Free energies for the discrete chain in a periodic potential and the dual Coulomb gas

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The partition function for a chain of particles connected by springs in a periodic potential is considered. This problem is dual to a one-dimensional Coulomb gas on a lattice. The free energies of both problems can be calculated from the eigenvalue of a transfer matrix. High-temperature expansions are obtained for free energies of both problems. The free energy of a system of alternating charges on a lattice is calculated exactly. Continuum results for the Coulomb gas and the sine-Gordon model are easily regained from the transfer-matrix approach. For the Villain potential the partition function can be written directly in terms of the kinks in the chain. The kinks are on sites of a lattice and interact through an exponential repulsion. The ground-state periodicity of this system exhibits a complete devil's staircase as a function of mismatch. For a similar potential the free energy can be calculated at all temperatures as the eigenvalue of a differential equation. A ladder of Josephson junctions is proposed as a new physical realization for this problem.

I. INTRODUCTION

In many physical systems there is a competition between some natural periodicity and the periodicity imposed by an underlying lattice. This competition results in an intriguing sequence of commensurate and incommensurate structures that have been extensively studied.[1–16] Examples of such phenomena have been observed in adsorbed layers,[1] charge-density-wave conductors,[2] and chain compounds such as $Hg_{3-\delta}AsF_6$.[3] To study the atoms in the vicinity of a dislocation core Frenkel and Kontorova[4] introduced the problem of a one-dimensional chain of particles connected by springs and subject to a periodic substrate potential. The Hamiltonian for the system is

$$\mathcal{H}=\sum_n \left[\frac{\hat{\mu}}{2}(u_{n+1}-u_n-\epsilon)^2+\frac{\hat{W}}{2}\cos(2\pi u_n) \right] . \quad (1.1)$$

The natural period ϵ of the chain competes with the substrate periodicity which is taken to be unity. This system has been studied by several authors. Since, in one dimension ordered phases occur only at zero temperature, the focus of most of the work has been to obtain the ground state of the chain by solving the force equations (Refs. 5–16) $\partial\mathcal{H}/\partial u_n=0$, i.e.,

$$\hat{\mu}(u_{n+1}-2u_n+u_{n-1})=\pi\hat{W}\sin(2\pi u_n) . \quad (1.2)$$

The incommensurability ϵ does not appear in the force equations. Therefore, the solution of Eq. (1.2) has to be selected that minimizes the energy for a given ϵ. Frank and van der Merwe[5] obtained the ground states in the continuum limit, where the difference on the left-hand side of Eq. (1.2) is replaced by a second derivative. For $\epsilon<\epsilon_c=2/\pi l_0$ [$l_0=(\hat{\mu}/2\hat{W})^{1/2}$], the commensurate structure with all particles located in the potential minima has the lowest energy. For $\epsilon>\epsilon_c$ the ground state is best described as a series of equally spaced kinks. Each kink (or soliton) is the boundary between roughly commensurate domains. Since the kink separation varies continuously with ϵ this phase is generally incommensurate with the underlying lattice and has a zero-frequency phonon mode. In the discrete problem there is a Peierls energy[6,7] (approximately[8] $4\pi^2\hat{\mu}e^{-\pi^2 l_0}$) for pinning the kinks to the substrate minima that gives rise to higher-order commensurate structures.[9]

The discrete force equations (1.2) are equivalent to a two-parameter mapping describing the time evolution of a sinusoidally driven pendulum and have been studied in the context of dynamical systems.[10,11] Typical trajectories for this map are chaotic. However, Aubry[12,13] has demonstrated that the trajectories that correspond to ground states of Eq. (1.1) are either fixed cycles (commensurate states), or smooth Kolmogorov-Arnold-Moser orbits. Many other results for the discrete problem such as the quasiperiodicity of the ground state are due to Aubry.[12,13] Certain questions, such as the scaling properties near the commensurate-incommensurate transitions, are still not entirely resolved.[14] A good review of these and other related problems can be found in the review article by Pokrovsky, Talapov, and Bak.[15]

Another approach is to calculate the partition function of the chain.[17–19] The ground-state energy can then be obtained as the zero-temperature limit of the free energy. The partition function also contains information about finite-temperature properties that are relevant to physical systems.[18,19] In this paper the relation between the discrete chain and a number of other one-dimensional problems is demonstrated by mappings of the partition function. In Sec. II it is shown that the problem is dual to a Coulomb gas on a one-dimensional lattice. Due to the long-range nature of the Coulomb interaction this problem cannot be treated directly. However, by rewriting the Hamiltonian in terms of electric fields the interactions become local, and the partition function can be calculated by a transfer-matrix method. At high temperatures successive approximations can be made by truncating the size

of the matrix, which is equivalent to restricting the possible values of the electric field. Thus in Sec. III we obtain a high-temperature expansion for the chain free energy, and also evaluate the free energy of the lattice Coulomb gas. Schotte and Truong[20] have demonstrated that for an alternating sequence of charges in the continuum limit, there is a phase transition if periodic boundary conditions are imposed. The analog of this result in the lattice problem is easily obtained from the transfer-matrix formalism. By letting the lattice spacing approach zero, results for the continuum Coulomb gas (such as the pressure of a many-component plasma[21–23]) are obtained in Sec. IV.

The Coulomb-gas description is not particularly useful for studying the discrete chain at zero temperature. However, in Sec. V it is shown that for the special case of the Villain potential the Hamiltonian can be written directly in terms of the kinks. The kinks are now pinned to the lattice and are subject to an exponential repulsion. The periodicity of the ground states exhibits a complete devil's staircase as a function of incommensuration. Finally a ladder of Josephson junctions is proposed as a new physical system where the predictions of this paper can be tested.

II. THE DUAL COULOMB GAS

The partition function for the chain is obtained from

$$Z=\int_{-\infty}^{\infty}\prod_{n=1}^{N}du_n\exp\left[\sum_n\left[\frac{\mu}{2}(u_{n+1}-u_n-\epsilon)^2+V(u_n)\right]-\Theta\frac{\mu}{2}(u_N-u_1)^2\right]. \tag{2.1}$$

where $\mu=\beta\hat{\mu}=\hat{\mu}/kT$, and $\Theta=0$ (1) corresponds to an open (closed) chain. A general periodic potential $kTV(u)$ is considered. Since $V(u)=V(u+n)$ it is possible to make a Fourier expansion

$$e^{-V(u_n)}=\sum_{\{m_n\}}e^{-\tilde{V}(m_n)+2\pi i m_n u_n}. \tag{2.2}$$

After substituting (2.2) into (2.1) it is possible to do the Gaussian integrals involving $\{u_n\}$, and

$$Z=Z_{\rm ph}\sum_{\{m_n\}}{}'\exp\left[-\sum_n[\tilde{V}(m_n)-2\pi i n m_n\epsilon]+\frac{\pi^2}{2\mu}\sum_{n,l}m_n m_l\times|n-l|\left[1-\Theta\frac{|n-l|}{N}\right]\right], \tag{2.3}$$

