PHYSICAL REVIEW A VOLUME 17, NUMBER 3 MARCH 1978

The sine-Gordon chain: Equilibrium statistical mechanics

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(Received 19 September 1977)

The equilibrium statistical mechanics of the sine-Gordon chain is studied using transfer-integral techniques. Implementation of formally exact expressions for the free energy, equilibrium averages, etc., rests upon solution of the transfer-integral (TI) problem. Away from the continuum limit the solution to the TI problem contains features that must be examined with some care. Several approximate schemes for solving the TI problem are described and subjected to numerical verification. The appropriate thermodynamic variables for describing the sine-Gordon chain are found to be temperature and phase; the mechanical variable conjugate to phase is torque. Examination of the Helmholtz free energy, torque, equilibrium averages, etc., shows that as $T \to 0^+$ the chain with nonzero phase is described by a gas of noninteracting solitons. At $T = 0$°K the chain with nonzero phase corresponds to a kink lattice. At $T = 0^+$ this lattice "melts" although the phase evolution continues to occur locally on the chain as solitons.

I. INTRODUCTION

In their pioneering work on the ϕ^4 system Krumhansl and Schrieffer[1] (KS) suggested that the low-temperature statistical mechanics of systems that admit the possibility of solitary waves (or solitons) might be described by the superposition of two essentially independent kinds of modes of motion; the conventional small oscillation modes (or phonons) and the solitary wave modes or solitons (KS made an explicit demonstration of this suggestion for ϕ^4). This suggestion has proved very fruitful in a phenomenologic description of many aspects of displacive transitions,[2] in the discussion of possible current carrying modes in one-dimensional conductors,[3] etc. Independent of the existence of specific physical manifestations, the idea that nonlinear systems, i.e., systems that admit solitary waves or solitons, possess intrinsically nonlinear modes that participate in the behavior of the system like a single-particle mode is very appealing and of great interest. Fogel *et al.*[4] have studied the motion of a sine-Gordon soliton at $T = 0$°K in the presence of an external field with damping and have found that the soliton exhibits single-particle properties; Gupta and Sutherland[5] (GS) and Currie *et al.*[6] have studied the equilibrium statistical mechanics of the sine-Gordon system. Currie *et al.*[6] argue that they find properties in reasonable agreement with the suggestion of Krumhansl and Schrieffer.

The purpose of this paper is to describe a number of results from the study of the equilibrium statistical mechanics of the sine-Gordon system. We do this with two purposes in mind. Firstly, to describe those particular features of the method of calculation and results that are important to understanding and using the solution to the equilibrium statistical mechanics. (In a paper to appear, referred to as II, we discuss a method of the solution to the nonequilibrium statistical mechanics that rests heavily on the results we obtain here.) Secondly, to call attention to a number of important differences between the calculational details and results obtained in this work and by GS and Currie *et al.*

In Sec. II we set up the problem of a system of physical pendula in Earth's gravitational field that are coupled by torsion springs and that are separately driven by an external torque. Here we set this external torque equal to zero. The equation of motion for a single pendulum, in the continuum limit, is the sine-Gordon equation. We formulate the calculation of the partition function, the free energy, and various statistical averages for this system in terms of a transfer-integral (TI) problem.

In Sec. III we discuss details of the solution of the TI problem. Particular attention is paid to methods of solution that are valid away from the continuum limit (in the continuum limit the TI problem reduces to the Mathieu equation) as it is this circumstance that governs most physical applications of the statistical mechanics. The TI problem involves a nonsymmetric kernel and the use of a nonsymmetric completeness relation. We describe methods of solution of the TI problem valid in various limits and make numerical tests of the convergence of an approximate solution.

Section IV is devoted to displaying and discussing the results of calculations of the thermodynamic properties of the sine-Gordon system. We pay particular attention to identifying the appropriate physical variables that describe the system. Gupta and Sutherland have discussed the equilibrium statistical mechanics in terms of a pressure (this physical system has no capacity to exert a pressure) and the chemical potential. We find that

the appropriate mechanical variable is the torque required to hold the system at a particular total phase. (It is the torque which is *called* the chemical potential by GS; these authors also inappropriately identify the Gibbs free energy with the pressure.) We examine the displacement fluctuations and show the system to behave like a gas of noninteracting particles. In the appendixes we work out various details that support the arguments and calculations in the main body of the paper.

II. THERMODYNAMIC AND STATISTICAL MECHANICAL RELATIONS

In this section we describe the formal thermodynamic and statistical mechanical relations that are employed in discussing the sine-Gordon system. For the purpose of giving this description definiteness and to aid in developing intuition we employ a particular realization of the sine-Gordon system. Consider $M+1$ physical pendula in Earth's gravitational field and coupled to one another by torsion springs.[7] The Hamiltonian of this system is

$$H = T + V(1, \ldots, M+1)$$
$$= \sum_{i=1}^{M+1} \left[\tfrac{1}{2} I \omega_i^2 - E_1 \cos\theta_i + \tfrac{1}{2} E_2 (\theta_{i+1} - \theta_i)^2 \right], \qquad (1)$$

where θ_i is the displacement of the ith pendulum from equilibrium, $E_1 = mgR$, and E_2 measures the strength of the torsion spring that couples the i and $i+1$ pendula (see Fig. 1). An external field of constant torque can be applied to each pendulum (by wrapping a string, with mass M, around each axle; see Fig. 1) in which case the Hamiltonian contains the added term

$$H_e = -\sum_{i=1}^{M+1} E_0 \theta_i . \qquad (2)$$

It is this external torque which generates the phase evolution of the individual pendulum and the phase current that is the subject of paper II. For the discussion in this paper $E_0 = 0$.

The system described by Eq. (1) is a linear array of $M+1$ physical pendula coupled by torsion springs. This system is embedded in a temperature reservoir at temperature T. The possible motions of the pendula are motion of the phase, e.g., the relative phase of a near-neighbor pair, $\theta_{i+1} - \theta_i$, the phase change along a segment of the chain, etc. The appropriate thermodynamic variables to describe the mechanical characteristic of this system are the *phase* and *torque* which generates it. The phase is defined by[5]

$$\Phi = \sum_{i=1}^{M+1} (\theta_{i+1} - \theta_i) = (\theta_{M+1} - \theta_1) \qquad (3)$$

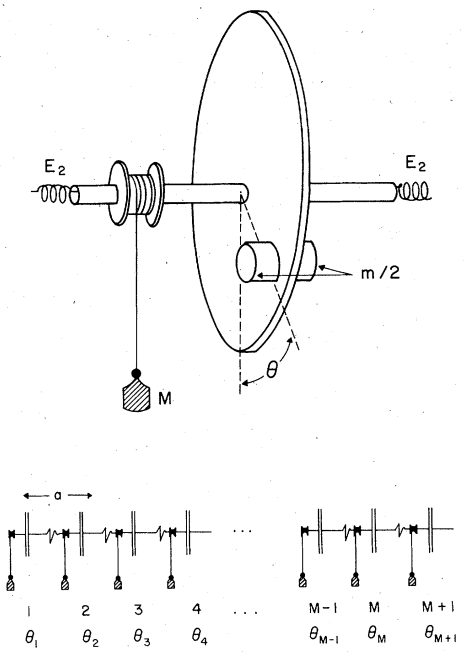

FIG. 1. Sine-Gordon chain. A physical system which is described by the Hamiltonian in Eq. (1) is a linear chain of torsion-coupled pendula. Each pendulum has mass m held by a weightless disk at distance R from the axle and is coupled to the neighboring pendula through a pair of torsion springs. The gravitational potential energy is measured from the height of the axle; the torsion springs attempt to hold pendula m and $m+1$ at relative angular displacement zero. An *external* torque is exerted on each pendulum by a mass hung over a spindle on the axle.

and measures the total phase evolution along the chain. The phase of the system, total phase evolution along the chain, is changed by changing the torque applied *across* the system, from 1 to $M+1$; e.g., the first pendulum is held fixed and a torque is applied to the $M+1$ pendulum to generate a change in the phase of the system. The phase is an extensive variable; it corresponds directly to the "kink number" of GS. To do the thermodynamics of the system described by Eq. (1) we employ the Helmholtz free energy

$$F(T, \Phi; M+1) = E - TS, \qquad (4)$$

where τ, the torque is the thermodynamic conjugate of the phase,

$$dE = T\,dS - \tau\,d\Phi, \qquad (5)$$

$$S = -(\partial F/\partial T)_{\Phi}, \qquad (6)$$

$$\tau = -(\partial F/\partial \Phi)_{T}; \qquad (7)$$

we write the free energy occasionally with a reminder that $M+1$ particles are involved. The num-

ber of particles in the system is a parameter; the length of the system L ($L = Ma$, where a is the spacing between pendula) is also a parameter and not a physical variable. Gupta and Sutherland use L as a physical variable analogous to the volume and they define a pressure, $-\partial F/\partial L$. This pressure has no physical meaning since the system described by Eq. (1) or by GS has no capacity to exert forces along the length of the chain. (Below we show that the "kink pressure" of GS is the Gibbs free energy.)

