PHYSICAL REVIEW B VOLUME 45, NUMBER 17 1 MAY 1992-I

Thermodynamics and correlations of the quantum Toda lattice

A. Cuccoli, M. Spicci, and V. Tognetti
Dipartimento di Fisica dell'Università di Firenze, Largo E. Fermi 2, I-50125 Firenze, Italy

R. Vaia
Istituto di Elettronica Quantistica del Consiglio Nazionale delle Ricerche, Via Panciatichi 56/30, I-50127 Firenze, Italy

(Received 16 January 1992)

The aim of the explicit evaluation of the equilibrium thermodynamic properties of the quantum Toda lattice is here reached by a method which reduces the evaluation of quantum statistical averages to a classical configurational integral. This is done by constructing an effective potential of the same form as the original one, whose parameters are renormalized by the quantum fluctuations. In addition to quantum specific heat (in agreement with Bethe ansatz calculations), explicit results for meaningful static correlation functions are reported.

The one-dimensional lattice with nearest-neighbor exponential interaction,[1-3] also known as the Toda lattice, has been widely studied in recent years.[4-15] Its main distinctive feature is that it is exactly solvable both in the classical and in the quantum regime, and the exact integrability is associated with a realistic interaction potential. Indeed the Toda lattice can either be assumed as a model for complex physical systems like, for example, the DNA molecule,[14,15] or it can be used to mimic the behavior of other nonlinear, more complicated, pairwise potentials, like the Lennard-Jones ones.

The problem of the classical dynamics of the model was already solved by Toda,[1,2,16] and the macroscopic thermodynamic properties of the classical system can be obtained in terms of the Euler Γ function and its derivatives.[4] Despite the full integrability, which has been shown by an algebraic method[17] and by quantum inverse scattering,[9] a complete, *explicit* solution for the quantum system is still lacking. Only global quantum thermodynamic quantities have been obtained by the Bethe ansatz.[10-12] However, the validity of such approaches for finding the exact energy eigenvalues cannot be proven in a rigorous way. Moreover, it has been recently shown that even though periodic boundary conditions are applied, the Bethe ansatz gives definitely incorrect results for the energy levels of finite quantum chains.[13]

In this paper we will present explicit results for the equilibrium thermodynamic properties of the quantum Toda lattice. They are obtained by reducing the evaluation of quantum statistical averages to classical configuration integrals through the introduction of an approximate effective potential. This procedure, already successfully applied to other nonlinear systems,[18-23] allows us not only to reproduce very easily the results of the much more cumbersome Bethe ansatz calculation for the thermodynamic quantities, but we are also able to evaluate quantum static correlation functions, showing peculiar quantum effects.

The Toda lattice models a chain of N distinguishable particles of mass m described by the Hamiltonian

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \left[\frac{\hat{p}_i^2}{2m} + v(\hat{x}_i - \hat{x}_{i-1}) \right] , \qquad (1)$$

where the nearest-neighbor interaction potential v is

$$v(r) = \frac{a}{b} \left[e^{-b(r-r_0)} - 1 \right] + a(r-r_0) . \qquad (2)$$

The constant b is a measure of the nonlinearity of the potential, while the ratio a/b sets the energy scale. The position r_0 of the minimum of $v(r)$, represents the equilibrium distance of two adjacent particles at zero temperature and zero pressure in the classical system. The characteristic frequency $\omega_0 = [v''(r_0)/m]^{1/2} = (ab/m)^{1/2}$ is used to define the coupling parameter $g \equiv (\hbar\omega_0)/(2a/b) = (\hbar b^{3/2})/(2\sqrt{am})$, which rules the strength of the quantum effects. We will consider the thermodynamic limit $N \to \infty$, and $L \to \infty$ with $d = L/N$ held constant, L being the total length of the chain; periodic boundary conditions are applied.

