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1989 J. Phys. A: Math. Gen. 22 3095

(http://iopscience.iop.org/0305-4470/22/15/023)

J. Phys. A: Math. Gen. 22 (1989) 3095-3101. Printed in the UK

Finite-temperature excitations of the Toda lattice in the semiclassical regime

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Received 27 January 1989

Abstract. The finite-temperature excitations of a large Toda lattice in the semiclassical regime are analysed using the Bethe ansatz, and a physical interpretation is presented, showing clearly that the lattice phonon excitation corresponds to the Bethe ansatz hole, even in the classical limit at finite temperature. Our method gives a simple derivation of the formulae for excitation energies and momenta, which were first written down by Gruner-Bauer and Mertens from a consistency argument, and it suggests why solitons do not apparently contribute to the Toda lattice free energy.

1. Introduction

Recently, a number of authors [1-5] have examined the problem of finding dispersion curves for excitations in the Toda lattice at finite temperatures. This is an interesting problem because the Toda lattice [6] is fully integrable, having both phonon- and soliton-type excitations, and thus is a soluble, reasonably physical [7], anharmonic one-dimensional system. Similar work has already been done for excitations in the sine-Gordon system where, for example, the temperature dependence of the soliton mass [8] is fairly well understood. The Toda lattice, however, is rather different from the sine-Gordon system in that the soliton is non-topological and there is no mass gap.

The analyses in the literature [1-5] of excitation spectra and thermodynamics for the large quantum Toda lattice are all based on the Bethe ansatz equations. In fact, despite the full integrability of the system, these equations are not precisely correct for the finite (periodic) lattice [9], but we have found they do become exact in the limit of a large lattice, so in this paper we always assume we are looking at a large system. (Actually, the Bethe ansatz analysis misses a fixed fraction of the states of the system [9], but this does not affect our arguments or conclusions here.)

The Bethe ansatz analysis of finite-temperature excitation energies is based on the work of Lieb and Liniger [10] and Yang and Yang [11] on the non-relativistic Bose gas with delta function interaction between particles. For the Bose gas, the interaction gives rise to a wavefunction of a quasifermionic nature in that it is defined in terms of a set of momentum-like variables $\{k_i\}$ which must all be distinct and, for the eigenstates in a system with periodic boundary conditions, each k_i has an associated integer quantum number I_i, corresponding to the total phase winding (kinetic plus phase shift) on moving that particle around the system. The ground state is thus a filled 'Fermi sea' from $-k_F$ to k_F, corresponding to the lowest possible set of these quantum numbers $\{I_i\} \equiv 0, \pm 1, \pm 2, \ldots$, and at zero temperature the excitations are

0305-4470/89/153095+07$02.50

holes in this sea and particles above it. The dispersion curves differ from the free-fermion case because moving one particle in momentum space causes a slight shift in all the other k_i, a 'backflow', renormalising the energy and momentum of the excitation. This renormalisation does not change the qualitative picture of the low-energy excitation structure, which still looks like that of a free-fermion gas. At finite temperatures, the dispersion curves are affected because the backflow now takes place in the thermal equilibrium distribution of k_i rather than the filled Fermi sea but, again, this is a rather minor effect, in that the energy scale is changed somewhat, but the allowed energy levels and occupation probabilities closely correspond to those for the free-fermion gas. In particular, near the Fermi surface there is particle-hole symmetry—at zero temperature, the low-energy ($k \ll k_F$) particle and hole excitations have identical dispersion curves, and for temperatures $T \ll E_F$, particles and holes are thermally excited in equal densities in symmetrical fashion. (Obviously, this is no longer true for excitations with bare momenta of order k_F.)

For the Toda lattice, if we assume it is legitimate to use the Bethe ansatz, a very similar picture emerges. The ground state is again a filled Fermi sea from $-k_F$ to k_F, corresponding to the lowest possible set of the associated quantum numbers, $\{I_i\} \equiv 0, \pm 1, \pm 2, \ldots$. Again, the zero-temperature elementary excitations are holes and particles. However, at this point the analogy ends. There is no particle-hole symmetry. In the classical limit, the particles become solitons, the holes phonons, differing in energy by order $\hbar$. On going to finite temperatures, the momentum space $\{k_i\}$ distribution, which has been computed numerically by Hader and Mertens, is rounded in just the way one expects of a Fermi distribution. Yet this apparent symmetry about a 'Fermi level' is deceptive—in the classical limit, the system must be entirely describable by Boltzmann statistics.