To develop the statistical mechanics of the system described by Eq. (1) we employ the canonical ensemble

$$Z(T,\Phi) = \int d\omega_1 \cdots d\omega_{M+1} \int d\theta_1 \cdots d\theta_{M+1} \times e^{-\beta H(1,\cdots M+1)}, \quad (8)$$

with

$$F(T,\Phi) = -k_B T \ln Z(T,\Phi). \quad (9)$$

Equations (4)–(9) give a complete prescription for the equilibrium statistical mechanics.

We calculate $Z(T,\Phi)$ subject to the constraints

$$\theta_1 = 0 \text{ and } \theta_{M+1} = \Phi = 2\pi\eta \quad (10)$$

for all time. For η an integer we use N, the "kink number" of GS. From Eq. (8) we have

$$Z(T,\Phi) = [(2\pi k_B T/I)^{1/2}]^{(M-1)/2} Z_V, \quad (11)$$

where the first term comes from $M-1$ ω integrals and

$$Z_V = \int d1 \cdots dM+1\, \delta(\theta_1)\delta(\theta_{M+1} - \Phi) e^{-\beta V(1,\cdots M+1)}; \quad (12)$$

here we use the shorthand 1 for θ_1, $d1$ for $d\theta_1$, etc. To evaluate Z_V we employ the complete set of states $\psi_\nu(\theta)$ with completeness relation

$$\delta(\theta - \theta') = \sum_\nu \phi_\nu(\theta)\psi_\nu(\theta') \quad (13)$$

to write

$$Z_V = \sum_{\mu\nu} \int d1 \cdots dM+1\, \phi_\nu(\Phi)\psi_\mu(0)\phi_\mu(\theta_1) \times e^{-\beta V(1,\cdots M+1)} \psi_\nu(\theta_{M+1}). \quad (14)$$

We choose ψ_ν and ϕ_ν to be the right- and left-hand eigenfunctions of a convenient transfer integral; i.e.,

$$\int d2\, e^{-K(1,2)} \psi_\nu(2) = e^{-\beta\epsilon_\nu} \psi_\nu(1), \quad (15R)$$

$$\int d1\, \phi_\nu(1) e^{-K(1,2)} = e^{-\beta\epsilon_\nu} \phi_\nu(2), \quad (15L)$$

with

$$K(1,2) = (-\lambda_1 \cos\theta_1) + \tfrac{1}{2}\lambda_2(\theta_2 - \theta_1)^2, \quad (16)$$

where $\lambda_1 = \beta E_1$ and $\lambda_2 = \beta E_2$. Equation (14) can be rewritten in the form

$$Z_V = \sum_{\mu\nu} \phi_\nu(\Phi)\psi_\mu(0) \times \int d1 \cdots dM+1\, \phi_\mu(1) e^{-K(1,2)} e^{-K(1,2)} \cdots \times e^{-K(M,M+1)} \psi_\nu(M+1) \quad (17)$$

so that repeated use of Eq. (15R) leads to

$$Z_V = \sum_{\mu\nu} \phi_\nu(\Phi)\psi_\mu(0) e^{-M\beta\epsilon_\mu} \int d1\, \phi_\mu(1)\psi_\nu(1). \quad (18)$$

The ϕ and ψ of Eq. (15) are chosen to be orthonormal so that Z_V reduces to

$$Z_V = \sum_\nu \phi_\nu(\Phi)\psi_\nu(0) e^{-M\beta\epsilon_\nu}. \quad (19)$$

The transfer-integral problem defined by Eqs. (15) and (16) is a homogeneous Fredholm equation of the second kind with a polar kernel[8]; i.e., it is not symmetric in 1 and 2; a properly symmetric kernel can be constructed from which all of the standard orthogonality, completeness, etc., relations can be established. These relations can then be transformed back to the unsymmetric form; e.g., Eq. (13). We employ the unsymmetric form of the TI kernel, which arises naturally in calculations of the type we do here, because wave functions, eigenvalues, etc., are simpler to calculate in this form. It is only in doing formal manipulations to show orthogonality, completeness, etc., that the symmetric kernel is useful.

Employing methods similar to those employed above we can derive formal expressions for single particle, pair,... averages,[1,9] e.g.,

$$\langle F(\theta_{n+1})\rangle = \frac{1}{Z_V} \sum_{\mu\nu} \phi_\nu(\Phi)\psi_\mu(0) F_{\mu\nu} e^{-(M-n)\beta\epsilon_\nu} e^{-n\beta\epsilon_\mu} \quad (20)$$

and

$$F_{\mu\nu} = \int d\theta\, \phi_\nu(\theta) F(\theta) \psi_\nu(\theta); \quad (21)$$

$$\langle F(\theta_{n+1}) G(\theta_{m+1})\rangle = \frac{1}{Z_V} \sum_{\mu\nu\nu'} \phi_\nu(\Phi)\psi_\mu(0) F_{\mu\nu'} G_{\nu'\nu} e^{-(M-n)\epsilon_\nu} \times e^{-(n-m)\beta\epsilon_{\nu'}} e^{-m\beta\epsilon_\mu}. \quad (22)$$

Equations (19) and (20) reduce the calculation of the equilibrium properties of the system described by Eq. (1) to the solution of the transfer-integral problem given by Eqs. (15). In Sec. III

we take up the discussion of the solution to Eqs. (15).

III. TRANSFER INTEGRAL

The basic transfer integral problem is given by Eqs. (15R) and (15L), i.e.,

$$\int_{-\infty}^{+\infty} d\theta_2\, e^{+\lambda_1\cos\theta_1} e^{-\lambda_2(\theta_2-\theta_1)^2/2}\psi_\nu(\theta_2) = e^{-\beta\epsilon_\nu}\psi_\nu(\theta_1)\,. \quad (23)$$

By inspection of Eqs. (15) the left-hand eigenfunction is related to the right-hand eigenfunction by

$$\phi_\nu(\theta) = e^{-\lambda_1\cos\theta}\psi_\mu^*(\theta)\,. \quad (24)$$

Because of the translational invariance of the single-particle potential under displacements $2\pi m$ we have

$$\psi_\mu(\theta+2\pi m) = \psi_\mu(\theta)e^{i\mu m}. \quad (25)$$

Equation (23) can be converted to a differential equation. Consider the general problem defined by

$$\int d2\, e^{-\beta V(1)} e^{-\beta W(12)}\psi_\nu(2) = e^{-\beta\epsilon_\nu}\psi_\nu(1)\,, \quad (26)$$

where $W(12)$ is a function of $|\theta_1-\theta_2|$. Then $\phi_\nu(1)$ has symmetry properties determined entirely by $\exp[-\beta V(1)]$. To convert Eq. (26) into a differential equation we use the translation operator

$$\psi_\nu(2) = e^{(\theta_2-\theta_1)D_1}\psi_\nu(1),$$

where $D_1 = d/d\theta_1$ and the cumulant expansion[10] to write

$$\int d2\, e^{-\beta W(12)}\,\frac{\int d2\, e^{-\beta W(12)}\, e^{(\theta_2-\theta_1)D_1}}{\int d2\, e^{-\beta W(12)}}\,\psi_\nu(1) = \exp[+C_0 + (1/2!)C_2D_1^2 + (1/4!)C_4D_1^4 + \cdots]\psi_\nu(1). \quad (27)$$

In this equation

$$C_0 = \int d2\exp[-\beta W(12)]\,,$$

$$C_2 = \langle\theta_{21}^2\rangle\,, \quad C_4 = \langle\theta_{21}^4\rangle - 3\langle\theta_{21}^2\rangle^2$$

with the averaging procedure

$$\langle\cdots\rangle = \frac{\int d\theta_{21}\, e^{-\beta W(\theta_{21})}\cdots}{\int d\theta_{21}\, e^{-\beta W(\theta_{21})}} \quad (28)$$

and $\theta_{21} = \theta_2 - \theta_1$. Here we have used $\langle\theta_{21}\rangle = \langle\theta_{21}^3\rangle = \cdots = 0$. For the special case of a harmonic potential only C_2 is nonzero, $C_2 = 1/\lambda_2$ and $C_0 = \ln(\lambda_2/2\pi)^{1/2}$. Using these results we can write Eq. (23) in differential form

$$e^{\lambda_1\cos\theta} e^{D^2/2\lambda_2}\psi_\nu(\theta) = e^{-\beta\tilde{\epsilon}_\nu}\psi_\nu(\theta)\,, \quad (29)$$

where $\exp(-\beta\tilde{\epsilon}_\nu) = (\lambda_2/2\pi)^{1/2}\exp(-\beta\epsilon_\nu)$. If we could combine the exponentials on the LHS of Eq. (29) into a single exponential we could reduce this equation to a Schrödinger equation and finally the Mathieu equation.[11] Eigenfunctions and eigenvalues could then be read out of tables. It is the unacceptability of this procedure that leads to the need for a careful discussion of the solution to Eq. (23) or (29). Let us consider several special cases.

