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Finite-Size Corrections to the Free Energy of Coulomb Systems with a Periodic Boundary Condition

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Classical Coulomb systems in d dimensions ($d \geqslant 2$) with a periodic boundary condition, period W, in the direction $x^{(d)}$ are considered. With the other directions of the confining volume of length L, it is shown that if the system is in a conducting phase, then the "strip" free energy $kTf_W, f_W = -\lim_{L\to\infty} L^{-(d-1)} \log Z$, has the large-$W$ expansion

$$f_W \sim Wf_\infty + \frac{(d/2-1)\,\Gamma(d/2-1)}{\pi^{d/2} W^{d-1}} \zeta(d) + O\left(\frac{1}{W^{d+1}}\right)$$

where kTf_∞ is the bulk free energy per unit volume, $\zeta(x)$ denotes the Riemann zeta function, and $\Gamma(x)$ denotes the gamma function. With $1/W$ identified as kT, this result is precisely the low-temperature behavior of the free energy of a $(d-1)$-dimensional Debye solid. This fact is explained in terms of an equivalence between the Coulomb gas and quantum fields. Also, the expansion is verified for some exactly solved models of Coulomb systems in two dimensions.

KEY WORDS: Coulomb systems; finite-size corrections; sine-Gordon field theory.

1. INTRODUCTION AND SUMMARY

1.1. The Strip Free Energy at a Conformal Critical Point

One of the fundamental predictions of the theory of conformal critical points in two dimensions is the finite-size correction to the strip free energy.

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Specifically, consider a lattice model with the parameters chosen to correspond to bulk critically, but in a strip geometry of length L and width W (the number of rows of the lattice) wrapped around a cylinder. Then the free energy kTf_W per unit length

$$f_W = -\lim_{L \to \infty} \frac{1}{L} \log Z \tag{1.1}$$

has the large-W behavior[1,2]

$$f_W \sim Wf_\infty - \frac{\pi c}{6W} + O\left(\frac{1}{W^2}\right) \tag{1.2}$$

where kWf_∞ is the bulk free energy per unit volume and c is the central charge of the Virasoro algebra of the underlying continuous field theory. Equivalently, for low temperatures T the specific heat C per unit volume of a conformally invariant one-dimensional quantum system has the behavior

$$C \sim \pi c k^2 T / 3\hbar v \tag{1.3}$$

where the dispersion relation of the low-lying excitations is assumed to be of the form $\omega \sim vk$.

In contrast to (1.2), away from critically the strip free energy kTf_W has the large-W behavior

$$f_W \sim Wf_\infty + O(e^{-W/\chi}) \tag{1.4}$$

where χ is the correlation length. Qualitatively, the different behaviors (1.2) and (1.4) are attributable to the divergence of the correlation length at criticality.

1.2. Objective and Plan of the Paper

In this paper we will consider the large-W expansion of the analogue of (1.1) for general classical Coulomb systems in dimensions $d \geqslant 2$. Periodic boundary conditions are imposed in one direction, $x^{(d)}$ say, and the system has length W in this direction. The "strip" free energy kTf_W is then defined as

$$f_W = -\lim_{L \to \infty} \frac{1}{L^{d-1}} \log Z \tag{1.5}$$

where L is the length of each side of the confining volume in each of the directions $x^{(1)}, \ldots, x^{(d-1)}$.

A Coulomb system in its conduction phase has a finite correlation length and is certainly not critical. However, in Section 2 we provide a general argument which shows that in the conducting phase, for $d \geqslant 2$, the free energy (1.5) has a universal large-W expansion

$$f_W \sim W f_\infty + \frac{(d/2-1)\,\Gamma(d/2-1)}{\pi^{d/2} W^{d-1}} \zeta(d) + O\left(\frac{1}{W^{d+1}}\right) \tag{1.6}$$

where $\zeta(d)$ is the Riemann zeta function

$$\zeta(d) = \sum_{n=1}^{\infty} \frac{1}{n^d} \tag{1.7}$$

and $\Gamma(x)$ is the gamma function. In Section 3 the result (1.6) for $d=2$ is verified in some special cases. These are the two-dimensional, one-component and two-component plasmas, at the special coupling $\gamma = 2$, where

$$\gamma = q^2/kT \tag{1.8}$$

for which exact results are known.