The goal of reducing to configurational integrals the evaluation of quantum statistical averages and thermodynamic functions, at the equilibrium temperature $T = 1/k_B\beta$, is achieved when an explicit expression for the matrix elements $\rho(\mathbf{X}',\mathbf{X}) = \langle \mathbf{X}' | \hat{\rho} | \mathbf{X} \rangle$ of the density operator $\hat{\rho} = e^{-\beta\hat{\mathcal{H}}}$ is obtained. Indeed, for every $p-x$ ordered[24] operator $\hat{A} \equiv A(\hat{\mathbf{p}},\hat{\mathbf{x}})$ $(\hat{\mathbf{p}} = \{\hat{p}_i\},\ \hat{\mathbf{x}} = \{\hat{x}_i\})$, we can write

$$\langle \hat{A} \rangle = \frac{1}{Z} \int d\mathbf{X}\, A(i\hbar\partial_{\mathbf{z}}, \mathbf{X} - \tfrac{1}{2}\mathbf{z}) \rho(\mathbf{X} - \tfrac{1}{2}\mathbf{z}, \mathbf{X} + \tfrac{1}{2}\mathbf{z}) \Big|_{\mathbf{z}=0} , \qquad (3)$$

where Z is the partition function.

Treating the pure quantum part of the fluctuations in the self-consistent Gaussian approximation, one can obtain the following expression for the density matrix:[25]

$$\rho(\mathbf{X}-\tfrac{1}{2}\mathbf{z},\mathbf{X}+\tfrac{1}{2}\mathbf{z})=\left(\frac{m}{2\pi\hbar^2\beta}\right)^{N/2}\int d\mathbf{x}\,e^{-\beta V_G(\mathbf{x})}\prod_k \exp\left[\frac{1}{2\hbar^2}\left(\gamma_k(\mathbf{x})+\frac{m}{\beta}\right)z_k^2\right]$$
$$\times\prod_k\frac{1}{[2\pi\alpha_k(\mathbf{x})]^{1/2}}\exp\left(-\frac{1}{2\alpha_k(\mathbf{x})}(X_k-x_k)^2\right). \qquad (4)$$

Here and in the following the subscript k denotes variables transformed by the orthogonal matrix $\mathbf{U}(\mathbf{x})=\{U_{ki}(\mathbf{x})\}$, which diagonalizes the frequency matrix

$$\omega_{ij}^2(\mathbf{x})=\frac{1}{m}\left\langle\frac{\partial^2 V}{\partial x_i\partial x_j}(\mathbf{x}+\boldsymbol{\xi})\right\rangle_{\mathbf{x}}, \qquad (5)$$

whose eigenvalues are $\omega_k(\mathbf{x})$. In Eq. (5) we have introduced the notation $\langle f(\boldsymbol{\xi})\rangle_{\mathbf{x}}$ for the ($\mathbf{x}$-dependent) Gaussian average over the *pure quantum fluctuation* variables $\boldsymbol{\xi}=\{\xi_i\}$, defined by

$$\langle f(\boldsymbol{\xi})\rangle_{\mathbf{x}}\equiv\int d\boldsymbol{\xi}\,f(\boldsymbol{\xi})\prod_k\frac{\exp[-\xi_k^2/2\alpha_k(\mathbf{x})]}{[2\pi\alpha_k(\mathbf{x})]^{1/2}}, \qquad (6)$$

where $\xi_k=U_{ki}\xi_i$. The parameters

$$\alpha_k(\mathbf{x})\equiv\frac{\hbar}{2m\omega_k(\mathbf{x})}\left(\coth f_k(\mathbf{x})-\frac{1}{f_k(\mathbf{x})}\right) \qquad (7)$$

and

$$\gamma_k(\mathbf{x})\equiv m^2\omega_k^2(\mathbf{x})\alpha_k(\mathbf{x}), \qquad (8)$$

are respectively the pure quantum quadratic average fluctuations of position and momemtum for a harmonic oscillator of frequency $\omega_k(\mathbf{x})$ and $f_k(\mathbf{x})=\frac{1}{2}\beta\hbar\omega_k(\mathbf{x})$. Finally, the effective potential $V_G(\mathbf{x})$ is given by

$$V_G(\mathbf{x})=\langle V(\mathbf{x}+\boldsymbol{\xi})\rangle_{\mathbf{x}}-\frac{1}{2}\sum_{ij}\alpha_{ij}(\mathbf{x})\left\langle\frac{\partial^2 V}{\partial x_i\partial x_j}(\mathbf{x}+\boldsymbol{\xi})\right\rangle_{\mathbf{x}}$$
$$+\frac{1}{\beta}\sum_k\ln\frac{\sinh f_k(\mathbf{x})}{f_k(\mathbf{x})}, \qquad (9)$$

and the expression for the partition function simplifies to

$$Z=e^{-\beta F}=\left(\frac{m}{2\pi\hbar^2\beta}\right)^{N/2}\int d\mathbf{x}\,e^{-\beta V_G(\mathbf{x})}. \qquad (10)$$