Case 1; $E_2 = 0$. This case corresponds to independent pendula. In Eq. (23) the θ_2 integral is unconstrained so that we have

$$\psi(\theta_1) \propto e^{+\lambda_1\cos\theta_1}\,. \quad (30)$$

We anticipate the single-particle density to be of the form $\rho(\theta) \propto \phi(\theta)\psi(\theta)$ so that this means (see Sec. IV)

$$\rho(\theta) \propto \exp(\lambda_1\cos\theta_1) \quad (31)$$

as we expect.

Case 2; $E_1 = 0$. This case corresponds to an $M+1$ particle elastic band or a piece of spring steel. Equation (29) reduces to

$$-\frac{1}{2\lambda_2}\frac{d^2}{d\theta^2}\psi_\nu(\theta) = \beta\tilde{\epsilon}_\nu\psi_\nu(\theta) \quad (32)$$

with

$$\beta\tilde{\epsilon}_\nu = \nu^2/2\lambda_2\,, \quad (33)$$

$$\psi_\nu(\theta) = e^{+i\nu\theta}/\sqrt{2\pi} \quad (34)$$

and $\phi_\nu(\theta) = \psi_\nu^*(\theta)$.

Case 3. $k_BT \to +\infty$. In this case $\lambda_1 \to 0$ and $\lambda_2^{-1} \to +\infty$. This case is equivalent to case 2 with ϵ_ν and ψ_ν given by Eqs. (33) and (34).

Case 4. $k_BT \to 0$ *and* $\lambda_2 \gg \lambda_1$. In this case $\lambda_1 \to L^+$ and $\lambda_2 \to L^+$ while the torsion spring is much stronger than the gravitational potential barrier; $E_2 \gg E_1$. If one pendulum is twisted through 2π then several neighbors will follow. In Appendix D we show, by one of several approximations that we have developed for this case, that $\psi_\nu(\theta)$ and $\beta\tilde{\epsilon}_\nu$ are well approximated by the solution of the Mathieu equation,[11] i.e.,

$$\left(-\frac{1}{2\lambda_2}\frac{d^2}{d\theta^2} - \lambda_1\cos\theta\right)\psi_\nu(\theta) = \beta\tilde{\epsilon}_\nu\psi_\nu(\theta) \quad (35)$$

even though the TI problem cannot be directly reduced to Eq. (35). However, as the solution to Eq. (35) is employed for $\lambda_1 \gg 1$, in this limit we must retain the asymmetry of the completeness relation and use

$$\phi_\nu^*(\theta) = e^{-\lambda_1\cos\theta}\psi_\nu^*(\theta)\,. \quad (36)$$

(Compare this requirement with the continuum approximation below.)

Case 5. Continuum approximations. The continuum approximation cannot be examined with the TI equation in the form in which we have developed it. We describe a discretization of a Hamiltonian density in Appendix A. We find that the continuum approximation maps onto Eq. (1) with

$$E_1 \longrightarrow V_1 \rho \Delta x \quad \text{and} \quad E_2 \longrightarrow \Gamma \rho / \Delta x \,,$$

where Δx is the length of the units over which the continuum is discretized. Using these expressions for E_1 and E_2 in Eq. (29) leads to

$$e^{\beta V_1 \rho \Delta x \cos\theta} e^{\Delta x D^2/2 \beta \Gamma \rho} \psi_\nu(\theta) = e^{-\beta \tilde{\epsilon}_\nu} \psi_\nu(\theta) \,. \quad (37)$$

Upon defining $\beta\tilde{\epsilon}_\nu$, $\beta\tilde{\epsilon}_\nu \rho \Delta x = \beta \tilde{\epsilon}_\nu$, we may take $\rho \Delta x \to 0$ and obtain

$$\left(-\frac{1}{2\beta\Gamma\rho^2} \frac{d^2}{d\theta^2} - \beta V_1 \cos\theta \right) \psi_\nu(\theta) = \beta \tilde{\epsilon}_\nu \psi_\nu(\theta) \,, \quad (38)$$

the Mathieu equation. In this case the asymmetry of the completeness relation is of no consequence as

$$\phi_\nu(\theta) = e^{-\beta V_1 \rho \Delta x \cos\theta} \psi_\nu^*(\theta) = \psi_\nu^*(\theta) \,. \quad (39)$$

(Compare to case 4 above where the asymmetry must be retained.) It is important to recognize that the continuum limit described here is a physical limit. For a physical system with density $\rho \simeq 1/\text{Å}$ [e.g., as in the case of a charge-density wave (CDW)[3]] at $k_B T \ll V_1$ we have $\beta V_1 \rho \Delta x \to 0$ only if we can make sense out of discretization over subatomic lengths (in the case of a CDW over $\Delta x \ll 1$ Å). Although the continuum limit is possible in mathematical models it must be used with caution in mapping those models onto physical systems.

We find that the basic TI problem we wish to solve can be reduced to one of several tractable differential equations under a variety of circumstances. See Fig. 2. The most important case for careful consideration is case 4 above, the low-temperature limit. We have solved the differential equation (35) for a variety of values of λ_1 and λ_2. As a test of how the resulting eigenfunctions and eigenvalues are related to the solution to the exact TI problem, Eq. (23), we have (a) calculated the average value of the LHS of Eq. (23) using the solution to Eq. (35) in order to compare the resulting "energy" expectation value with the eigenvalue obtained from Eq. (35); i.e., we compare

$$\ln \frac{\int d\theta_1 d\theta_2 \psi_0(\theta_1) e^{\lambda_1 \cos\theta_1} e^{-\lambda_2 (\theta_2 - \theta_1)^2/2} \psi_0(\theta_2)}{\int d\theta_1 \psi_0(\theta_1) \psi_0(\theta_1)} \,, \quad (40)$$

where $\psi_\nu(\theta)$ is given by the solution to Eq. (35), with $\beta\tilde{\epsilon}_\nu$ from solution of Eq. (35); and (b) calculated $\psi_\nu^{(1)}(\theta)$ from Eq. (23) according to the prescription

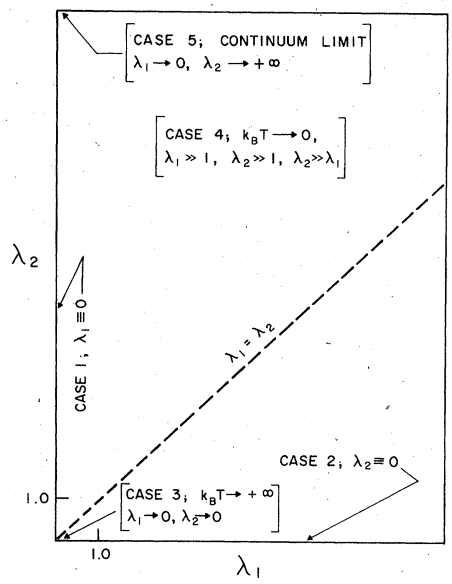

FIG. 2. Special cases of the transfer integral. The location of the five special cases of the transfer integral equation described in Sec. III are shown as a function of λ_1, λ_2. In four of these cases the transfer integral reduces to a differential equation and has a symmetric completeness relation, cases 1, 2, 3, and 5. These cases are on the boundary of the λ_1-λ_2 parameter space, i.e., either $\lambda_1 \to 0$, $\lambda_2 \to 0$ or both. In the fifth case, case 4, the transfer integral reduces approximately to a differential equation and has a nonsymmetric completeness relation. This latter case, case 4, is most often the case of interest in describing physical systems.

$$\psi_0^{(1)}(\theta_1) = e^{\beta \tilde{\epsilon} \nu} \int d\theta_2 \, e^{\lambda_1 \cos\theta_1} e^{-\lambda_2 (\theta_2 - \theta_1)/2} \psi_0(\theta_2) \,, \quad (41)$$

where $\psi_0(\theta_2)$ is given by the solution of Eq. (35), and compared $\psi_0^{(1)}(\theta)$ to $\psi_0(\theta)$ from Eq. (35). The first test, a comparison of "eigenvalues" is a measure of the suitability of the average shape of the wave function. We have used the second test to examine the behavior of the wave function at values of θ far from $\theta = 0, 2\pi, 4\pi, \ldots$. It is $\psi_0(\theta)$ near $\theta \simeq \pi, 3\pi$, that must be well approximated if the soliton properties of the system are to be correctly described. Our findings are that the energy eigenvalue for Eq. (23) is given to excellent approximation by the solution to Eq. (35). Equation (35) seems to be a good approximation well beyond the region in λ_1-λ_2 space where the discussion in Appendix D would lead us to expect it to be so. We show the results of test (a) in Fig. 3(b) where we show $\psi_\nu^{(1)}(\theta)$ given by Eq. (41) near $\theta \simeq \pi$ for comparison with $\psi_0(\theta)$ given by Eq. (35). In all cases the error in $\psi_0(\theta)$ in this most critical region of space is less than a factor of 2.

