-frequency peak is nearly the same as the quasiharmonic dispersion ω_p (figure 3). For not too large q values the half-width is also very well approximated by the harmonic value (35). Moreover, the peak structure is clearly Lorentzian (see figure 5). We therefore interpret the low-frequency peak as the contribution from quasiharmonic phonons.

We now discuss the soliton and phonon contribution relative to the total correlation function S_{ee}. Our results for $S^s_{ee}(q)$ in figure 2 show a decrease with increasing q (this static form factor is the area under $S^s_{ee}(q, \omega)$). We therefore expect a disappearance of the soliton peak with higher q values. It is also expected that the soliton contribution becomes less pronounced for lower temperatures, since there is a drastic decrease in the static form factor with decreasing temperatures (see figure 2). These effects are seen quite clearly in the results of Diederich (1981b). However, there is a quantitative disagreement: the numerical results show a much larger soliton contribution (e.g. at least 50% for small q at $T = 0.25$) than expected from our $S^s_{ee}(q)$, which yields 12% at most for small q values. A possible explanation for this discrepancy might be an enhancement of the soliton form factor by the soliton–phonon interaction (an example for such a coupling is the libron form factor for solid orthohydrogen (Bickermann *et al* 1974)). However, the results of a molecular dynamics calculation of Schneider and Stoll (1980, 1981) indicate that the soliton contribution may be rather small. In this calculation there is only one unresolved resonance structure in S_{ee}. The dispersion curve is for small q slightly above the harmonic value $\omega_h^2 = 2(1 - \cos q)$. With increasing q it follows this dispersion and finally approaches the quasiharmonic value ω_p (crosses in figure 3). Since the harmonic dispersion ω_h is situated between ω_p and ω_s, the resonance in S_{ee} may represent a superposition of a phonon and a soliton contribution, where the latter decreases with increasing q, as seen in figure 2. This interpretation is also supported by the behaviour of the half-wdith, which is linear for small q and nearly two times that of Γ_s (see figure 4).

We summarise that Diederich's (1981b) results as well as the results of the molecular dynamics simulation of Schneider and Stoll (1980, 1981) can be qualitatively understood in our simple soliton-gas picture. For quantitative details it might be necessary to include effects of phonon–soliton scattering.

Acknowledgments

We would like to thank T Schneider, E Stoll and S Diederich for several valuable discussions and preprints of their papers prior to publication.

Note added in proof. Yoshida and Sakuma (1982) included some effects of the soliton–phonon scattering in their calculation of the free energy, but they could not reproduce the exact result.

References

Bickermann A, Biem W and Mertens F G 1974 *Z. Phys.* **267** 31–9
Bolterauer H and Opper M 1981 *Z. Phys.* B **42** 155–61

Büttner H 1981 *Nonlinear Phenomena at Phase Transitions and Instabilities, NATO Adv. Study Inst.* ed T Riste (New York: Plenum)
Büttner H and Mertens F G 1979 *Solid State Commun.* **29** 663–5
Diederich S 1981a *Phys. Rev.* B **24** 3186, 3193
—— 1981b *Phys. Lett.* **86A** 294
Eilenberger G 1981 *Solitons, Springer Series in Solid State Science* vol 19 (Berlin: Springer) § 7
Flaschka H 1974 *Prog. Theor. Phys.* **51** 703
Leibfried G 1955 *Encyclopedia of Physics* vol VII/1 (Berlin: Springer) p 274
McLaughlin D W 1975 *J. Math. Phys.* **16** 96, 1704 (E)
Mertens F G and Büttner H 1981 *Phys. Lett.* **84A** 335–7
Mikeska H J 1973 *Solid State Commun.* **13** 73–6
Schneider T and Stoll E 1980 *Phys. Rev. Lett.* **45** 997–1000
—— 1981 *Phys. Rev.* to be published
Toda M 1967 *J. Phys. Soc. Japan* **22** 431
—— 1975 *Phys. Rep.* **18** 1
Yoshida F and Sakuma T 1982 *Phys. Rev.* A in press