The purpose of the present paper is to try to give a clear physical picture of the Bethe ansatz excitations in the Toda lattice, especially at finite temperature, so that the particle-hole asymmetry is seen to be natural. The first finite-temperature Bethe ansatz analysis of the Toda lattice was given by Theodorakopoulos [5], who set up and solved numerically the standard Yang and Yang [11] integral equation for $\hat{\varepsilon}(p)$, the classical version of the Yang and Yang function $\varepsilon(k)$. The thermodynamic function $\varepsilon(k)$ is defined by $\rho(k)/\rho_h(k) = e^{-\varepsilon(k)/T}$, where $\rho(k)$ is the density of filled states, $\rho_h(k)$ that of empty states, in the neighbourhood of momentum k. In the classical limit at finite temperature, of course, this ratio vanishes as $\hbar$, so $\hat{\varepsilon}$ is defined essentially by subtracting $T \ln \hbar$. From this analysis, Theodorakopoulos concluded that for the semiclassical case excitations were clearly of particle character since so few states were occupied. We believe this statement of his to be only partially correct—the phonon excitations are holes, and this large hole-to-particle ratio just reflects the large number of phonons in each mode near the classical limit. Another attempt at providing a physical interpretation of the Toda lattice Bethe ansatz equations was that of Takayama and Ishikawa [4], who presented a formulation of the equations closely resembling the phenomenological interacting gas model with phonons and solitons. However, as discussed by Gruner-Bauer and Mertens [1], this type of model, based on dividing the excitations into two classes by choosing a finite-temperature Fermi surface, has some unphysical features. Our analysis clarifies some of these points. Gruner-Bauer and Mertens also derived formulae for the finite-temperature excitation energies and momenta in terms of the Bethe ansatz ε function, by approaching the zero-temperature classical limit in two different ways. In this paper, we shall show how these formulae arise very naturally in our interpretation of the Bethe ansatz formalism.

In § 2, we review the zero-temperature Bethe ansatz results for the Toda lattice, then in § 3 we discuss the finite-temperature case, explaining why the particles and holes are in fact physically quite different types of excitation, in contrast to the apparently analogous Bose gas case.

2. Zero-temperature Bethe ansatz analysis for the Toda lattice

The Hamiltonian for the Toda system has the form

$$H=\sum p_i^2+4g\sum e^{2(q_{i+1}-q_i)}. \tag{2.1}$$

It was first observed by Sutherland [12] that, even though the wavefunction cannot be of Bethe ansatz form since the potential has finite extent, the Bethe ansatz equations nevertheless give the correct ground-state energy and low-energy excitation spectra for the infinite Toda lattice in the classical limit. For a dilute Toda gas, the Bethe ansatz wavefunction is correct asymptotically in the region where all particles are well separated. This non-trivial result is a consequence of the factorisability of the scattering matrix. Still, the energy levels are given correctly even when the gas is not dilute and there is no asymptotic region available. The exponential interaction leads to a scattering phase shift derivative

$$\delta'(k)=\sum_{n=1}^{S}\frac{n}{n^2+(k/2)^2} \tag{2.2}$$

where S is defined in terms of the coupling constant g by $g=2S(S+1)$.

The phase shift has this simple form only for the special coupling values corresponding to S integral, otherwise it must be expressed in terms of gamma functions. However, the classical limit is $g\to\infty$, so we can always approach it through integral S values. The phase shift can thus be written in the classical limit

$$\delta'=\tfrac{1}{2}\ln(1+(2S/k)^2). \tag{2.3}$$

The standard Bethe ansatz boundary condition for the quasimomenta

$$k=\frac{2\pi}{L}I(k)+\frac{1}{L}\sum\delta(k-k') \tag{2.4}$$

gives a ground-state density $\rho(k)$ satisfying

$$\frac{1}{2\pi}=\rho(k)+\frac{1}{2\pi}\int_{-k_F}^{k_F}\delta'(k-k')\rho(k')\,dk'. \tag{2.5}$$

Notice that $\delta'(k)$ has a maximum at $k=0$, $\delta'(0)=\Sigma^{s}\,1/n\simeq\ln S$, and δ' falls away as $2S^2/k^2$ for large k^2, a broad delta function with a weight $2\pi S$. This implies that in (2.5) above, the second term on the right-hand side swamps the first for $|k|<k_F$, so the first term can be neglected.