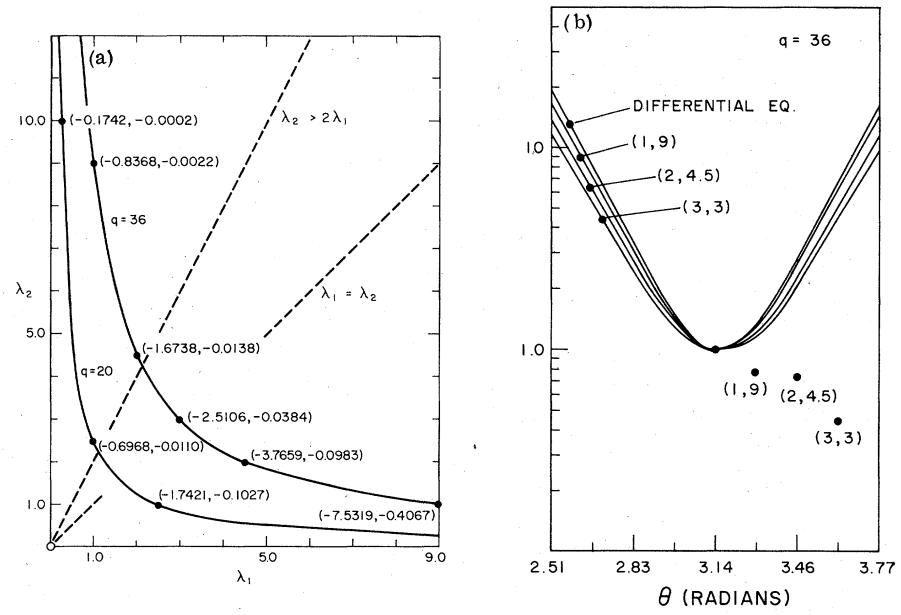

FIG. 3. Tests of the transfer integral equation. In (a) we show the energy eigenvalue found from solving the differential equation, Eq. (35), and the energy eigenvalue (40) from the expectation value of the transfer integral, Eq. (23), as the pair of numbers $(\beta\tilde{\epsilon}_\nu$, eigenvalue (40)$-\beta\tilde{\epsilon}_\nu)$, for several values of (λ_1,λ_2) at $q=20$ and $q=36$. The difference between the energy eigenvalue from Eq. (35) and the energy eigenvalue from Eq. (40) is always less than 2% for $\lambda_2 \geq \lambda_1$; e.g., at $\lambda_1=\lambda_2=3$, $\beta\tilde{\epsilon}_\nu=2.5106$, Eq. (40) $=-2.5490$ and the number pair plotted at $\lambda_1=3, \lambda_2=3$ is $(-2.5106, -0.0384)$. In (b) we show the evolution of the wave function near $\theta=\pi$. The continuous curves are the wave function (normed to 1 at π) from the solution of Eq. (35) and the wave function from Eq. (41) for three values of λ_1 and λ_2 at $q=36$. The ratio of the magnitude of $\psi^{(1)}(\theta)$ at $\theta=\pi$ from Eq. (40) to $\psi(\theta)$ at $\theta=\pi$ from Eq. (35) for three values of λ_1 and λ_2 at $q=36$ is shown by solid circles. The differential-equation approximation to the transfer-integral approximates the shape of the wave function near π very well as $\lambda_2/\lambda_1 \to L^+$ at fixed q. Similarly the magnitude of $\psi^{(1)}(\pi)/\psi(\pi) \to 1$ at $\lambda_2/\lambda_1 \to L^+$. These tests verify that the differential-equation approximation to the transfer integral does an excellent job of preserving the average shape of the wave function and the details of the wave function in the barrier at $\theta \simeq \pi$ when $\lambda_2/\lambda_1 \gg 1$.

IV. EQUILIBRIUM PROPERTIES

In this section we work out and discuss the physical content of the formulas for the free energy, torque, one- and two-particle correlation functions, etc., derived above. The basic orientation of our discussion is to establish the validity of a simple picture of the equilibrium behavior. We do this to confirm the conjecture of Krumhansl-Schrieffer and in preparation for a discussion of nonequilibrium behavior in II.

Case A; $\lambda_1=0$. This case corresponds to case 2 above, the gravitational field is set to zero and the system reduces to a $M+1$ particle elastic band or a piece of spring steel. From Eqs. (32)–(34)

$$\phi_\nu^*(\theta)=\psi_\nu(\theta)=(1/\sqrt{2\pi})e^{i\nu\theta}$$

and

$$\beta\tilde{\epsilon}_\nu=+\nu^2/2\lambda_2.$$

Equation (19) for $Z_\nu(T,\Phi)$ yields $[\Phi=2\pi N,\ \psi_\nu(\Phi)=e^{i\nu\Phi}/\sqrt{2\pi}]$;

$$Z_\nu(T,\Phi)=\left[\left(\frac{2\pi}{\lambda_2}\right)^{1/2}\right]^M\left(\frac{\lambda_2}{2\pi M}\right)^{1/2}\exp(-\tfrac{1}{2}\lambda_2\Phi^2). \quad (42)$$

Using Eq. (42) in Eqs. (9) and (11) yields

$$F(T,\Phi)=F_0(T,0)+\Delta F(T,\Phi), \quad (43)$$

where

$$F_0(T,0)=-(M-1)\tfrac{1}{2}k_BT\ln[(2\pi)^2/I\beta^2E_2]+\tfrac{1}{2}k_BT\ln M \quad (44)$$

and

$$\Delta F(T,\Phi)=\tfrac{1}{2}(E_2/M)\Phi^2. \quad (45)$$

From Eq. (7) for the torque we have

$$\tau(T,\Phi)=(-E_2/M)\Phi. \quad (46)$$

For the matrix elements of $F(\theta)$, $G(\theta)$, etc., called for to evaluate $\langle F(\theta_{n+1})\rangle$, we write

$$F_{\mu\nu}=\frac{1}{2\pi}\int d\theta\, F(\theta)e^{i(\nu-\mu)\theta}, \quad (47)$$

etc., so that the average value of $F(\theta)$ given by Eq. (20) is[5,12]

$$\langle F(\theta_{n+1})\rangle = \frac{1}{2}\,\frac{\int d\theta\, F(\theta)\int d\mu\int d\nu\, e^{+i(\nu-\mu)\theta}e^{-i\nu\Phi}e^{-[(M-n)/2\lambda_2]\nu^2}e^{-n\mu^2/2\lambda_2}}{\int d\nu\; e^{-M\nu^2/2\lambda_2}} \tag{48}$$

or

$$\langle F(\theta_{n+1})\rangle = \int d\theta F(\theta) P_{n+1}(\theta), \tag{49}$$

where

$$P_{n+1}(\theta) = (\alpha/\sqrt{2\pi})\exp(-\tfrac{1}{2}\alpha^2)(\theta_{n+1} - x_n\Phi)^2 \tag{50}$$

with $\alpha^2 = M\lambda_2/x_n(1-x_n)$ and $x_n = n/M$. Thus the probability of finding θ_n at θ is given by a Gaussian centered at $(n/M)\Phi$ of width proportional to $\sqrt{M}$ and the location of n along the chain. For the average position of the nth pendumum we have

$$\langle \theta_{n+1}\rangle = x_n\Phi \tag{51}$$

and

$$\langle \theta_{n+1}^2\rangle - \langle \theta_{n+1}\rangle^2 = (k_BT/E_2)Mx_n(1-x_n). \tag{52}$$

The behavior of the system in this limit is essentially the same as the behavior of a linear chain of compressional springs for which

$$H = \sum_i \frac{p_i^2}{2m} + \tfrac{1}{2}\Gamma\sum_i (x_{i+1} - x_i)^2, \tag{53}$$

with $x_1 = 0, x_{M+1} = L$ and

$$F(T, L) = F(T, 0) + \tfrac{1}{2}\Gamma(L^2/M). \tag{54}$$

where

$$F(T,0) = -(M-1)\tfrac{1}{2}k_BT\ln\frac{(2\pi)^2}{m\beta^2} + \tfrac{1}{2}k_BT\ln M. \tag{55}$$

The force required to produce extension to length L is $f = -\partial F/\partial L = -(\Gamma/M)L$. For this system we have

$$\langle x_{n+1}\rangle = x_nL \tag{56}$$

and

$$\langle x_{n+1}^2\rangle - \langle x_{n+1}\rangle^2 = (k_BT/\Gamma)Mx_n(1-x_n). \tag{57}$$

We note the correspondence between Φ and L and τ and f.