1.3. Relationship to the Free Field

The result (1.6) has an interpretation in terms of quantum fields. Consider a d-dimensional Coulomb gas with the particles constrained on lines along, say, the $x^{(d)}$ direction and forming a $(d-1)$-dimensional lattice. Furthermore, suppose that in the direction of $x^{(d)}$ the system is periodic of period W. Then, using the Gaussian transformation,[3] we have that for small fugacity

$$\Xi_{\mathrm{CG}}^{(d)}(W) = \frac{Z_I^{(d-1)}(kT = 1/W)}{Z_F^{(d-1)}(kT = 1/W)} \tag{1.9}$$

where $\Xi_{\mathrm{CG}}^{(d)}$ denotes the grand partition function of the d-dimensional Coulomb gas, while $Z_I^{(d-1)}$ and $Z_F^{(d-1)}$ denote the partition function of an interacting quantum field theory and the free field theory, respectively, with the Hamiltonians of the field theories defined on a $(d-1)$-dimensional lattice. Note the relationship between the temperature T of the quantum field theory and the width W of the periodic boundary of the Coulomb gas as indicated in (1.9). As an explicit example of the identity (1.9), when the Coulomb gas consists of positive and negative charges of equal magnitude, the interacting quantum field is the sine-Gordon theory.[4]

The identity (1.9) when combined with the free energy expansion (1.6) implies that for low temperatures T,

$$C_F^{(d-1)}(T) - C_I^{(d-1)}(T) \sim d(d-1)(d/2-1)\,\Gamma(d/2-1)\,\zeta(d)\,\pi^{-d/2}k^d T^{d-1} \tag{1.10}$$

where $C_F^{(d-1)}$ and $C_I^{(d-1)}$ denote the specific heats per unit volume of the free and interacting fields in (1.9), respectively. Here we have deduced the large-W behavior of the grand partition function from the large-W expansion of the partition function. This is possible since the thermodynamic relationship between the free energy and the grand potential implies

$$\left(\frac{\partial f_W}{\partial W}\right)_v = \left(\frac{\partial \Omega_W}{\partial W}\right)_\mu \tag{1.11}$$

where Ω_W denotes the grand potential per unit area A of the nonperiodic directions, v denotes the average number of particles per unit A, and μ denotes the chemical potential.

The crucial observation, which in turn allows the expansion (1.6) to be easily understood within the context of quantum fields, is that the right-hand side of (1.10) is precisely $C_F^{(d-1)}(T)$. To see this, we note that since the free field is a Bose system with dispersion relation $\omega \sim |\mathbf{k}|$, as $|\mathbf{k}| \to 0$, its low-temperature properties are that of a $(d-1)$-dimensional Debye solid. In particular, the total energy E is given by

$$\begin{aligned} E &= E_0 + \sum_k \frac{\omega_k}{\exp(\omega_k/kT) - 1} \\ &\sim E_0 + V^{d-1} \int_{R^{d-1}} \frac{d\mathbf{k}}{(2\pi)^{d-1}} \frac{|\mathbf{k}|}{\exp(|\mathbf{k}|/kT) - 1} \end{aligned} \tag{1.12}$$

Using spherical coordinates, the integral in (1.12) is easily evaluated to give

$$\varepsilon \sim \varepsilon_0 + \frac{(d-1)!\, s_{d-1}\zeta(d)}{(2\pi)^{d-1}} (kT)^d \tag{1.13}$$

where

$$s_{d-1} = \frac{2\pi^{(d-1)/2}}{\Gamma((d-1)/2)} \tag{1.14}$$

is the surface area of a $(d-1)$-dimensional sphere and ε is the energy per volume. Differentiating (1.13) with respect to T gives the specific heat, which we can identify with the right-hand side of (1.10) after using the identity

$$\Gamma\left(\frac{d-1}{2}\right)=\frac{\pi^{1/2}}{2^{d-3}}\frac{(d-3)!}{\Gamma(d/2-1)} \tag{1.15}$$

in (1.14).