where $Z_{\rm ph}=(2\pi/\mu)^{N/2}$ is the contribution of phonons to the partition function. The summation over $\{m_n\}$ is restricted such that $\sum_n m_n=0$, and hence Eq. (2.3) represents the partition function of an overall neutral gas of charged particles on a lattice. An energy $\tilde{V}(m)$ is associated with creating a charge of magnitude m [$\tilde{V}(m)=\tilde{V}(-m)$ for an even potential $V(u)$], and the charges are subject to an *imaginary* electric field $2\pi i\epsilon$. In the presence of a mismatch ϵ the Coulomb-gas Hamiltonian is no longer Hermitian, although the positivity of the partition function is assured. The Coulomb interaction in one dimension is $U(r)=|r|$ for charges on a line (open chain, $\Theta=0$), and $U(r)=|r|(1-|r|/N)$ for charges on a circle of length N (closed chain, $\Theta=1$).[20] In the thermodynamic limit ($N\to\infty$) the two potentials are equivalent, although there can be differences if only restricted charge configurations are examined.[20] The one-dimensional lattice Coulomb gas is dual to the discrete sine-Gordon chain in the sense that the high-temperature properties of one problem are related to the low-temperature properties of the other. Unfortunately there is no obvious interpretation for the charges as excitations in the original problem.

Due to the long-range nature of the Coulomb interaction, it is not easy to evaluate the partition function, Eq. (2.3), directly. However, it can be rewritten in terms of electric fields (bond variables), instead of electric charges (site variables). In one dimension since the number of sites is equal to the number of bonds, either set of variables can be used in the partition function sum. The charges m_n are related to the fields e_n on bonds by

$$m_n=e_n-e_{n-1}, \tag{2.4}$$

and the partition function takes the particularly simple form

$$Z_c=\sum_{\{e_n\}}\exp\left[-\sum_n\left[\tilde{V}(e_n-e_{n-1})-2\pi i\epsilon e_n+\frac{2\pi^2}{\mu}e_n^2\right]\right]. \tag{2.5}$$

For the Coulomb gas on a line the boundary conditions are $e_0=e_N=0$, which ensure overall charge neutrality. This condition in conjunction with Eq. (2.4) restricts $\{e_n\}$ to integer values. On a circle (2.4) automatically ensures charge neutrality, while the extra condition $\sum_{n=1}^{N}e_n=0$ must be satisfied (for the continuity of the electric potential). In this case $\{e_n\}$ are no longer restricted to integer values, as will be demonstrated in the next section.

Since the interactions in Eq. (2.5) are nearest neighbor, a transfer matrix T can be used to evaluate the partition function. The elements of T,

$$\langle m|T|n\rangle=\exp\left[-\left[\tilde{V}(m-n)+\frac{2\pi^2}{\mu}m^2-2\pi i\epsilon m\right]\right], \tag{2.6}$$

decay exponentially with temperature, and this approach is most useful at high temperatures. The partition function is calculated from $Z_c=\langle 0|T^N|0\rangle\simeq\lambda_{\rm max}^N$, where $\lambda_{\rm max}$ is the largest eigenvalue of the transfer matrix. Alternatively, the transfer matrix can be written in Fourier space, where

$$T(q)=e^{-V(q)}\exp\left[\frac{1}{2\mu}\frac{d^2}{dq^2}-\epsilon\frac{d}{dq}\right],$$

and the eigenvalue equation becomes

$$\exp\left[\frac{1}{2\mu}\frac{d^2}{dq^2}\right]e^{-V(q)}y(q)=\lambda y(q+\epsilon). \tag{2.7}$$

The eigenfunction $y(q)$ has to be periodic in q. It is not easy to deal with this nonlocal equation. The WKB approximation is applied to (2.7) in Appendix A, and the results of Frank and van der Merwe[5] are rederived by this method. For a potential composed of quadratic segments, Eq. (2.7) can be reduced to a simple second-order differential equation as shown in Appendix B.

The differential equation in (2.7) can also be written as an integral equation, using the identity

$$\exp\left[\frac{1}{2\mu}\frac{d^2}{dq^2}-\epsilon\frac{d}{dq}\right]F(q) = -\int_{-\infty}^{\infty}K(q-q',\epsilon,\mu^{-1})F(q')dq' . \quad (2.8)$$

The kernel $K(q-q',\epsilon,\mu^{-1})$ satisfies the equation $\partial K/\partial(1/\mu)=\frac{1}{2}\partial^2 K/\partial q^2$. Together with the boundary condition $K(q-q',\epsilon,0)=\delta(q-q'-\epsilon)$ this implies

$$K=\left[\frac{\mu}{2\pi}\right]^{1/2}\exp\left[-\frac{\mu(q-q'-\epsilon)^2}{2}\right] .$$

Therefore, Eq. (2.7) is equivalent to the integral equation

$$\left[\frac{\mu}{2\pi}\right]^{1/2}\int_{-\infty}^{\infty}dq' e^{-\mu/2(q-q'-\epsilon)^2-V(q')}y(q')=\lambda y(q) . \quad (2.9)$$

This integral equation could have been obtained by applying the transfer-matrix method directly to the partition function in Eq. (2.1), and provides a check on the validity of previous transformations. Equation (2.9) has been used in calculating free energies for the discrete chain.[18]

III. THE FINITE-FIELD APPROXIMATION

A. The discrete chain

The elements of the transfer matrix $\langle m \mid T \mid n \rangle$, Eq. (2.6), decay as $e^{-(2\pi^2/\mu)m^2}$ for large m at finite temperatures. Therefore, to a good approximation the infinite matrix can be replaced by a finite-sized matrix. Successive approximations would correspond to increasing the size of the matrix. To order of x^3 ($x=e^{-2\pi^2/\mu}$) it is sufficient to consider a 3×3 matrix with m restricted to -1, 0, and $+1$. The eigenvalue equation is

$$\lambda^3-e^{-\tilde{V}(0)}[1+2x\cos(2\pi\epsilon)]\lambda^2+x[2(e^{-2\tilde{V}(0)}-e^{-2\tilde{V}(1)})\cos(2\pi\epsilon)+x(e^{-2\tilde{V}(0)}-e^{-2\tilde{V}(2)})]\lambda - x^2(e^{-3\tilde{V}(0)}-e^{\tilde{V}(0)-2\tilde{V}(2)}+2e^{-2\tilde{V}(1)-\tilde{V}(2)}-2e^{-\tilde{V}(0)-2\tilde{V}(1)})=0 . \quad (3.1)$$

Since this equation is valid to $O(x^3)$, the free energy $-\beta f=\ln\lambda$ can also be expanded to this order as

$$-\beta f=\tilde{V}(0)+2xz_1^2\cos(2\pi\epsilon)-2x^2z_1^2[1-z_2-\cos^2(2\pi\epsilon)(2-3z_1^2)] -2x^3z_1^2\cos(2\pi\epsilon)[3-2z_2-8z_1^2-z_2^2+8z_1^2z_2-2\cos^2(2\pi\epsilon)(2-6z_1^2+5z_1^4)]+O(x^4) , \quad (3.2)$$

where $z_n=e^{-\tilde{V}(n)+\tilde{V}(0)}$. Note that the variation of free energy (and hence other thermodynamic quantities) with the incommensuration ϵ decays exponentially with temperature (as $z_1^2e^{-2\pi^2kT/\hat{\mu}}$). By contrast for the continuum sine-Gordon chain a much slower decay (as $[\hat{\mu}^2\hat{V}^2/(kT)^4]$) is expected.[17,19] Thus the effect of springs is masked much faster at high temperatures for a discrete chain. The ratio of eigenvalues is related to the correlation function, and the correlation length ξ goes to zero as $\xi\simeq\hat{\mu}/(2\pi^2kT)$. The variation of the free energy with ϵ at zero temperatures is very complex (describing a devil's-staircase structure). This complexity is washed out at finite temperatures, and at high temperatures is replaced by $\cos(2\pi\epsilon)$. In particular the amplitude for a $\cos(2\pi p\epsilon)$ variation goes to zero as $e^{-2\pi^2p^2\hat{\mu}/kT}$.