Case B. $1 \ll \lambda_1 \ll \lambda_2$. This case corresponds to case 4 above; the temperature is small compared to E_1 and E_2 while at the same time the strength of the torsion spring is large compared to the gravitational potential energy. For the wave function that solves Eq. (35), we have (see Appendixes C and D)

$$\phi_\nu^*(\theta) = e^{-\lambda_1\cos\theta}\psi_\nu^*(\theta), \tag{58}$$

$$\psi_\nu(\theta) = \frac{1}{\sqrt{2\pi}}\sum_l e^{i\nu l}\chi_0(\theta - 2\pi l). \tag{59}$$

The behavior of $\chi_0(\theta - 2\pi l)$ is described in Appendix C. The energy eigenvalue appropriate to $\psi_\nu(\theta)$ given by Eq. (59) is

$$\beta\tilde{\epsilon}_\nu = -\lambda_1 + \tfrac{1}{2}(\lambda_1/\lambda_2)^{1/2} - \beta|t|\cos 2\pi\nu. \tag{60}$$

The quantity $|t|$ in Eq. (60) is the tunneling rate calculated in the tight-binding approximation; $\beta|t|$ is proportional to the number of solitons.[1,6] Using Eq. (60) in Eq. (19) leads to

$$Z_\nu = |\chi_0(0)|^2\exp M\left[C_0 + \lambda_1 - \frac{1}{2}\left(\frac{\lambda_1}{\lambda_2}\right)^{1/2}\right] \times \int d\nu\, e^{+M\beta|t|\cos 2\pi\nu}e^{-i\nu\Phi} \tag{61}$$

or

$$Z_\nu = |\chi_0(0)|^2\exp M\left[C_0 + \lambda_1 - \frac{1}{2}\left(\frac{\lambda_1}{\lambda_2}\right)^{1/2}\right] I_N(M\beta|t|), \tag{62}$$

where $\Phi = 2\pi N$. Using Eq. (62) and Eqs. (11) and (9) we have

$$F(T,\Phi) = F_0(T,0) + \Delta F(T,\Phi), \tag{63}$$

where

$$F(T,0) = -k_BT\frac{M-1}{2}\ln\frac{(2\pi)^2}{I\beta\lambda_2} - \frac{k_BT}{2}\ln\frac{2\pi}{\lambda_2} - ME_1 + M\tfrac{1}{2}k_BT\left(\frac{E_1}{E_2}\right)^{1/2} \tag{64}$$

contains the contribution to the free energy that dominate as $T \to 0\,^\circ$K and the thermally activated solitons leave the chain and

$$\Delta F(T,\Phi) = k_BT\ln I_N(M\beta|t|) \tag{65}$$

contains the contribution to the free energy due to both thermally excited solitons and the solitons created on the chain by the external torque. From Eq. (7) for the torque we have

$$\tau = +\frac{k_BT}{2\pi}\frac{\partial}{\partial N}\ln I_N(N(T)), \tag{66}$$

where $N(T) = M\beta|t|$ is the number of thermally excited solitons.[1,6]

We postpone the discussion of Eqs. (63)–(66) and write out the basic equations for the average value of θ_n, θ_n^2, and $\theta_n\theta_m$. Using the tight-binding wave functions and eigenfunctions from above in Eqs. (20) and (21) yields

$$\langle F(\theta_{n+1})\rangle = \sum_{l=-\infty}^{+\infty}\frac{F(l)I_{N-l}(v-u)I_l(u)}{I_N(v)}, \tag{67}$$

where $v = M\beta|t|$, $u = n\beta|t|$. In achieving Eq. (67) we have assumed $F(ll')$ to be diagonal, i.e.,

$$F(ll') \equiv \int d\theta\, \xi_0(\theta - 2\pi l) F(\theta) \chi_0(\theta - 2\pi l')$$

$$\simeq F(ll)\delta_{l,l'},$$

where ξ_0 is the left-hand function appropriate to χ_0, Eq. (C.8). As the tight-binding wave functions are very compact this is a good approximation (corrections are of order $\beta|t|$). For $F(\theta) = \theta$, $F(l) = l$ and use of Eq. (B4) in Eq. (67) yields

$$\langle \theta_{n+1} \rangle = (x_n) N. \tag{68}$$

For $\langle \theta_{n+1}^2 \rangle$ $[F(\theta) = \theta^2,\ F(l) = l^2]$

$$\langle \theta_{n+1}^2 \rangle = \sum_{l=-\infty}^{+\infty} \frac{l^2 I_{N-l}(v-u) I_l(v)}{I_N(v)} \tag{69}$$

which upon use of Eq. (B5) yields

$$\langle \theta_{n+1}^2 \rangle - \langle \theta_{n+1} \rangle^2 = n(1 - x_n)\beta|t| \frac{d}{dv} \ln I_N(v) \tag{70}$$

for $\langle \theta_{n+1}\theta_{m+1} \rangle$ $[F(\theta) = \theta,\ F(l) = l;\ G(\theta) = \theta,\ G(l') = l']$

$$\langle \theta_{n+1}\theta_{m+1} \rangle = \sum_{l=-\infty}^{+\infty} \sum_{l'=-\infty}^{+\infty} ll' I_{N-l'}(v-u) I_{l'-l}(u-w) I_l(w) / I_N(v) \tag{71}$$

which upon use of Eq. (B6) yields

$$\langle \theta_{n+1}\theta_{m+1} \rangle - \langle \theta_{n+1} \rangle \langle \theta_{m+1} \rangle = m(1 - x_n)\beta|t| \frac{d}{dv} \ln I_N(v). \tag{72}$$

Finally we calculate the one particle density. To do this we use Eq. (20) with $F(\theta_{n+1}) = \delta(\theta_{n+1} - \theta)$. Then,

$$\rho_{n+1}(\theta) \equiv \langle \delta(\theta_{n+1} - \theta) \rangle$$

$$= \sum_l \xi_0(\theta - 2\pi l) \chi_0(\theta - 2\pi l) \frac{I_{N-l}(v-u) I_l(u)}{I_N(v)}. \tag{73}$$

By comparison with Eq. (67) or (69) we identify

$$P_{n+1}(l) = I_{N-l}(v-u) I_l(u) / I_N(v) \tag{74}$$

with the probability that particle $n+1$ on an $M+1$ particle chain has phase $2\pi l$ given that the total phase evolution along the chain is $\Phi = 2\pi N$. Then, from Eq. (73), $\xi_0(\theta - 2\pi l)\chi_0(\theta - 2\pi l)$ is the probability of finding the particle at θ near $2\pi l$. (We anticipated this result in the discussion of case 1 in Sec. III.) Results similar to Eqs. (73) and (74) can be achieved for the two-particle density using Eq. (22), etc.[1,9]

In Eqs. (63)–(66) and Eqs. (68), (70), and (72) we have expressions for the free energy, the torque, displacement fluctuation, etc., that we wish to examine. We are already at low temperature, $\lambda_1\lambda_2 \gg 1$. We consider 2 limits; case B-1, in which the number of thermally excited solitons is far fewer than the number of solitons generated by the torque τ and case B-2, in which the number of thermally excited solitons is far greater than the number of solitons generated by the torque. We write

$$I_N(v) = I_N(Nz), \tag{75}$$

where $z = M\beta|t|/N$ is the ratio of the number of thermally excited solitons to the number of solitons generated by the torque. We use $N(T) = M\beta|t|$ to denote the number of thermally excited solitons and N to denote the number of solitons generated by the torque. Thus cases B-1 and B-2 correspond to $z \ll 1$ and $z \gg 1$ respectively.