When the quantum effects of nonlinearity are small, a low coupling approximation (LCA) can be introduced,[18] which removes the implicit dependence on $\mathbf{x}$ of the renormalization parameters.[20,25] For the system we are interested in, we thus obtain

$$V_G(\mathbf{x})=\sum_{i=1}^{N}v_{\rm eff}(x_i-x_{i-1}), \qquad (11)$$

where

$$v_{\rm eff}(r)=\frac{a}{b}e^{Db^2/2}e^{-b(r-r_0)}+a(r-r_0)$$
$$-\frac{a}{b}\left(1+\frac{Db^2}{2}e^{Db^2/2}e^{-b(d-r_0)}\right)+H. \qquad (12)$$

In the last formula

$$H=(N\beta)^{-1}\sum_k(\ln\sinh f_k-\ln f_k) \qquad (13)$$

is the term which restores the quantum behavior of the harmonic excitations, and

$$D=N^{-1}\sum_k 4\sin^2(kd/2)\alpha_k \qquad (14)$$

is a renormalization parameter typical of a one-dimensional system with nearest-neighbor interaction only. Both H and D in Eq. (12) are evaluated starting from the eigenvalues $\omega_k\equiv\omega_k(\mathbf{x}_0)$ of the matrix (5), where $\mathbf{x}_0$ is the configuration corresponding to the self-consistent absolute minimum of the effective potential subjected to the constraint of fixed length or fixed pressure. Due to the translational invariance of the system, such configuration corresponds to a uniform spacing of the atoms with lattice constant d, so that the transformation $\mathbf{U}$ reduces to a space Fourier transformation. We note also that $Db^2/2\ll 1$ is a consistency test for the validity of the LCA.

The effective potential (12) can also be rewritten in the form

$$v_{\rm eff}(r)=\frac{a'}{b}\left(e^{-b(r-r_0)}-1\right)+a'(r-r_0)+p'r+C, \qquad (15)$$

by defining the new renormalized constants

$$a'=ae^{Db^2/2},\quad p'=a(1-e^{Db^2/2}), \qquad (16)$$

$$C=ar_0(e^{Db^2/2}-1)$$
$$-\frac{a}{b}\left(1-e^{Db^2/2}+\frac{Db^2}{2}e^{Db^2/2}e^{-b(d-r_0)}\right)+H. \qquad (17)$$

Once the effective potential has been obtained, the standard procedure for classical chains described in Ref. 26 can be used to evaluate the thermodynamic functions and statistical averages. The final result for the quantum specific heat at constant length is

$$c=k_B\left\{\frac{1}{2}+\zeta-\frac{1}{\psi'(\zeta)}-\frac{TH_{TT}}{k_B}+b^2T\left(\frac{1}{\psi'(\zeta)}-\zeta\right)D_T+\frac{b^2T^2}{2}\left[\frac{a'}{bk_BT}e^{-b(d-r_0)}\left(1+\frac{Db^2}{2}\right)-\zeta\right]D_{TT}\right.$$
$$\left.+\frac{b^4T^2}{4}\left[\frac{a'}{bk_BT}e^{-b(d-r_0)}\left(2+\frac{Db^2}{2}\right)-\frac{1}{\psi'(\zeta)}\right]D_T^2\right\}, \qquad (18)$$

where the subscripts T denote derivatives in respect to the temperature, ψ' is the derivative of the digamma function, and

ζ is the solution of the saddle-point condition

$$d = r_0 - \frac{1}{b}\left[\ln\left(\frac{bk_BT}{a'}\right) + \psi(\zeta)\right] \tag{19}$$

for the integral (10).