Note that for $d=2$, the right-hand side of (1.10) gives the conformal result (1.3) with $c=1$ [when $d=2$, $(d/2-1)\,\Gamma(d/2-1)=1$ and $\zeta(d)=\pi^2/6$; we also have $\hbar=v=1$]. This is consistent with the above discussion, as a central charge $c=1$ corresponds to the free field in $1+1$ dimension.[1,2]

In contrast to the polynomial approach to zero of the specific heat of the free field, the specific heat of the interacting field should decrease to zero with the temperature exponentially fast, provided the Coulomb gas is in a conducting phase. This is a consequence of the exponential decay of the correlations in the conducting phase.[5] The correlation length is thus finite, which, from the identity (1.9), implies that there is a gap between the energy of the ground state and the energy of the first excited state. The identity (1.9) thus explains why although the Coulomb gas in the conducting phase is not a critical system, its strip free energy behaves analogously to that of a critical system: the behavior of the free energy is governed by that of the free field, which is a critical system, but the correlations are determined by the properties of a massive field theory, which is not critical.

2. FREE ENERGY SUM RULE

We are interested in general n-component Coulomb systems in which the components interact via the d-dimensional ($d\geqslant 2$) Coulomb potential $\Phi_W(\mathbf{x}^{(d)})$, where $\mathbf{x}^{(d)}=(x^{(1)}, x^{(2)},..., x^{(d)})$. In the direction $x^{(d)}$ a periodic boundary condition period W is imposed. The potential is then given by the summation

$$\Phi_W(\mathbf{x}^{(d)})=\Phi_\infty(|\mathbf{x}^{(d)}|) + \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [\Phi_\infty(x^{(1)},..., x^{(d-1)}, x^{(d)}+nW)-\Phi_\infty(0,..., 0, nW)] \tag{2.1}$$

where $\Phi_\infty(|\mathbf{x}^{(d)}|)$ is the Coulomb potential in free boundary conditions

$$\Phi_\infty(|\mathbf{x}^{(d)}|)=\begin{cases}-\log|\mathbf{x}^{(2)}|, & d=2\\ |\mathbf{x}^{(d)}|^{-(d-2)}, & d>2\end{cases} \tag{2.2}$$

The second term in the summand of (2.1) corresponds to the subtraction of the self-energy of the infinite array of periodic images.

Due to the singularity of the Coulomb potential at small distances, to obtain well-defined thermodynamics, it is necessary to regularize $\Phi_{\infty}(|\mathbf{x}^{(d)}|)$ at the origin by the addition of a short-range potential $\Phi_s(|\mathbf{x}^{(d)}|)$. Alternatively, the positive and negative charges may be restricted to separate subdomains. For definiteness it will be assumed that the potential has been modified at short distances, and this will be indicated by use of the superscript r, so we will write $\Phi_{\infty}^{(r)}(|\mathbf{x}^{(d)}|)$, for example. However, our results are still valid if the opposite charges are restricted to separate subdomains.

We will confine the system to a box of length W in the direction $x^{(d)}$ and of lengths L in the directions $x^{(1)},..., x^{(d-1)}$. The n different charge species will be taken to have charges qQ_{α}, $\alpha = 1,..., n$, where q is the "unit" charge, and the coordinates of a particle of species α will be denoted by $\mathbf{x}_j^{(d)}(\alpha)$, $j = 1,..., N_{\alpha}$, where N_{α} is the number of particles of species α. Global charge neutrality is assumed, which together with an appropriately regularized potential, should ensure the existence of the thermodynamic limit.