Case B-1. $N(T) \ll N$, $z \ll 1$. From 9.7.7[11]

$$\ln I_N(Nz) = -\tfrac{1}{2} \ln 2\pi N + N \ln \frac{N(T)}{2N} + N + O\left(\frac{1}{N}\right), \tag{76}$$

$$\frac{d}{dN} \ln I_N(N(T)) = \ln \frac{N(T)}{2N} + \frac{1}{2N} + O\left(\frac{1}{N^2}\right), \tag{77}$$

and

$$\frac{d}{dN(T)} \ln I_N(N(T)) = \frac{N}{N(T)} + O\left(\frac{N(T)}{N}\right). \tag{78}$$

For the free energy we have

$$\Delta F(T, \Phi) = N(E_\Phi - k_B T) - N k_B T \ln(M\beta|t_0|/2N) + \tfrac{1}{2} k_B T \ln 2N + O\left(\frac{1}{N}\right), \tag{79}$$

where we have used $|t| = |t_0| e^{-\beta E_\Phi}$, $\beta|t_0|$ is independent of T (see Appendix C). For the entropy we have

$$\Delta S = -\frac{\partial \Delta F}{\partial T} = -\frac{\Delta F - N E_\Phi}{T} \tag{80}$$

so that

$$\Delta U = \Delta F + T\Delta S = N E_\Phi. \tag{81}$$

Using Eq. (79) in Eq. (7) for the torque yields

$$\tau = -\frac{1}{2\pi} \frac{\partial \Delta F}{\partial N} = +\frac{k_B T}{2\pi} \left[\ln \frac{N(T)}{2N} - \frac{1}{2N} + O\left(\frac{1}{N^2}\right) \right] \tag{82}$$

or

$$\tau = -\frac{1}{2\pi} \left(E_\Phi - k_B T \ln \frac{M\beta|t_0|}{2N} + \frac{k_B T}{2N} + \ldots \right). \tag{83}$$

From Eq. (70) using Eq (78) we have

$$\langle \theta_{n+1}^2 \rangle - \langle \theta_{n+1} \rangle^2 \simeq x_n (1 - x_n) N \tag{84}$$

and similarly from Eq. (72) we have

$$\langle \theta_{n+1}\theta_{m+1} \rangle - \langle \theta_{n+1} \rangle \langle \theta_{m+1} \rangle \simeq x_m (1 - x_n) N. \tag{85}$$

Case B-2. $N(T) \gg N$; $z \gg 1$. From 9.7.7[11]

$$\ln I_N(Nz) = -\tfrac{1}{2} \ln 2N - \tfrac{1}{2} \ln z + Nz - N/2z + O(z^{-2}),$$

$$\frac{d}{dN} \ln I_N(N(T)) = -\frac{N}{N(T)} + O\left(\frac{N}{N(T)^2}\right), \tag{86}$$

and

$$\frac{d}{dN(T)}\ln I_N(N(T)) = 1 - \frac{1}{2N(T)} + O\left(\frac{N^2}{N(T)^2}\right). \quad (87)$$

For the free energy we have

$$\Delta F(T,\Phi) = \tfrac{1}{2}k_B T \ln 2N - \tfrac{1}{2}k_B T \ln[N(T)/N] + k_B T N(T) + O(N^2/N(T)^2). \quad (88)$$

For the entropy we have

$$\Delta S = -\frac{\partial \Delta F}{\partial T} = -\frac{\Delta F}{T} - k_B[N(T) - \tfrac{1}{2}]\beta E_\phi \quad (89)$$

and

$$\Delta U = E_\phi N(T). \quad (90)$$

Using Eq. (88) in Eq. (7) for the torque yields

$$\tau = -\frac{1}{2\pi}\frac{\partial \Delta F}{\partial N} = -\frac{k_B T}{2\pi}\frac{N}{N(T)}. \quad (91)$$

Using Eq. (87) in Eq. (70) we have

$$\langle \theta_{n+1}^2 \rangle - \langle \theta_{n+1} \rangle^2 \simeq x_n(1 - x_n)N(T) \quad (92)$$

and

$$\langle \theta_{n+1}\theta_{m+1} \rangle - \langle \theta_{n+1} \rangle \langle \theta_{m+1} \rangle = x_n(1 - x_m)N(T). \quad (93)$$

Case B-3: $N = 0, 1, 2, 3, \ldots; N(T) \ll 1$. We consider the case in which $N(T) \to 0, N \to 0$ to see how the system behaves as $T \to 0$ and to compare these results with the limits of the results above. We have $N(T) = M\beta|t| = M\beta|t_0|e^{-\beta E_\phi} \equiv me^{-\beta E_\phi}$

$$\ln I_0(N(T)) = \tfrac{1}{4}m^2 e^{-\beta E_\phi}, \quad (94)$$

$$\ln I_1(N(T)) = \ln(m/z) - \beta E_\phi + \tfrac{1}{8}m^2 e^{-2\beta E_\phi}, \quad (95)$$

and

$$\ln I_1(N(T)) - \ln I_0(N(T)) = \ln \tfrac{1}{2}m - \beta E_\phi - \tfrac{1}{8}m^2 e^{-2\beta\phi}, \quad (96)$$

and

$$\tau \equiv -(1/2\pi)\{\Delta F(T,1) - \Delta F(T,0)\} = -(1/2\pi)E_\phi. \quad (97)$$

Torque: In Fig. 4 we show the evolution of the torque as a function of temperature at fixed N given by Eqs. (46), (83), and (97). For fixed E_1 and E_2 as $T \to L^+, k_B T \to E_\phi$, the number of solitons is so great that the chain is completely covered, $N(T) \gg M$. The concept of a soliton loses its meaning, the chain can be twisted without attention to the subtleties of soliton formation; a twist goes on the chain nonlocally or uniformly. Thus the chain responds like a piece of spring steel—no amount of temperature can override E_2 and the torque is given by

$$\tau = -(E_2/M)2\pi N \quad .$$

A torque similar to this arises if $E_1 \to 0$ at any $k_B T$ for also in this limit the phase $2\pi N$ is evolved uniformly along the chain like a piece of spring steel. For fixed E_1 and E_2 as $T \to 0$, $k_B T \ll E_\phi$ and $N(T) \ll N \ll M$, creation of phase 2π occurs locally on the chain and requires torque $-E_\phi/2\pi$. In the intermediate regime, $k_B T \ll E_\phi$ and $N(T) \gg N$, the torque behaves as given by Eq. (83). For $N \gg M$ the chain is uniformly twisted at any temperature.

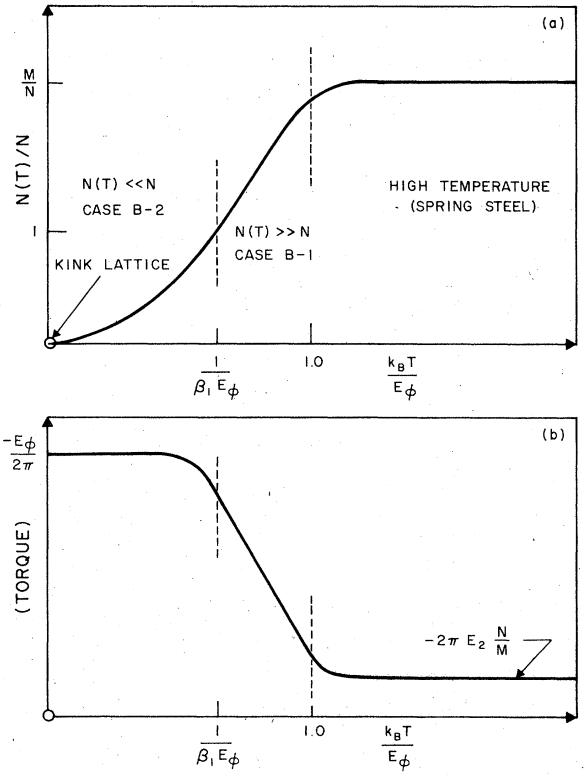

FIG. 4. Behavior of the torque as a function of temperature. The number of thermally activated solitons on the chain is proportional to $\exp(-\beta E_\phi)$. At $T = 0$ °K the phase of the chain evolves from 0 to $2\pi N$ and is described by an N soliton kink lattice. At $T = 0^+$ °K this lattice melts; at $T > 0$ °K thermal solitons join those already present from the melted kink lattice (the nonthermal solitons). The torque required to hold the phase on the chain does not change appreciably from $-E_\phi/2\pi$ until the number of thermal solitons is comparable to the number of nonthermal solitons, $\exp(-\beta E_\phi) \approx N$. As the temperature is raised beyond $\beta E_\phi \approx 1$ the number of solitons on the chain becomes comparable to M, solitons lose their meaning, the chain behaves like a piece of spring steel. In this limit $k_B T \gg E_1$, $k_B T \gg \gg E_2$, and $k_B T \gg E_\phi$; the thermal energy is greater than any basic energy associated with the system.