In Fig. 1 we report the specific heat as a function of the reduced temperature $t = bk_BT/2a$ for some values of the quantum coupling g, together with the results for the same quantity obtained by Hader and Mertens[11] by the Bethe ansatz for $g = 0.5$. The overall agreement between both approaches confirms the validity of these data. From the figure it is clearly seen that quantum harmonic features are dominant only at lowest temperatures, while in the intermediate region, whose width increases with the coupling, both quantum and nonlinear effects play an important role. Eventually, the classical behavior is approached at highest temperatures.

At difference with the Bethe ansatz method, we also are able to compute static correlation functions of the quantum Toda lattice through Eqs. (3) and (4). Here we explicitly consider the position-position, $C_{xx}(n)$, and displacement-displacement, $C_{rr}(n)$, quantum correlation functions, defined by

$$C_{xx}(n) = \langle (x_{i+n} - x_i - nd)^2 \rangle \tag{20}$$

and

$$C_{rr}(n) = \langle (r_{i+n} - d)(r_i - d) \rangle , \tag{21}$$

$r_i = x_{i+1} - x_i$ being the distance between two adjacent particles. Such functions, already studied in the classical dynamical case,[5,6,8] are symmetric functions of n, and can be easily related with the correlation function of the density fluctuations and with the force-force correlation, respectively.

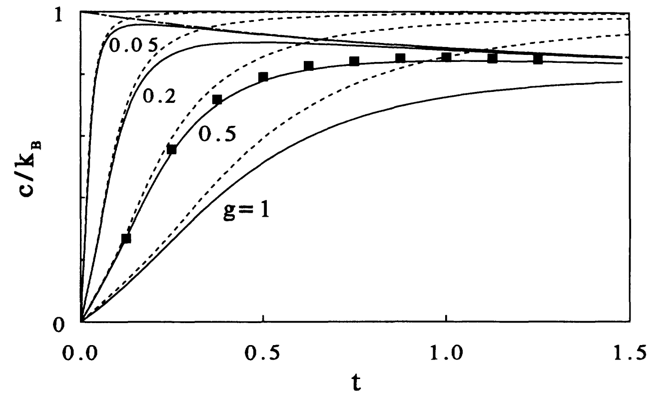

FIG. 1. Specific heat per particle at constant length of the Toda lattice vs the reduced temperature t (see text). The dot-dashed line is the classical result; the solid lines are the quantum results for the value of g showed beside, and the dashed lines are the harmonic approximation for the same value of g. The solid squares are the Bethe ansatz results (Ref. 11) for $g = 0.5$.

The LCA expression for the average of functions depending only on the configuration $\mathbf{x}$ and translationally invariant when evaluated in $\mathbf{x}_0$ can be obtained by[25]

$$\langle A(\mathbf{x}) \rangle = \langle A(\mathbf{x}) \rangle_G + \frac{1}{2N}\sum_k \left[\alpha_k + \delta_k \left(\frac{\langle v''(x)\rangle_G - v''(d)}{v''_{\mathrm{eff}}(d)}\right)\right] A_k , \tag{22}$$

where $A_k = \sum_{i,j} U_{ki} U_{kj} A_{ij}(\mathbf{x}_0)$ is the spatial Fourier transform of $A_{ij}(\mathbf{x}_0) = [\partial^2 A(\mathbf{x})/\partial x_i \partial x_j]_{\mathbf{x}=\mathbf{x}_0}$,

$$\delta_k = \frac{\omega_k}{2}\frac{\partial \alpha_k}{\partial \omega_k} = -\frac{\hbar}{4m\omega_k}\left(\coth f_k + \frac{f_k}{\sinh^2 f_k} - \frac{2}{f_k}\right) , \tag{23}$$

and we have denoted with $\langle \cdots \rangle_G$ the configurational average

$$\langle \cdots \rangle_G = \frac{1}{Z}\int d\mathbf{x} (\cdots) e^{-\beta V_G(\mathbf{x})} . \tag{24}$$