The expansion in (3.2) is valid for any potential. For the cosine potential $V(u)=W\cos(2\pi u)$, an expansion in powers of W yields

$$-\beta f=\frac{W^2}{2}[\tfrac{1}{2}+x\cos(2\pi\epsilon)+x^2\cos(4\pi\epsilon)+x^3\cos(6\pi\epsilon)] -\frac{W^4}{16}\{\tfrac{1}{4}+4x\cos(2\pi\epsilon)+x^3[2+3\cos(4\pi\epsilon)] +6x^3\cos(6\pi\epsilon)\}+O(W^6,x^4) . \quad (3.3)$$

The above expansion suggests that the complete coefficient of W^2, to all orders in x, is

$$\tfrac{1}{4}+\tfrac{1}{2}\sum_{n=1}^{\infty}x^n\cos(2\pi n\epsilon)=\frac{1}{4}\frac{1-x^2}{1-2x\cos(2\pi\epsilon)+x^2} .$$

This is, in fact, correct and can be readily observed from an expansion of the partition function in (2.3), since a pair of charges ± 1 separated a distance n contributes

$$z_1^2\exp\left[-\frac{2\pi^2}{\mu}n\pm 2\pi i\epsilon n\right]\rightarrow\frac{W^2}{2}x^n\cos(2\pi n\epsilon)$$

(adding the two dipole directions) to the partition function. The charge configurations leading to Eq. (3.2) are $+\cdots-$, $+\cdots\bullet\cdots-$, $+\cdots=\cdots+$, and their charge conjugates.

B. The lattice Coulomb gas

The Hamiltonian for the one-dimensional lattice Coulomb gas in the grand canonical ensemble is

$$-\beta\mathcal{H}=\frac{\beta e^2}{2}\sum_{i,j}m_im_jV(\mid i-j\mid)-\sum_{i=1}^{N}\beta\mu(m_i) , \quad (3.4)$$

where e^2 characterizes the strength of the Coulomb interaction $U(r)=\mid r\mid[1-\Theta(\mid r\mid/N)]$, and $z_n=e^{-\beta\mu(n)}$ is the fugacity of a charge of n units. For a one-component

plasma only z_1 is nonzero. As demonstrated in Sec. II the partition function for the Coulomb gas can be written in terms of electric fields and evaluated by a transfer-matrix method. Approximating the transfer matrix by finite-size matrices corresponds to restricting the maximum value of the electric field (or asserting that the system undergoes electric breakdown for fields exceeding a critical value). This is in fact a physically appropriate restriction.

It is necessary to examine the effects of boundary conditions more carefully. For the Coulomb gas on a line ($\Theta=0$) the boundary conditions $e_0=e_N=0$ together with (2.4) restrict $\{e_n\}$ to integer values. For the Coulomb gas on a circle the nonlocal constraint $\sum_{n=1}^{N}e_n=0$ has to be satisfied, and although the differences between the fields are integral, the fields $\{e_n\}$ are no longer restricted to integer values. For any configuration of charges $\{m_n\}$ on the circle, the fields can be written as $e_n=q_n+d$, where q_n are integers [$m_n=q_n-q_{n-1}$ from (2.4)] and d has to be chosen such that $\sum_{n=1}^{N}e_n=0$. This nonlocal constraint can be incorporated by a Hamiltonian minimization principle.[24] The Hamiltonian (3.4) can be rewritten in terms of electric fields as

$$-\beta\mathscr{H}(d)=-\sum_n[\beta e^2(q_n+d)^2+\beta\mu(q_n-q_{n-1})]\ . \tag{3.5}$$

Let us regard d as a variable. For any configuration $\{q_n\}$ the minimum of $\mathscr{H}(d)$ is obtained for

$$\frac{\partial\mathscr{H}(d)}{\partial d}=0\Longrightarrow\sum_n(q_n+d)=\sum_n e_n=0\ . \tag{3.6}$$

Thus for any configuration of $\{q_n\}$ evaluating $\mathscr{H}(d)$ at its minimum ensures that the condition $\sum_{n=1}^{N}e_n=0$ is satisfied. This Hamiltonian minimization in fact defines a new Hamiltonian, and it can be shown that the free energy of the minimized Hamiltonian is obtained by minimizing the free energy of the original Hamiltonian as a function of d.[24] Therefore, the free energy on a circle is given by $\beta f=\min[-\ln\lambda_{\max}(d)]_d$, where $\lambda_{\max}(d)$ is the largest eigenvalue of the transfer matrix

$$\langle m\mid T(d)\mid n\rangle=z_{m-n}\exp\left[-\frac{\beta e^2}{2}[(m+d)^2+(n+d)^2]\right]\ . \tag{3.7}$$

In most cases in the thermodynamic limit ($N\to\infty$) the boundary conditions are not important, and the minimum occurs at $d=0$. However, only when restricted charge configurations are considered boundary conditions become important.[20]

An example is provided by allowing only sequences of alternating charges ±1, which is equivalent to a series of dipoles with the same orientation. The continuum version of this problem has been studied by Schotte and Truong.[20] In this case the electric field can only take two possible values, e.g., $e_n=d-\frac{1}{2}$, $d+\frac{1}{2}$ (note the shift of d by $\frac{1}{2}$ which is just a convenient change of variables). The corresponding transfer matrix is 2×2, and using (3.7, is given by

$$T(d)=e^{-\beta e^2(d^2+1/4)}\begin{bmatrix}e^{-\beta e^2 d} & z_1\\ z_1 & e^{\beta e^2 d}\end{bmatrix}\ . \tag{3.8}$$

Since on the line ($\Theta=0$) the fields $\{e_n\}$ must be integers the free energy is obtained by setting $d=\frac{1}{2}$ or $-\frac{1}{2}$, and is given by

$$\beta f=-\ln[\lambda_{\max}(\tfrac{1}{2})]=\frac{\beta e^2}{2}-\ln\left\{\cosh\left[\frac{\beta e^2}{2}\right]+\left[\sinh^2\left[\frac{\beta e^2}{2}\right]+z_1^2\right]^{1/2}\right\}\ . \tag{3.9}$$

By contrast, on a circle the free energy is obtained from

$$\beta f=\min(\beta e^2(d^2+\tfrac{1}{4})-\ln\{\cosh(\beta e^2 d)+[\sinh^2(\beta e^2 d)+z_1^2]^{1/2}\})_d\ . \tag{3.10}$$

The function to be minimized has the typical Landau double-well dependence on d. Expanding about $d=0$ gives

$$\frac{f}{e^2}=\min\left[\tfrac{1}{4}-\ln(1+z_1)+d^2\left[1-\frac{\beta e^2}{2z_1}\right]+\frac{d^4}{3}\left[\frac{\beta e^2}{2z_1}\right]^3(3-z_1^2)+O(d^6)\right]_d\ . \tag{3.11}$$

There is a classical second-order phase transition for $\beta e^2=2z_1$. The low-temperature phase is a gas of similarly oriented dipoles that dissociate at the transition temperature. The phase boundary is identical to that obtained by Schotte and Truong in the continuum limit,[20] which is rather surprising since the actual free energies are very different. (These results do not apply to the sine-Gordon chain where all configurations have to be considered.)