Sutherland [12] solved (2.5) for ρ by replacing $\ln(1+(2S/k)^2)$ with $\ln(2S/k)^2$, dropping the negligible first term on the right-hand side, and then differentiating with respect to k' to get

$$0=\int_{-k_F}^{k_F}\frac{\rho(k')}{k-k'}\,dk' \tag{2.6}$$

with the solution $\rho(k)=C/(k_F^2-k^2)^{1/2}$.

The particle density $d = N/L = \int \rho(k)\, \mathrm{d}k$, so $C = d/\pi$,

$$k_\mathrm{F} = 4S\mathrm{e}^{-1/d}. \tag{2.7}$$

The energy is given by

$$E_0/L = \int k^2 \rho(k)\, \mathrm{d}k = \mathrm{d}k_\mathrm{F}^2/2$$

so

$$E_0/N = 8S^2\,\mathrm{e}^{-2/d} = 4g\,\mathrm{e}^{-2/d}. \tag{2.8}$$

This is the correct value for the infinite Toda lattice. Notice that, in the classical Toda lattice, this is all potential energy, since the particles are at rest, yet here it is formally a sum over kinetic energies, in a part of configuration space the particles do not reach. To realise these momenta, one could take a static Toda lattice of finite length held by walls on an infinite line, remove the walls at its end and let the particles spring apart. The final configuration would be widely separated particles with just this set of momenta. Strictly speaking, as we have noted elsewhere, this result is not quite right for *finite* Toda lattices; the Bethe ansatz result differs from the exact classical ground-state energy by a term of order N^{-2} for an N-particle system.

We turn now to a discussion of the particle and hole excitations above this ground state. Continuing to follow Sutherland's [12] adaptation of the Bose gas analysis of Lieb and Liniger [10], the energy and momentum of the excitation are given by

$$\Delta E(k) = \hbar^2|\varepsilon(k) - \varepsilon(k_\mathrm{F})| \tag{2.9a}$$

$$\Delta K(k) = 2\pi\hbar \int_{k_\mathrm{F}}^{k} \rho(k')\, \mathrm{d}k' \tag{2.9b}$$

where $\varepsilon(k)$ is determined by

$$-\mu + k^2 = \varepsilon(k) - \frac{1}{2\pi}\int_{-k_\mathrm{F}}^{k_\mathrm{F}} \delta'(k-k')\, \mathrm{d}k' \tag{2.10}$$

μ being the chemical potential.

Following precisely the same steps as those after equation (2.5) gives the Hilbert transform for $\varepsilon(k)$

$$2k = \frac{1}{2\pi}\int_{-k_\mathrm{F}}^{k_\mathrm{F}} \frac{\varepsilon(k')}{k-k'}\, \mathrm{d}k' \tag{2.11}$$

yielding

$$\varepsilon(k) = -4\sqrt{k_\mathrm{F}^2 - k^2}.$$

This gives two dispersion curves.

Type I, holes: $|k| < k_\mathrm{F}$, $k = k_\mathrm{F}\cos\theta$:

$$\begin{aligned} \Delta K &= 2\hbar\, \mathrm{d}\theta \\ \Delta E &= 4\sqrt{k_\mathrm{F}^2 - k^2} = 4\hbar^2 k_\mathrm{F}|\sin\theta|. \end{aligned} \tag{2.12}$$

Type II, particles: $|k| > k_\mathrm{F}$, $k = k_\mathrm{F}\cosh\phi$;

$$\begin{aligned} \Delta K &= \hbar\mathrm{d}k_\mathrm{F}(\phi\cosh\phi - \sinh\phi) \\ \Delta E &= \hbar^2 k_\mathrm{F}^2|\cosh\phi\sinh\phi - \phi|. \end{aligned} \tag{2.13}$$

The point we wish to emphasise with this rather lengthy recapitulation is that in the semiclassical regime, where k_F is of order $\hbar^{-1}$, the $\hbar$ factors cancel for particle-like excitations but not for hole-like excitations. Why is this system so different in this respect from the Bose gas? One might first think that the singularity in the density of states at the Fermi surface is leading to singular backflow effects, renormalising particles and holes in a different way. However, we shall see that this not the explanation.