The final expressions we obtain for the two correlation functions for $n \geq 0$ are therefore

$$C_{xx}(n) = \frac{1}{b^2}\left(n\psi'(\zeta) + \frac{2b^2}{N}\sum_k (\alpha_k + W\delta_k)[1 - \cos(nkd)]\right) \tag{25}$$

and

$$C_{rr}(n) = \frac{1}{2b^2}\left[[(n+1) + |n-1| - 2n]\psi'(\zeta) + \frac{8b^2}{N}\sum_k (\alpha_k + W\delta_k)\sin^2\left(\frac{kd}{2}\right)\cos(nkd)\right] , \tag{26}$$

where the constant W is given by

$$W = e^{-Db^2/2}\left(\zeta \frac{bk_BT}{a'} e^{b(d-r_0)} - 1\right) . \tag{27}$$

We can observe that the terms in Eqs. (25) and (26) involving the digamma function corresponds to the classical results, although calculated with renormalized parameters, whereas the additional terms are of purely quantum origin.

In Fig. 2 we report $C_{xx}(n=1)$ as a function of the reduced temperature for $g = 0.5$ and $d = r_0$, together with the results for the same quantity for the classical Toda chain. The corresponding curves in the harmonic approximation are also plotted, showing the relevance of both the quantum and the nonlinear effects. For increasing values of n, the quantum contribution to the correlation function $C_{xx}(n)$ tends towards a constant value (which becomes smaller and smaller as the temperature is raised), so that the behavior of $C_{xx}(n)$ is soon ruled out by the first term of the right-hand side of Eq. (25), and it displays the same

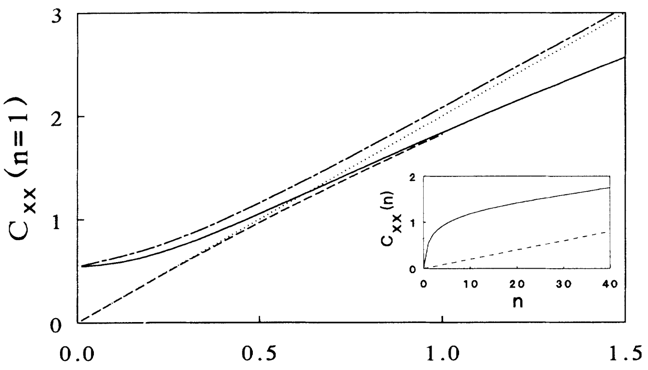

FIG. 2. Position-position correlation function $C_{xx}(n=1)$ for $g=0.5$ vs the reduced temperature t (see text). The units of the y axis are $1/b^2$. Solid line, quantum Toda chain; dash-dotted line, quantum harmonic chain; dashed line, classical Toda chain; dotted line, classical harmonic chain. In the inset $C_{xx}(n)$ at $t=0.01$ is plotted vs the lattice site n.

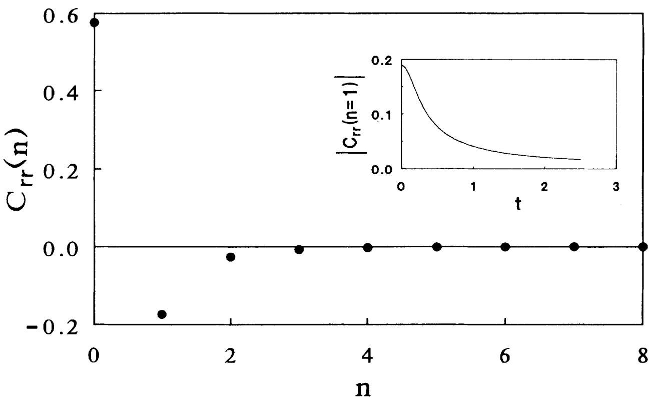

FIG. 3. Displacement-displacement correlation function $C_{rr}(n)$ for $g=0.5$ vs the lattice site n at $t=0.1$ (see text). The units of the y axis are $1/b^2$. In the inset the absolute value of $C_{rr}(n=1)$ as a function of the reduced temperature is plotted.

linear growth (generally with a different slope, due to the quantum renormalization) of the classical correlation function, as it is shown in the inset of Fig. 2. Only for low values of n and for low temperatures, the classical and quantum behavior are significantly different.