There is a close correspondence between the alternating sequence of charges and the one-dimensional Ising model. Comparison of the low-temperature expansions for the nearest-neighbor Ising model with the alternating Coulomb gas on a line indicates that the two partition functions become proportional with the identification $2H=e^2$ and $z_1=e^{-2\beta K}$ (K is the nearest-neighbor interaction and H is the magnetic field in the Ising model). Similarly the alternating Coulomb gas on a circle is related to a one-dimensional Ising model subject to both nearest-neighbor and infinite-range interactions, which also has a classical phase transition.[25]

In the next level of approximation the field is allowed to take on three values, $e_n=d-1$, d, $d+1$. This would again correspond to examining a sequence of dipoles, but the dipoles are not required to point in the same direction anymore. The 3×3 transfer matrix from (3.7) is

$$T(d)=e^{-\beta e^2 d^2}\begin{bmatrix} e^{-\beta e^2(2d+1)} & z_1 e^{-\beta e^2(d+1/2)} & z_2 e^{-\beta e^2} \\ z_1 e^{-\beta e^2(d+1/2)} & 1 & z_1 e^{-\beta e^2(-d+1/2)} \\ z_2 e^{-\beta e^2} & z_1 e^{-\beta e^2(-d+1/2)} & e^{-\beta e^2(-2d+1)} \end{bmatrix} . \tag{3.12}$$

The largest eigenvalue $\lambda_{\max}(d)$ is always maximized for $d=0$, and hence in this case the free energies of the Coulomb gases on the line and the circle are identical and given by

$$\beta f=-\ln\left\{\frac{1+e^{-\beta e^2}(1+z_2)}{2}+\left[\left[\frac{1-e^{-\beta e^2}(1+z_2)}{2}\right]^2+2z_1^2 e^{-\beta e^2}\right]^{1/2}\right\} . \tag{3.13}$$

There is no longer a transition between the gas of dipoles at low temperatures and the dissociated plasma at high temperatures. For a one-component plasma $z_2=0$, and expressions (3.10) and (3.13) for the free energy are similar except that z_1^2 is replaced by $2z_1^2$. This result has a simple physical interpretation. For the Coulomb gas on a line the energy of a sequence of dipoles is independent of their orientations. For $e_n=0,1$ each dipole has a unique orientation and a fugacity of z_1^2, while for $e_n=-1,0,1$ both orientations are possible with an effective fugacity of $2z_1^2$. The convergence of the finite-field approximation for the one-component plasma with $\mu_1=e^2$ is demonstrated in Fig. 1. The free energies corresponding to (3.13) and the next level of approximation with $e_n=0,\pm1,\pm2$ (calculated by numerically diagonalizing a 5×5 matrix) are plotted.

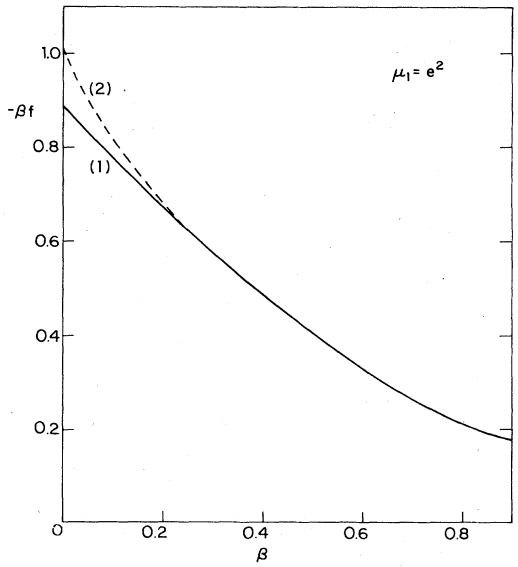

FIG. 1. Free energies of the discrete one-component Coulomb plasma with possible electric fields $e_n=0,\pm1$ (solid line) and $e_n=0,\pm1,\pm2$ (dashed line). The free energy with e_n unrestricted is not distinguishable from the dashed line on this scale.

The free energies converge rapidly and in fact the free energy of the unrestricted one-component plasma on a lattice cannot be distinguished from the $|e_n|\leq2$ approximation on the scale of Fig. 1.

IV. THE CONTINUUM LIMIT

A number of results are known for the continuum Coulomb gas and sine-Gordon systems in one dimension.[17,19,21–23] In this section it is demonstrated that these results can be obtained easily be taking the appropriate continuum limit of the equations in previous sections. Consider an interval of length L, subdivided into a lattice of N sites separated by a distance (a). The continuum limit is obtained by letting $a\to0$ and $N\to\infty$, while $L=Na$ is fixed. The appropriate way to scale the parameters of the Coulomb gas is $-\beta e^2\to-\beta e^2 a$, $-\beta f\to\beta p a$, and $z_n\to z_n a$. Since $-\beta e^2$ and $-\beta f$ represent energies per bond (energy densities) it is clear that they should scale with a, while the scaling form $z_n\to z_n a$ is necessary to keep the density of charges finite as $a\to0$.

For a many-component plasma, a potential $V(q)$ can be constructed from

$$e^{-V(q)}=\sum_n e^{-\tilde{V}(n)+inq}=1+2a\sum_{n\neq0}z_n\cos(nq)\underset{a\to0}{=}\exp\left[2a\sum_n z_n\cos(nq)\right] . \tag{4.1}$$

The transfer-matrix equation in Fourier space corresponding to Eq. (2.7) with $\epsilon=0$ is

$$\exp\left[\beta e^2 a\frac{d^2}{dq^2}\right]\exp\left[2a\sum_n z_n\cos(nq)\right]y(q)=e^{\beta a p}y(q) , \tag{4.2}$$

with $y(q+2\pi)=y(q)$. As $a\to0$, $e^{aA}e^{aB}$ can be replaced by $e^{a(A+B)}$, and the pressure p is obtained from the largest eigenvalue of

$$\left[\beta e^2\frac{d^2}{dq^2}+2\sum_n z_n\cos(nq)\right]y(q)=\beta p y(q) . \tag{4.3}$$

For a one-component plasma only z_1 is nonzero, and Eq. (4.3) reduces to Mathieu's equation.[26] The pressure is then given by $p=-(e^2/4)a_0(4z_1/\beta e^2)$, the result obtained by Lenard[21] and Prager[22] (a_0 is the lowest characteristic value of the Mathieu equation[26]). Equation (4.3) is the generalization of this result to a many-component plasma.[23]