The resolution to the paradox becomes apparent if we consider a finite Toda system, N particles, say, with periodic boundary conditions, and N sufficiently large that the errors in the Bethe ansatz approach mentioned earlier [9] are negligible. Even with N finite, we can still of course take the classical limit in which the phonon (hole) energy becomes vanishingly small compared with the soliton (particle) energy, so the problem is still there. Of course, the ground-state momentum distribution is now a sequence of N points in k space, in fact the solution of (2.4), taking the quantum number $I(k)$ to be integer from $-(N-1)/2$ to $(N-1)/2$, assuming N odd. For reasonably large N, the k_i will distribute themselves close to the $C(k_F^2-k^2)^{-1/2}$ distribution, and the ground-state energy will be $\Sigma\, p_i^2=\hbar^2\,\Sigma\, k_i^2$. From (2.8) above, this is a macroscopic quantity, and so the p_i are finite in the classical limit—and all the k_i are infinite, of order $\hbar^{-1}$. Sutherland's neglect of the finite term in (2.5) is equivalent to neglecting the integers in (2.4).

We can now see the essential difference between particles and holes. Let us begin by considering a hole excitation in the ground state. This means in terms of the quantum numbers that some n ($n<(N-1)/2$) is missing and there is an extra quantum number at $(N+1)/2$, say. How does this affect the k_i distribution? To leading order, it does not affect it at all because, as we have just argued, the integers are negligible in (2.4)! Thus the effect is of order $\hbar$, a slight shift to the right for k_n, and at the same time some shifts in the other k_i. Since there are a finite number N of these, this remains a quantum (order $\hbar$) effect. Thus in terms of the k_i distribution, the hole excitation does not look like a missing k_i—it looks like a very slightly enlarged gap.

The point to be emphasised here is that in the classical limit the *phase shifts* between particles become infinite, of order $\hbar^{-1}$. Thus the relative phase shifting, not the sequence of quantum numbers, is the major determinant of the configuration of k_i in the ground state. In contrast, for the Bose gas analysis of Lieb and Liniger, the interval between adjacent k_i in the ground state is largely determined by the *quantum number* difference, so a single hole excitation corresponds to a gap between adjacent filled k_i close to twice the interval in the ground state.

For the particle distribution, if the excitation from the ground state is created by shifting the quantum number $N/2$ to $N/2+n$, with n finite, then in the classical limit the excitation energy again goes to zero. But the particle excitation is actually defined by making a *finite* momentum change in the top p_i ($\simeq\hbar k_F$) which in the classical limit implies an infinite n. The p_i are classical momenta of the Toda particles, so naturally this is a macroscopic excitation.

3. Finite-temperature excitations of the Toda lattice

Yang and Yang define the function $\varepsilon(k)$ in terms of the local densities of filled and empty states in thermal equilibrium

$$\rho(k)/\rho_h(k)=e^{-\varepsilon(k)/T}. \tag{3.1}$$

Minimising the free energy leads to the well known integral equation for $\varepsilon(k)$,

$$-\mu+k^2=\varepsilon(k)+\frac{T}{2\pi}\int_{-\infty}^{\infty}\delta'(k-k')\ln(1+\mathrm{e}^{-\varepsilon(k')/T})\,\mathrm{d}k'. \tag{3.2}$$

In the limit $T\to 0$ this gives (2.10) above.

The classical limit of this equation is given by noting that at finite temperatures Boltzmann statistics are appropriate, $\rho/\rho_{\mathrm{h}}\ll 1$, and so

$$-\mu+k^2=\varepsilon(k)+\frac{T}{2\pi}\int_{-\infty}^{\infty}\delta'(k-k')\,\mathrm{e}^{-\varepsilon(k')/T}\,\mathrm{d}k'. \tag{3.3}$$

This is the equation solved by Theodorakopoulos.

For the Bose gas, described by equation (3.2) (but with the appropriate phase shift) Yang and Yang argued that even at finite temperature it is reasonable to define excitations above the thermal equilibrium state in a way analogous to (2.12) above, except that now there is no natural base line fermion energy, so an excitation is one particle plus one hole, generated by moving a single quantum number from I to I' corresponding to a bare quasimomentum shift from k to k', say. The resulting excitation does have an explicit two-component form, the energy is $\varepsilon(k')-\varepsilon(k)$, and the momentum can be written analogously. Consequently, the term 'excitation energy' is often used for $\varepsilon(k)$ alone.