For the displacement-displacement correlation function $C_{rr}(n)$, the quantum corrections do affect more strongly the dependence on n, because the first term on the right-hand side of Eq. (26) is not zero for $n=0$, so that $C_{rr}(n)$ for $n \neq 0$ has an entirely quantum origin. Figure 3 shows $C_{rr}(n)$ for the Toda lattice, for $g=0.5$ and $t=0.1$ and in the inset $C_{rr}(n=1)$ is reported as a function of temperature. We notice that, within the LCA, the nonlinear contribution to $C_{rr}(n=1)$ only arises from the term proportional to W, and for the Toda potential W tends to 0 not only for $t \to 0$, but also for $t \to \infty$, so that $C_{rr}(n=1)$ differs from the corresponding correlation function of a purely harmonic chain only for intermediate temperatures.

Equations (3) and (4) also allow us to evaluate averages of functions depending on both **x** and **p**; typical quantities are the frequency moments of the spectral shape. Work is in progress in this direction in order to approach the dynamical correlations.

Useful discussions with Professor A. R. Bishop are gratefully acknowledged.

---

[1] M. Toda, J. Phys. Soc. Jpn. **22**, 431 (1967).

[2] M. Toda, J. Phys. Soc. Jpn. **23**, 501 (1967).

[3] M. Toda, *Theory of Nonlinear Lattices* (Springer, Berlin, 1981).

[4] M. Toda and N. Saitoh, J. Phys. Soc. Jpn. **52**, 3703 (1983).

[5] T. Schneider and E. Stoll, Phys. Rev. Lett. **45**, 997 (1980).

[6] S. Diederich, Phys. Rev. B **24**, 3186 (1980); **24**, 3193 (1980).

[7] S. Diederich, Phys. Lett. **85A**, 233 (1981).

[8] S. Diederich, Phys. Lett. **86A**, 294 (1981).

[9] E. K. Sklyanin, in *Non-Linear Equations in Classical and Quantum Field Theory*, edited by N. Sanchez (Springer, Berlin, 1983).

[10] F. G. Mertens, Z. Phys. B **55**, 353 (1984).

[11] M. Hader and F. G. Mertens, J. Phys. A **19**, 1913 (1986).

[12] R. Fowler and Nai-Chang Yu, J. Phys. A **22**, 3095 (1989).

[13] R. Fowler and H. Frahm, Phys. Rev. B **39**, 11 800 (1989).

[14] A. Muto, A. C. Scott, and P. L. Christiansen, Phys. Lett. A **136**, 33 (1989).

[15] A. Muto, A. C. Scott, and P. L. Christiansen, Physica D **44**, 75 (1990).

[16] M. Toda, Prog. Theor. Phys. Suppl. **45**, 174 (1970).

[17] M. A. Olshanetsky and A. M. Perelomov, Lett. Math. Phys. **2**, 7 (1977).

[18] R. Giachetti and V. Tognetti, Phys. Rev. B **33**, 7647 (1986).

[19] R. Giachetti, V. Tognetti, and R. Vaia, Phys. Rev. A **38**, 1521 (1988).

[20] A. Cuccoli, V. Tognetti, and R. Vaia, Phys. Rev. B **41**, 9588 (1990).

[21] A. Cuccoli, A. Macchi, M. Neumann, V. Tognetti, and R. Vaia, Phys. Rev. B **45**, 2088 (1992).

[22] S. Liu, G. K. Horton, and E. R. Cowley, Phys. Lett. A **152**, 79 (1990).

[23] A. Cuccoli, V. Tognetti, P. Verrucchi, and R. Vaia, Phys. Rev. B **44**, 903 (1991).

[24] F. A. Berezin, Usp. Fiz. Nauk **132**, 497 (1980) [Sov. Phys. Usp. **23**, 763 (1980)].

[25] A. Cuccoli, A. A. Maradudin, A. R. McGurn, V. Tognetti, and R. Vaia (unpublished).

[26] A. Cuccoli, V. Tognetti, and R. Vaia, Phys. Lett. A **160**, 184 (1991).