Similarly the pressure of a gas of alternating charges is obtained by taking the continuum limits of Eqs. (3.9) and (3.10) as

$$p=-\frac{e^2}{2}\left\{1-\left[1+\left[\frac{2z_1}{\beta e^2}\right]^2\right]^{1/2}\right\} \tag{4.4}$$

on a line, and

$$p=e^2\min\left\{d^2+\frac{1}{4}-\left[d^2+\left[\frac{z_1}{\beta e^2}\right]^2\right]\right\}_d \tag{4.5}$$

on a circle. These results are identical to those obtained by Schotte and Truong[20] who directly examined the continuum problem. Finally, the continuum analog of Eq. (3.13), describing a two-component plasma with the electric field restricted to $e(x)=0,\pm1$, is given by

$$p=-\frac{e^2}{2}\left\{1-\frac{z_2}{\beta e^2}-\left[\left[1-\frac{z_2}{\beta e^2}\right]^2+2\left[\frac{2z_1}{\beta e^2}\right]^2\right]^{1/2}\right\}. \tag{4.6}$$

The continuum sine-Gordon model[17] is obtained by replacing $\sum_n(u_n-u_{n-1}-\epsilon)^2$ in Eq. (1.1) with $\int dn(\partial u/\partial n-\epsilon)^2$, and regarding n as a continuous variable. This is a good approximation to the discrete chain when (Ref. 5) $l_0=(\hat{\mu}/2\hat{W})^{1/2}\gg1$ and $\epsilon\ll1$. At finite temperatures the free energy per unit length is obtained from an eigenvalue equation as in Eq. (2.7), with

$$T(q)=e^{-V(q)}\exp\left[\frac{1}{2\mu}\frac{d^2}{dq^2}-\epsilon\frac{d}{dq}\right]$$
$$\approx\exp\left[\frac{1}{2\mu}\frac{d^2}{dq^2}-\epsilon\frac{d}{dq}-V(q)\right].$$

Correction terms in the exponential operator, of the order of $\epsilon V'$ and $V/\mu\approx1/l_0^2$, are ignored. The free energy is then obtained as the eigenvalue of the operator

$$\mathscr{H}=\frac{1}{2\mu}\frac{d^2}{dq^2}-\epsilon\frac{d}{dq}-V(q).$$

This eigenvalue is calculated by Burkov and Talapov[19] using a WKB approximation. The free energy obtained in this approximation fails to describe the discrete chain at high temperature, where Eq. (3.2) is appropriate.

V. DEVIL'S-STAIRCASE STRUCTURES AT ZERO TEMPERATURE

A. The discrete chain and the Villain potential

The most interesting properties of the discrete chain occur at zero temperature, where many ground states of different periodicities are expected. The dual Hamiltonian, Eq. (2.5), is only useful at high temperatures. However, by using the Poisson summation formula it can be converted to a form appropriate to low temperatures. The Poisson summation formula replaces $\sum_{e_n}$ by $\int de_n\sum_{k_n}e^{-2\pi ik_ne_n}$. It will then be possible to do the integration over $\{e_n\}$ for a Villain potential, defined by its Fourier components $\tilde{V}(m)=m^2/W$. Equation (2.5) is now transformed to

$$Z_c=\sum_{\{k_n\}}\int_{-\infty}^{\infty}\prod_n de_n\exp\left\{-\sum_n\left[\left[\frac{2}{W}+\frac{2\pi^2}{\mu}\right]e_n^2-\frac{2}{W}e_ne_{n-1}+2\pi i(k_n-\epsilon)e_n\right]\right\}. \tag{5.1}$$

Setting the Gaussian integration over $\{e_n\}$ gives

$$Z_c\propto Z_k=\sum_{\{k_n\}}\exp\left[-\frac{1}{\tau}\sum_{n,m}(k_n-\epsilon)e^{-|n-m|/l}(k_m-\epsilon)\right], \tag{5.2}$$

where τ is proportional to temperature and given by

$$\tau=\frac{2}{\pi l_0 W}\left[1+\frac{\pi^2}{4l_0^2}\right]^{1/2}, \tag{5.3}$$

and the length scale l is related to $l_0=(\mu/2W)^{1/2}$ by

$$\frac{1}{l}=\ln\left[1+\frac{\pi^2}{2l_0^2}+\frac{\pi}{l_0}\left[1+\frac{\pi^2}{4l_0^2}\right]^{1/2}\right]. \tag{5.4}$$

Since τ behaves like temperature Z_k can provide information about low-temperature properties of the system. In fact the variables k_n will be identified with kinks in the original chain. The constant of proportionality between the chain [Eq. (2.3)] and kink [Eq. (5.2)] partition functions is $\exp N[\ln(\pi/l_0)-1/2l]$ which is independent of temperature. Since Z_K is invariant under $k_n\to k_n+j$, $\epsilon\to\epsilon+j$, it is manifestly periodic in ϵ. Also, Z_K is even in ϵ and it is sufficient to consider the interval $0\le\epsilon\le\frac{1}{2}$.

For $\epsilon=0$, the ground state of the kink Hamiltonian has all k_n equal to zero, while for $\epsilon>0$, positive values of k_n are favored. Since there is roughly an energy $(m-\epsilon)^2$ associated with creating a kink $k_n=m$, close to zero temperature and for $\epsilon>0$ it is sufficient to consider $k_n=t_n=0,1$. Larger kink values are not energetically favorable in this system.[27] The kinks $\{t_n\}$ interact through a Hamiltonian

$$\mathscr{H}_K=[1-2\epsilon\coth(1/2l)]\sum_n t_n-\sum_{n\neq m}t_nt_me^{-|n-m|/l}+N\epsilon^2\coth(1/2l). \tag{5.5}$$

The mismatch ϵ has to exceed a critical value $\epsilon_c=[2\coth(1/2l)]^{-1}$ before any kinks appear in the system. Kinks separated by a distance x feel a repulsive interaction $e^{-|x|/l}$. In the limit $l_0\gg1$, $1/l=\pi/l_0$, and the interaction between kinks agrees with that calculated from the continuum sine-Gordon model.[5] It is interesting that in this model the kinks interact only through two-body interactions. Ignoring the lattice and balancing the energy gain for kink creation with their repulsion indicates that for $\epsilon>\epsilon_c$ the separation of kinks is roughly $x\approx-l\ln[\coth(1/2l)(\epsilon-\epsilon_c)]$.