Displacement: It is difficult from the examination of Eqs. (45), (79) and (88) to develop a picture of what the solitons are doing. Let us examine Eqs. (52), (84), and (92) for the mean-square fluctuation of the angle at station $n+1$ along the chain. We show the behavior of $\langle \theta_{n+1} \rangle$ and $\langle \theta_{n+1}^2 \rangle$

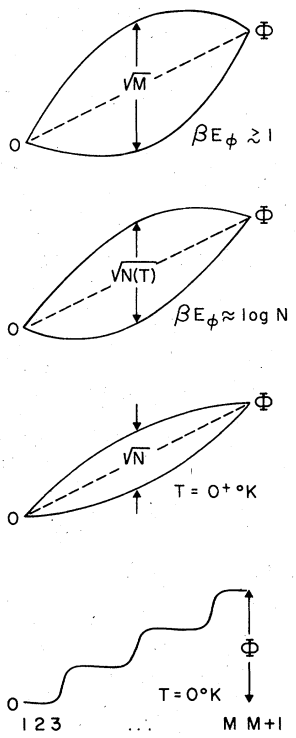

FIG. 5. Average value of θ, θ^2. At $T = 0$ °K the phase on the chain is in the form of a kink lattice. At $T = 0^+$ °K the lattice melts and $\langle\theta_n\rangle$ lies on the dashed line from 0 to Φ. The fluctuations in the displacement of the nth pendulum is proportional to the number of nonthermal solitons on the chain, $\langle\theta_n^2\rangle \propto N$. As T increases $\langle\theta_n\rangle$ continues to lie on the dashed line, the fluctuations become greater, $\langle\theta_n^2\rangle \propto N(T)$ for $N(T) > N$ and $\langle\theta_n^2\rangle \propto M$ at the highest temperatures.

in Fig. 5. From this figure we see that the behavior of the $n+1$ pendulum is analogous to a constrained random walk. If there are nonthermal solitons on the chain and $T = 0^+$ °K the average position of the $n+1$ pendulum on the chain is at $(n/m)N$ and the pendulum fluctuates from this average position by $\sqrt{M}$, $\sqrt{N(T)}$, or $\sqrt{N}$ depending on the number of solitons or the temperature. The number of phase kinks—therefore the number of steps in the randon walk is given by the number of solitons (for $k_B T \ll E_\phi$); thus $\delta\theta_v \propto \sqrt{N}$ and $\sqrt{N(T)}$. For $T \gg E_\phi$, the concept of soliton is without meaning and the number of effective phase kinks is M, $\delta\theta_n \propto \sqrt{M}$. These results for $\delta\theta_n^2$ provide rather convincing evidence that the solitons on a chain behave to very good approximation like a system of noninteracting particles that are free to move from one end of the chain to the other. This picture of soliton behavior persists even as $T \to 0$ °K from above. On the other hand we have the result of GS that the $T = 0$ °K equilibrium state for a chain with total phase evolution Φ is given by the kink lattice with $N = \Phi/2\pi$ solitons. The result of GS was derived in the continuum approximation—we complement it with our result here at $T > 0$ °K (also valid in the continuum approximation) and confirm the conclusion of GS that the $T = 0$ °K kink lattice is unstable to thermal fluctuations. We do not mean to say that the solitons disappear from the chain at $T > 0$ °K, but rather that their $T = 0$ °K localization on the chain is destroyed immediately at $T = 0^+$ °K. This conclusion is demonstrated in the continuum approximation. Certainly its sources is one-dimensional thermal fluctuations. Thus it is plausible that this conclusion also obtains for the discrete chain although it has not been so demonstrated.

It is appropriate to comment briefly on the relationship of the calculation of GS to those presented here. Gupta and Sutherland constructed the Helmholtz free energy $Z(T, \Phi)$ according to the same prescription as that used above. They then go to a torque (pressure) ensemble by using

$$\sum_\Phi e^{-\beta\tau\Phi} Z(T, \Phi).$$

The resulting thermodynamic potential is the Gibbs free energy[13]

$$G(T, \tau) = \sum_\Phi e^{-\beta\tau\Phi} Z(T, \Phi).$$

Gupta and Sutherland then write $G(T, \tau) = \beta PL$, where L is the length of the system, and define the pressure

$$P = (1/L) G(T, \tau).$$

The discussion by GS of the chemical potential-pressure relationship is a discussion of the relationship of torque (called μ) to the Gibbs free energy (called pressure).

Currie *et al.* have argued, by comparison of the torque (presumed by them to be the chemical potential) at $T \to 0$ °K and $N \gg N(T)$ with the chemical potential of an ideal gas, that at $T \neq 0$ °K the solitons behave like a noninteracting gas of particles. This conclusion is justified at low temperature by making the correspondence; phase is generated by a torque reservoir ⟷ "kinks" are generated by a "chemical potential" reservoir. It is explicitly demonstrated by the calculations of $\langle\theta_n^2\rangle$.

If the solitons behave like a noninteracting gas of particles one might hope to derive an ideal gas law for them, e.g., $\tau\Phi \propto k_B T$. Such a result is complicated by two essential features of the physics. (i) The torque τ does two jobs. It creates the particles of the ideal gas, the kinks, and it sustains the total phase evolution along the chain against collisions of the kinks at the end of the

chain that try to unravel it. (ii) The particles on the chain may be of two types, kinks and antikinks, so that the collisions at the end of the chain twist it both clockwise and counterclockwise.

V. CONCLUSION

We have studied the equilibrium statistical mechanics of the sine-Gordon system. We have employed transfer-integral techniques to work out the free energy, torque, average value of θ_{n+1}^2, etc. Formally exact expressions for these quantities can be implemented once the solution to the appropriate transfer-integral problem is in hand. We discuss a number of subtleties associated with the TI problem. Approximate solutions to the TI problem in various limits are discussed and numerical and other evidence for the validity of these approximations is presented.

The equilibrium statistical mechanics in the canonical ensemble, depends upon the identification of the Helmholtz free energy and physically meaningful thermodynamic variables. We argue that the appropriate thermodynamic variables for the sine-Gordon chain are temperature and phase, that phase is generated by a torque reservoir, etc. Our use of these variables is to be contrasted to the thermodynamics of Gupta and Sutherland which employs a chemical potential (equivalent to our torque) and pressure (which does not exist).

We examine a variety of thermodynamic functions and statistical mechanical averages at both high and low temperature. By studying the average of θ_{n+1} we find compelling evidence that the solitons behave at low temperature like a gas of noninteracting particle

ACKNOWLEDGMENT

Work partially supported by the NSF under Grant No. DMR-76-14447.

APPENDIX A: THE CONTINUUM APPROXIMATION

The total energy is given by the Hamiltonian density

$$E(\pi,\phi)=\int_0^L [\tfrac{1}{2}I\omega^2+\tfrac{1}{2}\Gamma(\phi')^2+V(\phi)]\rho\,dx, \qquad \text{(A1)}$$

where ρ is a suitably defined density. The equation of motion for ϕ has a solution asymptotic to $\pm\pi$ at $x\to\pm\infty$ of the form $[V(\phi)=-V_1\cos\phi]$

$$\phi(x,t)=4\tan^{-1}\left[\exp\left(\pm\frac{x-vt}{d(1-v^2/c^2)^{1/2}}\right)\right] \qquad \text{(A2)}$$

which describe the sine-Gordon solitons ($c^2=\Gamma/I$ and $d^2=\Gamma/V_1$). The energy of the system with a single static soliton present is

$$E_\phi=8\sqrt{V_1\Gamma}\rho. \qquad \text{(A3)}$$

The length of a static soliton is

$$d=\sqrt{\Gamma/V_1}. \qquad \text{(A4)}$$

To discretize the continuum field we divide the line $(0,L)$ into M equal units of length Δx:

$$\Delta x=L/M.$$

Then we have

$$\rho\int dx\,V(\phi)\to\sum_{i=1}^{M}\rho\Delta x\,V(\phi_i)$$

and

$$\rho\int dx\,\frac{\Gamma}{2}(\phi')^2\to\sum_{i=1}^{M}\rho\Delta x\Gamma\,\frac{(\phi_{i+1}-\phi_i)^2}{\Delta x^2}.$$

Comparison with Eq. (1) leads to

$$V_1\rho\Delta x\to E_1 \qquad \text{(A5)}$$

and

$$\Gamma\rho/\Delta x\to E_2. \qquad \text{(A6)}$$

In terms of the variables of Eq. (1) the soliton energy is $E_\phi=8\sqrt{E_1E_2}$ and the length of the soliton, measured in units Δx, is $d/\Delta x=\sqrt{E_2/E_1}$.