With the above definitions and specifications, the "strip" free energy (1.5) is given by

$$f_W = -\lim_{L\to\infty} \frac{1}{L^{d-1}} \log\left[\left(\prod_{\alpha=1}^{n} \frac{1}{N_{\alpha}!} \prod_{l=1}^{N_{\alpha}} \int_V d\mathbf{x}_l^{(d)}(\alpha)\right) e^{-\gamma H_W}\right] \tag{2.3}$$

where γ is defined by (1.8), the volume of each integration is $L^{d-1} \otimes W$, and

$$H_W = \frac{1}{2} \sum_{\alpha=1}^{n} \sum_{\gamma=1}^{n} \sum_{j=1}^{N_{\alpha}} \sum_{k=1}^{N_{\gamma}}{}^{*} Q_{\alpha} Q_{\gamma} \Phi_W^{(r)}(\mathbf{x}_k^{(d)}(\gamma) - \mathbf{x}_j^{(d)}(\alpha)) \tag{2.4}$$

(here the asterisk on the final summation denotes that if $\alpha = \gamma$, the term $j = k$ is to be omitted).

Rather than studying the large-W behavior of (2.3) directly, we will study the behavior of the partial derivative $\partial f_W/\partial W$. To calculate the partial derivative, we note that both the volume V and potential Φ_W are functions of W. However, by changing variables

$$x^{(d)} = W X^{(d)} \tag{2.5}$$

in the direction $x^{(d)}$, the dependence of V on W can be removed. Denoting the position vector $\mathbf{x}^{(d)}$ with this change of variables by $\mathbf{X}^{(d)}$ and the volume V by $\hat{V}$ ($\hat{V} = L^{d-1} \otimes [0, 1]$), we thus have

$$\frac{\partial f_W}{\partial W} = -\rho + \lim_{L\to\infty} \frac{1}{2kTL^{d-1}} \int_{\hat{V}} \int_{\hat{V}} d\mathbf{X}^{(d)}\, d\mathbf{Y}^{(d)} \times \left(\frac{\partial}{\partial W} \Phi_W^{(r)}(\mathbf{X}^{(d)} - \mathbf{Y}^{(d)}) \right) C_W(\mathbf{X}^{(d)}, \mathbf{Y}^{(d)}) \tag{2.6}$$

where $C_W(\mathbf{X}^{(d)}, \mathbf{Y}^{(d)})$ denotes the charge–charge correlation defined with the change of variables (2.5) (see, e.g., ref. 6 for the explicit definition of this quantity), and ρ denotes the bulk density. Changing back to the original variables, we thus have

$$\frac{\partial f_W}{\partial W} = -\rho + \lim_{L\to\infty} \frac{1}{2kTL^{d-1}} \int_{V} \int_{V} d\mathbf{x}^{(d)}\, d\mathbf{y}^{(d)} \times \psi_W(\mathbf{x}^{(d)} - \mathbf{y}^{(d)})\, C_W(\mathbf{x}^{(d)}, \mathbf{y}^{(d)}) \tag{2.7}$$

where

$$\psi_W(\mathbf{x}^{(d)} - \mathbf{y}^{(d)}) = \frac{\partial}{\partial W} \Phi_W^{(r)}(\mathbf{X}^{(d)} - \mathbf{Y}^{(d)}) \Big|_{\substack{X^{(d)} = x^{(d)}/W \\ Y^{(d)} = y^{(d)}/W}} \tag{2.8}$$

In the directions $x^{(j)}$, $j = 1,..., d-1$, since we are taking $L \to \infty$, the charge–charge correlation is a function of the difference $x^{(j)} - y^{(j)}$, so that the double integration can be reduced to a single integration. Also, since the $x^{(d)}$ direction is periodic, this is true for $j = d$. Thus, without any approximation, (2.7) can be rewritten as

$$\frac{\partial f_W}{\partial W} = -\rho + \frac{W}{2kT} \int_V d\mathbf{x}^{(d)}\, \psi_W(\mathbf{x}^{(d)})\, C_W(\mathbf{x}^{(d)}) \tag{2.9}$$