In the sine-Gordon model the kinks are pinned to the lattice by a Peierls potential.[6–9] In contrast, in Eq. (5.5) the kinks are constrained to lie on the sites of the lattice. It is this pinning of kinks to lattice sites that results in a devil's-staircase structure for ground states. The $\{t_n\}$ in (5.5) are binary variables, and in fact $\mathcal{H}_K$ is equivalent to an Ising Hamiltonian with exponentially decaying antiferromagnetic interactions and subject to a magnetic field. Bak and Bruinsma[28] have recently demonstrated how the ground states of such Hamiltonians with general long-range antiferromagnetic interactions can be calculated. Their results are valid as long as the interactions $J(n)$ are a convex function of the range n. For the Hamiltonian $\mathcal{H}_K$,

$$J(n+1)+J(n-1)-2J(n)=2e^{-n/l}[\cosh(1/l)-1]>0\ , \tag{5.6}$$

and this condition is satisfied. Let q denote the density of kinks $[q=(1/N)\sum_n t_n]$. Then the ground states of the system have the following properties.[28]

(a) For every rational $q=m/n$, there is an n-fold degenerate ground state, such that the positions x_i of the ith kink are related by[29,30]

$$x_{i+p}-x_i=\text{Int}\left[p\frac{n}{m}\right] \text{ or Int}\left[p\frac{n}{m}\right]+1\ , \tag{5.7}$$

where Int denotes the integer part. For example, for $q=\frac{2}{9}$, first-neighbor kinks are separated by $\delta x_1=4$ or 5, second-neighbor kinks are separated by $\delta x_2=9$, etc. This kink structure is indicated in Fig. 2(a). These correspond to possible commensurate ground states of the chain.

(b) Each of the above states is stable for a range of mismatch values $\epsilon_-(q)<\epsilon<\epsilon_+(q)$. This range is obtained by requiring that the addition or removal of a single kink, and the subsequent rearrangement of kinks, does not reduce the energy. This is similar to obtaining ϵ_c by calculating when it is energetically favorable to add a kink to the system. The range of stability of each commensurate phase is

$$\delta\epsilon\left[\frac{m}{n}\right]=\frac{n}{\coth(1/2l)}\left[\frac{\sinh(1/2l)}{\sinh(n/2l)}\right]^2\ , \tag{5.8}$$

which depends on n but is independent of m.

(c) The kink density q exhibits a devil's staircase as a function of the mismatch ϵ, i.e., there are steps for every rational value of q. Adding the stability intervals, Eq. (5.8), for the rational values of q, indicates that the devil's staircase is *complete;* i.e., the rational values of q cover the whole $0\le\epsilon\le\frac{1}{2}$ interval, and there is no room for irrational q values.

This last result is surprising, since incommensurate states (corresponding to irrational q) are expected in the sine-Gordon chain. This is due to the nature of the Villain potential. It is continuous at finite temperatures, but becomes singular at zero temperature, where it is equivalent to a series of parabolas as indicated in Fig. 2(b). In fact, Aubry[13] has obtained the ground state of particles moving in such a potential by solving the force equation (1.2) explicitly. This work therefore demonstrates the equivalence of the complete devil's staircases obtained in a continuous system by Aubry,[13] and in an Ising model by Bak and Bruinsma.[28] The absence of incommensurate states results from the nondifferentiability of the potential and the failure of the Kolmogorov-Arnold-Moser theorem, as discussed by Aubry[13] and elsewhere.[14] It would be interesting to know if there are generalizations of Eq. (5.5) that allow incommensurate states.

Some of the transformations outlined in this paper can also be carried out in higher dimensions. The dual two-dimensional Coulomb gas has been considered by Nelson and Halperin,[31] while a two-dimensional analog of the kink Hamiltonian in (5.2) is obtained by Schulz.[32] For $\epsilon=\frac{1}{2}$, the kink Hamiltonian (5.5) becomes an Ising model with antiferromagnetic interactions,

$$\mathcal{H}=\sum_{i,j}\sigma_i\sigma_j e^{-|i-j|/l}\ .$$

This is the antiferromagnetic version of the Kac-Baker model,[33] where the free energy is obtained by undoing the transformations leading to (5.5), and solving an integral equation similar to (2.9).

The Villain potential actually changes shape with temperature, and is continuous at finite temperatures. By contrast the Aubry potential can be defined to have the form in Fig. 2(b) at all temperatures, i.e.,

$$V(q)=W\pi^2[q-\text{Int}(q+\tfrac{1}{2})]^2\ . \tag{5.9}$$

The free energy for this potential can be obtained at all temperatures as the eigenvalue of a simple differential equation. The differential equation is calculated from Eq. (2.7) with the details given in Appendix B. The free energy $-\beta f$ is the eigenvalue of the equation $(0\le\epsilon\le\frac{1}{2})$

$$-\beta f y(q)=K\left[\frac{1}{2\mu}\frac{d^2}{dq^2}-\epsilon\frac{d}{dq}-W\pi^2q^2-\frac{W\pi^2}{\mu}q\frac{d}{dq}+W^2\pi\epsilon q+\frac{\mu\epsilon^2}{2}(1-K^{-1})-\frac{W\pi^2}{2\mu}\right]y(q)\ , \tag{5.10}$$

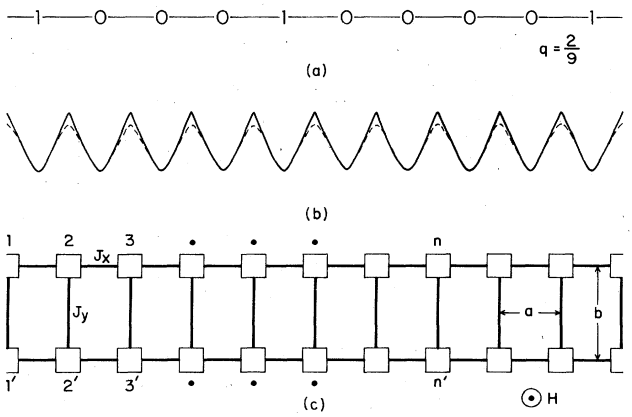

FIG. 2. (a) The kink structure for the ground state with $q=\frac{2}{9}$. (b) The zero-temperature Villain potential (solid line) and the cosine potential (dashed line). (c) The Josephson-junction ladder. The superconducting regions on the sites of the ladder are coupled to their nearest neighbors.

with $K=2/\pi^2 Wl\tau$, and periodic boundary conditions $y(\frac{1}{2})=y(-\frac{1}{2})$ and $dy/dq(\frac{1}{2})=dy/dq(-\frac{1}{2})$. For $\epsilon=0$, Eq. (5.10) is the Schrödinger equation for a particle in the Aubry potential. I am unaware of any other context, where Eq. (5.10) with $\epsilon\neq 0$ may have been studied.