APPENDIX B: MODIFIED BESSEL FUNCTION IDENTITIES

In this appendix we list the collection of identities and several asymptotic expansions for the modified Bessel functions that are useful in the evaluation of various averages. From Abramowitz and Stegun we have (9.6.26)

$$I_{\nu-1}(z)-I_{\nu+1}(z)=2(\nu/z)I_\nu(z) \qquad \text{(B1)}$$

and

$$I_{\nu-1}(z)+I_{\nu+1}(z)=2\frac{d}{dz}I_\nu(z). \qquad \text{(B2)}$$

The Bessel function addition theorem (9.1.75),

$$J_\nu(v)=\sum_{l=-\infty}^{\infty}J_{\nu-l}(v-u)J_l(u)$$

and the identity (9.6.3),

$$I_\nu(z)=(-i)^\nu J_\nu(iz),\quad -\pi<\arg z\le\tfrac{1}{2}\pi$$

yield

$$I_\nu(v)=\sum_{l=-\infty}^{+\infty}I_{\nu-l}(v-u)I_l(u), \qquad \text{(B3)}$$

for real u and v. We may combine (B1) and (B2) to obtain

$$\sum_{l\infty}^{+\infty}lI_{\nu-l}(v-u)I_l(u)=u\nu I_\nu(v)/v, \qquad \text{(B4)}$$

$$\sum_{l=-\infty}^{+\infty} l^2 I_{\nu-l}(v-u) I(u) = \frac{u^2}{v^2}\nu^2 I_\nu(v) + u\left(1-\frac{u}{v}\right)\frac{dI_\nu(v)}{dv}, \quad \text{(B5)}$$

and

$$\sum_{ll'} ll' I_{\nu-l'}(v-u) I_{l'-l}(u-w) I_l(w) = \frac{wu}{v^2}\nu^2 I_\nu(v) + w\left(1-\frac{u}{v}\right)\frac{dI_\nu(v)}{dv}. \quad \text{(B6)}$$

APPENDIX C: SOLUTION TO THE TRANSFER-INTEGRAL EQUATION IN THE TIGHT-BINDING APPROXIMATION

The TI equation can be reduced to the Schrödinger equation in the form, Eq. (35) (see Fig. 6)

$$\left(-\frac{1}{2\lambda_2}\frac{d^2}{d\theta} - \lambda_1\cos\theta\right)\psi_\nu(\theta) = \beta\bar{\epsilon}_\nu\psi_\nu(\theta). \quad \text{(C1)}$$

In the limit $\lambda_1 \gg 1, \lambda_2 \gg 1$, we may solve this equation in the tight-binding approximation:

$$\psi_\nu(\theta) = \frac{1}{\sqrt{2\pi}}\sum_l e^{il\nu}\chi_0(\theta - 2\pi l) \quad \text{(C2)}$$

with $|\nu| \leq (n/2P)$ [n is an integer, $|n| \leq P$ and $\psi_\nu(\theta)$ is assumed to be periodic over $2\pi P$] and energy eigenvalue

$$\beta\bar{\epsilon}_\nu = -\lambda_1 + \tfrac{1}{2}(\lambda_1/\lambda_2)^{1/2} - \beta|t|\cos 2\pi\nu. \quad \text{(C3)}$$

In Eq. (C3) $|t|$ is related to the rate of tunneling from localization near $2\pi m$ to localization near $2\pi(m+1)$:

$$\beta|t| = 4(\lambda_1/\lambda_2)^{1/2}|\chi_0(0)|^2\exp(-8\sqrt{\lambda_1\lambda_2}). \quad \text{(C4)}$$

The parameters for the sine-Gordon soliton are its energy

$$\beta E_\phi = 8\sqrt{\lambda_1\lambda_2} \quad \text{(C5)}$$

and a measure of its size

$$d = \sqrt{\lambda_1/\lambda_2}. \quad \text{(C6)}$$

For the left-hand eigenfunction appropriate to the solution of Eq. (23) we have

$$\phi_\nu(\theta) = \frac{1}{\sqrt{2\pi}}\sum_l e^{-\nu l}\xi_0(\theta - 2\pi l), \quad \text{(C7)}$$

where [cf. Eq. (C2)]

$$\xi_0(\theta) = e^{-\lambda_1\cos\theta}\chi_0(\theta). \quad \text{(C8)}$$

Equation (C1) can be converted to the Mathieu equation (20.1.1), upon making the change of variable:

$$2\varphi + \pi = \theta, \quad \text{(C9)}$$

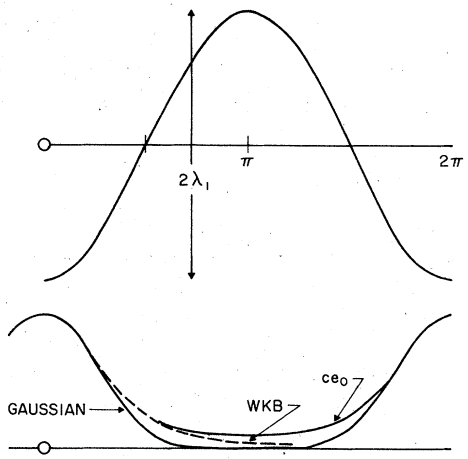

Fig. 6. The differential equation. Equation (35) or (C1) describes a particle of mass λ_2 in a periodic potential of amplitude $2\lambda_1$. As $T \to 0$ °K, $\lambda_1 \to L^+$, $\lambda_2 \to L^+$ and the differential equation becomes the Schrödinger equation for a heavy particle in a deep well. The particle is localized near $\theta, 2\pi, 4\pi, \ldots$ and well approximated (for the purpose of discussing the energy) by a Gaussian. The bandwidth of the particles is related to the rate of tunneling from $2\pi m$ to $2\pi(n+1)$. To calculate this rate accurately, the wave function and its derivative must be known at the barrier. The analytic results for the Mathieu equation may be used or the WKB wave function may be used to calculate the tunneling rate. The ground-state wave function $ce_0(\theta)$ is well approximated by the $k \to 0$ superposition of Gaussians (with suitably doctored WKB tails) centered at 0, 2π, $4\pi, \ldots$.

$$q = 4\lambda_1\lambda_2, \quad \text{(C10)}$$

and

$$a = 8\lambda_2\beta\bar{\epsilon}_\nu. \quad \text{(C11)}$$

Thus we may take over many of the known results for the Mathieu equation to check numerical work on Eq. (C1) and to obtain various analytic limits. The Mathieu equation is parametrized in terms of q and we use this variable in our discussion of the numerical work (Sec. III) and Fig. 3.

APPENDIX D: THE TRANSFER INTEGRAL AT LOW TEMPERATURE

As $T \to 0$ °K both λ_1 and λ_2 in Eq. (23) are large compared to 1. We take the solution to Eq. (29) in the form

$$\psi_\nu(\theta) = \frac{1}{\sqrt{2\pi}}\sum_l e^{i\nu l}\chi_0(\theta - 2\pi l) \quad \text{(D1)}$$

with $\chi_0(\theta - 2\pi l)$ solving Eq. (23) approximately near $\theta - 2\pi l$. We assume $\chi_0(\theta)$ to be given approximately by a Gaussian centered at $2\pi l$:

$$\chi_0(\theta) = A\exp(-\tfrac{1}{2}\alpha^2)(\theta - 2\pi l)^2. \quad \text{(D2)}$$

Substituting into Eq. (23) and integrating on θ_2 leads to

$$\beta\epsilon_0 = -\lambda_1 - \tfrac{1}{2}\ln\frac{2\pi}{\lambda_2}\ln\frac{2\pi}{\lambda_2} + \tfrac{1}{2}\sqrt{\lambda_1/\lambda_2} + \tfrac{1}{4}\lambda_1/\lambda_2 + O(\lambda_1/\lambda_2)^{3/2} \quad \text{(D3)}$$

and

$$\alpha^2 = \sqrt{\lambda_1\lambda_2}\,[1 + \tfrac{1}{2}\sqrt{\lambda_1\lambda_2} + O(\lambda_1/\lambda_2)]\,. \quad \text{(D4)}$$

Comparison with Appendix C shows that as $\lambda_1/\lambda_2 \to 0$ these values approach the values obtained from solution of the Mathieu equation. Thus the exact integral equation is solved to excellent approximation by the Mathieu equation for $\lambda_1 \gg 1$, $\lambda_2 \gg 1$, and $\lambda_2 \gg \lambda_1$. This result is verified in the numerical work discussed in Sec. III.

Since Eq. (23) admits a variational principle a solution in terms of the superposition of Gaussians, etc., is tractable.

A far more elegant demonstration of the reduction of the exact integral equation [or Eq. (29)] to the Mathieu equation in the limit $\lambda_1 \gg 1$, $\lambda_2 \gg 1$ is possible using a second cumulant expansion. We write Eq. (29) in the form

$$\exp\left(\frac{1}{2\lambda_2}\frac{d^2}{d\theta^2}\right)\psi_\nu(\theta) = e^{-\beta\epsilon_\nu}e^{-\lambda_1\cos\theta}\psi_\nu(\theta).$$

Multiply by $\psi_\nu(\theta)$ from the left [or $\phi_\nu(\theta)$] and integrate on θ. On the LHS this amounts to an average of $\exp[(1/2\lambda_2)(d^2/d\theta^2)]$, on the RHS this is the same average of $\exp(-\lambda_1\cos\theta)$. We exponentiate the average by using a cumulant expansion on the right and the left. Equating the leading cumulants on the right and left leads to the Mathieu equation The higher-order cumulants go to zero as $(\lambda_1/\lambda_2)^{n/2}$, etc.

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