This whole Yang and Yang analysis has been taken and applied to the finite-temperature Toda lattice, but the interpretation of $\varepsilon(k)$ in terms of the known Toda excitations in the classical limit has been unclear. As we mentioned in the introduction, there are some important differences between the Bose gas and the Toda lattice, despite the formal similarity. One way to illuminate the difference is to look separately at the quantum number distributions $\{I_i\}$ and the quasimomentum distributions $\{k_i\}$ for the two cases. At zero temperature, as discussed above, the ground state of the Bose gas has $\{I_i\}=0, \pm1, \pm2, \ldots$ to $\pm I_{\max}$, the corresponding k_i also fill a sea to a maximum momentum $\hbar k_{\mathrm{F}}$ of order $N\hbar$, for N particles in a system of unit length. For the Toda lattice, the $\{I_i\}$ distribution is again $0, \pm1, \pm2, \ldots$ and the k_i fill a sea, but this time the maximum sea momentum $\hbar k_{\mathrm{F}}$ is macroscopic—on the quantum scale, the k_i are spread far apart by the macroscopic phase shifts. At finite temperatures, for the Bose gas, the $\{I_i\}$ and $\{k_i\}$ distributions look very similar—they look like typical Fermi distributions, and the hole and particle distributions are very like those for a free Fermi gas. For the semiclassical Toda lattice, on the other hand, these two distributions behave quite differently. In the classical limit, at any finite temperature the quantum number distribution $\{I_i\}$ necessarily goes to the classical Boltzmann distribution. This means the Fermi sea evaporates instantly on heating, and the I_i have vast distances between them. In contrast, the $\{k_i\}$ distribution at finite temperature looks like the $\{k_i\}$ distribution at zero temperature, rounded off a little. It looks like a typical heated Fermi sea, but it is not. The phonons are the holes in the I_i distribution; that is to say the number of states between neighbouring I_i, i.e. $I_{i+1}-I_i-1$, is the occupation number of that particular phonon mode, of order $\hbar^{-1}$ in the classical limit. This causes a macroscopic speading of the k_i, but they were already (at zero temperature) macroscopically spread by the phase shifts, also of order $\hbar^{-1}$. Thus the rounding of the apparent 'Fermi sea' is a completely macroscopic phenomenon!

It is not difficult to understand the result of Gruner-Bauer and Mertens [1] in terms of this picture. By taking the classical zero-temperature limit in two different ways, they find the phonon energy ε_{ph} to be given in terms of the 'excitation energy' ε by

$$\varepsilon_{ph} = kT e^{-\beta\varepsilon}. \tag{3.4}$$

Since $e^{-\beta\varepsilon} = \rho/\rho_h$, and the phonon occupation per mode, from the argument above, is just ρ_h/ρ, (3.4) is merely the statement of equipartition of energy.

It is easy to verify in more detail that this interpretation is correct. In the Bethe ansatz formulation, a phonon is created at k_j by moving all I_i for $i>j$ to I_i+1. This yields

$$\Delta E = \sum_{i>j} [\varepsilon(I_i+1) - \varepsilon(I_i)] = \int d\varepsilon(k)\rho/\rho_h = \int e^{-\beta\varepsilon(k)}\, d\varepsilon(k) = \beta^{-1} e^{-\beta\varepsilon(k)}$$

$$\Delta P = \sum_{i>j} [h(I_i+1) - h(I_i)] = \int dh\rho/\rho_h = \int \rho(k)\, dk$$

where $h(I_i)$ is the number of integers less than I_i measured from an appropriate baseline. These are just the formulae of Gruner-Bauer and Mertens for phonons.

It is clearly not easy to separate out the soliton and phonon excitations at finite temperatures. A single k_i far above the rest would of course be a soliton, but the thermal equilibrium distribution has a smoothly decreasing density of k_i out to infinite k in the limit of a large system. Thus one can write down a free energy as an integral over k space simply in terms of the phonon modes between occupied k_i. We believe this explains why attempts to formulate the free energy as a sum of phonon and soliton contributions have not met with much success.

Acknowledgment

The authors would like to thank Holger Frahm for useful discussions of this topic.

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