B. Josephson-junction ladders

Yet another system with a behavior similar to the discrete chain is a ladder of Josephson junctions in a magnetic field. This system was pointed out to me by T. C. Halsey. Two-dimensional Josephson-junction arrays have been constructed, and studied both experimentally[34–36] and theoretically.[37,38] It should also be possible to construct arrays in the form of ladders as indicated in Fig. 2(c). The superconducting regions, placed at the sites of the ladder, are assumed to couple only to their nearest neighbors. Let θ_n ($\theta_{n'}$) denote the phase of the superconducting wave function on site n (n') of the upper (lower) branch of the ladder. The Hamiltonian for the system is then given by

$$-\beta\mathcal{H}_L=J_x\sum_n[\cos(\theta_{n+1}-\theta_n-A_{n+1,n}) +\cos(\theta_{n'+1}-\theta_{n'}-A_{n'+1,n'})] +J_y\sum_n\cos(\theta_n-\theta_{n'}-A_{n,n'}) , \tag{5.11}$$

where the phase $A_{m,n}$ is related to the line integral of the vector potential $\vec{A}$ between sites m and n by

$$A_{m,n}=\frac{2e}{\hbar c}\int_m^n \vec{A}\cdot d\vec{l} . \tag{5.12}$$

Around each plaquette on the ladder, the sum of $A_{m,n}$ is related to the magnetic flux penetrating the plaquette,

$$A_{n+1,n}+A_{n,n'}+A_{n',n'+1}+A_{n'+1,n+1} =\frac{2e}{\hbar c}\oint\vec{A}\cdot d\vec{l}=\frac{2e}{\hbar c}Hab=2\pi\epsilon , \tag{5.13}$$

where H is the magnetic field perpendicular to the ladder surface, ab is the area of a plaquette, and $\epsilon=Hab/\Phi_0$ is the ratio of the flux penetrating the plaquette to the flux unit $\Phi_0=hc/2e$.

The partition function is obtained by integrating over the phases θ_n,

$$Z_L=\int_0^{2\pi}\prod_n\frac{d\theta_n d\theta_{n'}}{(2\pi)^2} \times\exp\left[\sum_n\{J_x[\cos(\theta_{n+1}-\theta_n-A_{n+1,n}) +\cos(\theta_{n'+1}-\theta_{n'}-A_{n'+1,n'})] +J_y\cos(\theta_n-\theta_{n'}-A_{n,n'})\}\right] . \tag{5.14}$$

It is convenient to use bond variables $\varphi_n=\theta_{n+1}-\theta_n-A_{n+1,n}$, $\varphi'_n=\theta_{n'+1}-\theta_{n'}-A_{n'+1,n'}$, and $\psi_n=\theta_n-\theta_{n'}-A_{n,n'}$. Around each plaquette, Eq. (5.13) constrains the bond variables such that

$$\sigma_n=\varphi'_n+\psi_{n+1}-\varphi_n-\psi_n=2\pi\epsilon(\mathrm{mod}\,2\pi) . \tag{5.15}$$

The integration over site variables can be replaced by an integration over bond variables provided that above constraint is satisfied. Therefore,

$$Z_L=\sum_{\{e_n\}}\int_0^{2\pi}\prod_m\frac{d\varphi_m d\varphi'_m d\psi_m}{(2\pi)^3} \times\exp\left[\sum_n\{[J_x\cos\varphi_n+J_x\cos\varphi'_n+J_y\cos\psi_n] -ie_n(\varphi'_n+\psi_{n+1}-\varphi_n-\psi_n -2\pi\epsilon)\}\right] , \tag{5.16}$$

where

$$\sum_{e_n}e^{-ie_n(\sigma_n-2\pi\epsilon)}=2\pi\delta[(\sigma_n-2\pi\epsilon)(\mathrm{mod}\,2\pi)] \tag{5.17}$$

is used to impose the constraint. Integrating the bond variables results in

$$Z_L=\sum_{\{e_n\}}\exp\left[-\sum_n[2\tilde{V}_x(e_n)+\tilde{V}_y(e_n-e_{n+1})-2\pi i\epsilon e_n]\right] , \tag{5.18}$$

where

$$e^{-\tilde{V}_{x,y}(e)}=\int_0^{2\pi}\frac{d\theta}{2\pi}e^{J_{x,y}\cos(\theta)-ie\theta} . \tag{5.19}$$

Equation (5.18) is analogous to the electric field partition function, Eq. (2.5), and represents the dual of the Josephson-junction ladder problem. Again finite-sized transfer matrices can be used to calculate the free energy of the system at high temperatures. Equation (3.2) yields

$$-\beta f=-2\tilde{V}_x(0)-\tilde{V}_y(0)+\frac{J_x^2J_y^2}{8}\cos(2\pi\epsilon) +\frac{J_x^4J_y^2}{32}\cos(4\pi\epsilon)+O(J^8) . \tag{5.20}$$

If the Villain approximation to the cosine potential is used [$\tilde{V}_{x,y}(e)=e^2/2J_{x,y}$], it again becomes possible to use the Poisson summation formula, and integrate out the variables $\{e_n\}$. The result is

$$Z_L=\sum_{\{k_n\}}\exp\left[\frac{N}{2}\left[\ln(2\pi J_y)-\frac{1}{l}\right] -\frac{1}{\tau}\sum_{n,m}(k_n-\epsilon)(k_m-\epsilon)e^{-|n-m|/l}\right] , \tag{5.21}$$

which is similar to the kink partition function, Eq. (5.2), with

$$\frac{1}{l}=\ln\left[1+\frac{J_y}{J_x}+\left[\frac{J_y^2}{J_x^2}+2\frac{J_y}{J_x}\right]^{1/2}\right] \tag{5.22}$$

and

$$\tau=\frac{1}{\pi^2 J_x}\left[1+2\frac{J_x}{J_y}\right]^{1/2} . \tag{5.23}$$

The discussion of ground states of the kink Hamiltonian given in the previous section also applies to the ladder problem. Thus as the magnetic field (and hence ϵ) is increased, the system will go through a sequence of phases forming a complete devil's staircase. The kinks are now related to the currents circulating a plaquette. It is possible to write a partition function similar to (5.21) in two dimensions. However, the "charges" $\{k_n\}$ in two dimensions interact logarithmically rather than exponentially.[37] Despite this difference, some two-dimensional ground states found for the square lattice[38] are closely related to the one-dimensional ground states of the kink Hamiltonian.

If the cosine potential is used in place of the Villain potential, there will be incommensurate ground states in addition to the commensurate ones found above. The connection between the discrete chain (1.1) and the Josephson-junction ladder becomes clear if the London gauge is used. In this gauge $A_{n,n+1}=A_{n',n'+1}=0$, and $A_{n,n'}=2\pi n\epsilon$. Also in the ground state there is a symmetry $\theta_n=-\theta_n$, which reduces the Hamiltonian (5.11) to

$$-\beta\mathcal{H}_L=\sum_n[2J_x\cos(\theta_{n+1}-\theta_n)+J_y\cos(2\theta_n-2\pi n\epsilon)] . \tag{5.24}$$

A change of coordinates $\theta_n=\pi(u_n+n\epsilon)$, together with the approximation

$$\cos(\theta_{n+1}-\theta_n)\simeq 1-\tfrac{1}{2}(\theta_{n+1}-\theta_n)^2 ,$$

which is valid since successive phases θ_n are close, yields

$$-\beta\mathcal{H}_L=\sum_n[2J_x-\pi^2 J_x(u_{n+1}-u_n-\epsilon)^2+J_y\cos(2\pi u_n)] . \tag{5.25}$$

This is identical to the chain Hamiltonian with the identification $\mu=2\pi^2 J_x$ and $W=2J_y$. An experimentally relevant quantity is the critical current, which is defined in terms of the stability of current-carrying states at zero temperature, but it is not calculated here.