It thus remains to expand the derivative of the potential and the charge–charge correlations for large W. At this stage we make an assumption in our argument: the dependence of the charge–charge correlation on W decreases exponentially for large W. This assumption is supported by the expected exponential decay of the correlations in all directions with periodic boundary conditions. On the other hand, the derivative of the potential can be expanded in inverse powers of W. A short calculation using (2.1) and (2.2) shows

$$\psi_W(\mathbf{x}^{(d)}) \sim \frac{1}{W} \frac{(x^{(d)})^2}{|\mathbf{x}^{(d)}|} \Phi_S'(|\mathbf{x}^{(d)}|) - \frac{d-2}{W} \frac{(x^{(d)})^2}{|\mathbf{x}^{(d)}|^d} - \frac{(d-2)\,\zeta(d)}{W^{d+1}} \{(d-2)(d-1)(x^{(d)})^2 - d[(x^{(1)})^2 + \cdots + (x^{d-1})^2]\} + O\left(\frac{1}{W^{d+3}}\right) \tag{2.10}$$

where $\zeta(d)$ denotes the Riemann zeta function as defined by (1.7) and $\Phi'_S(r)$ is the derivative of the short-range potential. For $d=2$ the factor $(d-2)$ multiplying the second term and the same factor outside the brackets $\{\cdots\}$ (but not the one inside) are to be replaced by 1.

Substituting (2.10) in (2.9), we obtain

$$\frac{\partial f_W}{\partial W}=\left.\frac{\partial f_W}{\partial W}\right|_{W=\infty}-\frac{(d-2)\,\zeta(d)}{2kTW^d}\Bigg[(d-2)(d-1)\int_{\mathbb{R}^d} d\mathbf{x}^{(d)}(x^{(d)})^2\,C_\infty(\mathbf{x}^{(d)})$$
$$-d\sum_{j=1}^{d-1}\int_{\mathbb{R}^d} d\mathbf{x}^{(d)}(x^{(j)})^2\,C_\infty(\mathbf{x}^{(d)})\Bigg]+O\left(\frac{1}{W^{d+2}}\right) \tag{2.11}$$

where

$$\left.\frac{\partial f_W}{\partial W}\right|_{W=\infty}=-\rho+\frac{1}{2kT}\int_{\mathbb{R}^d} d\mathbf{x}^{(d)}$$
$$\times\left[\frac{(x^{(d)})^2}{|\mathbf{x}^{(d)}|}\,\Phi'_S(|\mathbf{x}^{(d)}|)-(d-2)\frac{(x^{(d)})^2}{|\mathbf{x}^{(d)}|^d}\right]C_\infty(\mathbf{x}^{(d)}) \tag{2.12}$$

For $d=2$ all factors of $(d-2)$ except the one multiplying $(d-1)$ are to be replaced by 1. Our final task is thus to evaluate the integrals in (2.11). Their value is given by the Stillinger–Lovett second moment sum rule (see, e.g., ref. 7), which states that for a Coulomb system in its conducting phase

$$\int_{\mathbb{R}^d} d\mathbf{x}^{(d)}(x^{(p)})^2\,C_\infty(\mathbf{x}^{(d)})=-\frac{2kT}{\kappa_d},\qquad p=1,2,\ldots,d \tag{2.13}$$

where κ_d is such that the Fourier transform of $\Phi_\infty(|\mathbf{x}^{(d)}|)$ is $\kappa_d/|\mathbf{k}|^2$. Explicitly (see, e.g., ref. 5)

$$\kappa_d=\frac{4\pi^{d/2}}{\Gamma(d/2-1)} \tag{2.14}$$

where $\Gamma(x)$ denotes the gamma function. Substituting (2.13) in (2.11) and antidifferentiating with respect to W, we obtain (1.6).