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APPENDIX A: THE WKB METHOD

The results of Frank and van der Merwe[5] on the continuum model can be regained from the transfer-matrix formulation. The eigenfunction y of Eq. (2.7) can be written as $y(q)=e^{V(q)+\psi(q)}$. The function $\psi(q)$ scales as $1/T$ as the temperature T goes to zero. Then

$$\frac{d^2}{dq^2}e^{\psi}=(\psi''+\psi'^2)e^{\psi}\approx\psi'^2 e^{\psi}$$

in the WKB approximation. Since

$$\psi'^2\propto\frac{1}{T^2}\gg\psi''\propto\frac{1}{T} ,$$

as $T\to 0$ this approximation improves. In general

$$\left[\frac{d}{dq}\right]^n e^{\psi}\approx\psi'^n e^{\psi} ,$$

and the transfer-matrix equation $T(q)y(q)=e^{\bar{f}}y(q)$ gives

$$\frac{\psi'^2}{2\mu}-\epsilon\psi'+V=\bar{f} . \tag{A1}$$

The solution to this quadratic equation is

$$\psi'=\mu\epsilon-[\mu^2\epsilon^2+2\mu(\bar{f}-V)]^{1/2} . \tag{A2}$$

Periodicity of the function y, $y(q+1)=y(q)$, implies $\int_0^1 dq\,\psi'=0$, or

$$\mu\epsilon=\int_0^1 dq[\mu^2\epsilon^2+2\mu(\bar{f}-V)]^{1/2} . \tag{A3}$$

For the cosine potential $V(q)=W/2\cos(2\pi q)$, let $\bar{f}=-\mu\epsilon^2/2-W/2+W/k^2$. Then

$$\epsilon=\frac{1}{l_0 k}\int_0^1 dq[1-k^2\cos^2(\pi q)]^{1/2}=\frac{2}{\pi l_0}\frac{E(k)}{k} , \tag{A4}$$

where $E(k)$ is the complete elliptic function of the second kind.[26] This result is identical to that obtained by directly considering the kink structure in the sine-Gordon problem.[5,17] The solution ψ' in Eq. (A2) is valid for $\epsilon>\epsilon_c=2/\pi l_0$. For $\epsilon<\epsilon_c$, Eq. (A3) has no solution. The function ψ' becomes discontinuous and $\bar{f}=W/2-\mu\epsilon^2/2$. Equation (A3) is valid for any potential $V(q)$, and the critical value ϵ_c for formation of kinks is in general given by[15]

$$\epsilon_c=\int_0^1 dq\left[\frac{2}{\mu}[V_{\max}-V(q)]\right]^{1/2} . \tag{A5}$$

The WKB method in connection with this problem has also been used by Burkov and Talapov.[19]

APPENDIX B: THE AUBRY POTENTIAL AT FINITE TEMPERATURES

The Baker-Campbell-Hausdorff (BCH) formula[39] can be used to write the transfer operator

$$T(q)=\exp\left[\frac{1}{2\mu}\frac{d^2}{dq^2}-\epsilon\frac{d}{dq}\right]e^{-V(q)}$$

as a single exponential. For a general potential $V(q)$ the resultant exponential cannot be obtained in closed form. However, for the Aubry potential, Eq. (5.9), composed of quadratic pieces $V(q)=W\pi^2 q^2$, the BCH summation can be carried out exactly. Let $p=d/dq$ and consider the

operators $A=\frac{1}{2}(p-\mu\epsilon)^2$, $B=\frac{1}{2}q^2$, and $C=[A,B]=qp-\mu\epsilon q+\frac{1}{2}$. The three operators form a complete set with commutation rules

$$[A,B]=C,\quad [A,C]=2A,\quad [B,C]=-2B\ . \tag{B1}$$

This completeness implies that[39]

$$U=e^{\mu\epsilon^2/2}T(q)=e^{(1/\mu)A}e^{-2\pi^2WB}=e^{rA+sB+tC} \tag{B2}$$

with r, s, and t to be determined. Consider the linear transformation caused by $U(\lambda)=e^{\lambda(rA+sB+tC)}$ on the vector space $V=xA+yB+zC$:

$$x(\lambda)A+y(\lambda)B+z(\lambda)C=U(\lambda)(x_0A+y_0B+z_0C)U(\lambda)^{-1}\ . \tag{B3}$$

Differentiating with respect to λ results in

$$[rA+sB+tC,\quad xA+yB+zC]=x'A+y'B+z'C\ . \tag{B4}$$

Equating the coefficients of A, B, and C results in a set of linear equations with the solution

$$\begin{bmatrix}x\\y\\z\end{bmatrix}=M(r,s,t)\begin{bmatrix}x_0\\y_0\\z_0\end{bmatrix}=\exp\left[\lambda\begin{bmatrix}-2t & 0 & 2r\\ 0 & 2t & -2s\\ -s & r & 0\end{bmatrix}\right]\begin{bmatrix}x_0\\y_0\\z_0\end{bmatrix}\ . \tag{B5}$$

The operator equation (B2) can now be written as a matrix equation ($\lambda=1$)

$$M(r,s,t)=M\left[\frac{1}{\mu},0,0\right]M(0,-2\pi^2W,0)$$
$$=\begin{bmatrix}1+4\pi^2\frac{W}{\mu}+4\pi^2\frac{W^2}{\mu^2} & \frac{1}{\mu^2} & \frac{2}{\mu}+4\pi^2\frac{W}{\mu}\\ 4\pi^4W^2 & 1 & 4\pi^2W\\ 2\pi^2W+4\pi^4\frac{W^2}{\mu} & \frac{1}{\mu} & 1+4\pi^2\frac{W}{\mu}\end{bmatrix}\ . \tag{B6}$$

The coefficients r, s, and t are determined as follows. The vector (r,s,t) has to be an eigenvector with eigenvalue 1, implying $r=-(1/\pi^2W)t$ and $s=2\mu t$. The eigenvalues of the left-hand side are 1, e^{λ}, and $e^{-\lambda}$ with

$$\lambda=2(t^2-sr)^{1/2}=\left[1+\frac{2\mu}{\pi^2W}\right]^{1/2}t\ .$$

Equating the traces of the two sides gives

$$1+e^{\lambda}+e^{-\lambda}=3+8\pi^2\frac{W}{\mu}+4\pi^4\frac{W^2}{\mu^2}\ . \tag{B7}$$

The solution $\lambda=-2/l$ implies $t=-2/\mu l\tau$ with l and τ as defined in Eqs. (5.3) and (5.4). Therefore, $r=(1/\mu)K$, $s=-2\pi^2WK$, $t=-(W\pi^2/\mu)K$, ($K=2/\pi^2Wl\tau$), and

$$e^{\mu\epsilon^2/2}T(q)=\exp\left[K\left[\frac{1}{2\mu}(p-\mu\epsilon)^2-W\pi^2q^2-\frac{W\pi^2}{\mu}(qp-\mu\epsilon q+\tfrac{1}{2})\right]\right]\ . \tag{B8}$$

The equation $T(q)y(q)=e^{-\beta f}y(q)$ now leads to the differential equation in (5.10). Note that only the interval $-\frac{1}{2}\le q\le\frac{1}{2}$ has to be considered when periodic boundary conditions are imposed. In the limit $l_0\gg1$, $K\approx1$ and $t\approx0$.

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