The working only requires minor modification to include the case when the system is in a dielectric phase, characterized by a finite static dielectric constant ε. The Stillinger–Lovett condition (2.11) then reads[7]

$$\int_{\mathbb{R}^d} d\mathbf{x}^{(d)}(x^{(p)})^2\,C_\infty(\mathbf{x}^{(d)})=-\frac{2kT}{\kappa_d}\left(1-\frac{1}{\varepsilon}\right) \tag{2.15}$$

so the only change needed to the sum rule (1.6) is the inclusion of the factor $(1-1/\varepsilon)$ in the finite-size correction. Similarly, the only required alteration to the formula (1.10) is the inclusion of the factor $(1-1/\varepsilon)$ on the right-hand side. Recalling that the exact value of $C_F(T)$ is given by $\varepsilon \to \infty$, (1.10) thus gives

$$C_I(T) \sim (1/\varepsilon)\, d(d-1)(d/2-1)\, \Gamma(d/2-1)\, \zeta(d)\, \pi^{-d/2} k^d T^{d-1} \quad (2.16)$$

From the discussion in Section 1.2, we can conclude that the interacting quantum field theory is now massless.

3. VERIFICATION OF THE SUM RULE

3.1. Two-Dimensional, One-Component Plasma at $\gamma = 2$

The derivation of (1.6) has been given for general n-component Coulomb systems, $n \geqslant 2$. A one-component system can be obtained by considering a two-component system of N particles of charge q and N' particles of charge $-q'$, and taking the limit $N' \to \infty$, $q' \to 0$ with $Nq = N'q'$ so that the system is overall charge neutral. The species of infinite particle density then forms a perfect gas, the free energy of which must be subtracted in the limiting procedure to obtain the free energy of the one-component system. Also

$$C_\infty(\mathbf{x}^{(d)}) \to q^2 \rho_{(2)}^T(\mathbf{x}) \quad (3.1)$$

where $\rho_{(2)}^T$ denotes the truncated two-particle distribution of the mobile species. Hence, with ρ now denoting the particle density of the mobile species, and the short-range potential Φ_s identically zero, (2.12) reads

$$\left.\frac{\partial f_W}{\partial W}\right|_{W=\infty} = -\rho - \frac{d-2}{2kT} \int_{\mathbb{R}^d} d\mathbf{x}^{(d)} \frac{(x^{(d)})^2}{|\mathbf{x}^{(d)}|^d} C_\infty(\mathbf{x}^{(d)}) \quad (3.2)$$

where for $d=2$ the factor $d-2$ is to be replaced by 1. For $d=2$ the potential (2.1) can be summed to give[8,9]

$$\Phi_W(x, y) = -\log[|\sinh \pi(x+iy)/W|\ (W/\pi)] \quad (3.3)$$

Using this potential, the free energy of the one-component strip system at the special coupling $\gamma = 2$ has been evaluated exactly[8] with the result

$$f_W = W(\tfrac{1}{2}\rho \log \rho/2\pi^2) + \pi/6W \quad (3.4)$$

This is in agreement with the sum rule (1.6) with $d=2$, and has the further remarkable that all additional correction terms are identically zero.

The result (2.10) can also be tested. Since the system in the bulk is rotationally invariant,

$$\int_{\mathbb{R}^2} d\mathbf{x}^{(2)} \frac{(x^{(2)})^2}{|\mathbf{x}^{(2)}|^2} C_\infty(\mathbf{x}^{(2)}) = \int_{\mathbb{R}^2} d\mathbf{x}^{(2)} \frac{(x^{(1)})^2}{|\mathbf{x}^{(2)}|^2} C_\infty(\mathbf{x}^{(2)}) \tag{3.5}$$

so that their common value is given by their mean value, which is

$$\frac{1}{2}\int_{\mathbb{R}^2} d\mathbf{x}^{(2)}\, C_\infty(\mathbf{x}^{(2)}) \tag{3.6}$$

But by (3.1) and the perfect screening sum rule,[7] (3.6) is equal to

$$\frac{-q^2}{2}\rho \tag{3.7}$$

The sum rule (3.2) thus reduces to

$$\left.\frac{\partial f_W}{\partial W}\right|_{W=\infty} = -\rho\left(1-\frac{\gamma}{4}\right) \tag{3.8}$$

With $\gamma = 2$, this result agrees with that which can be obtained from the exact result (3.4) (note that $\rho = v/W$, where $v = N/L$ is a constant in the partial derivative).

3.2. Two-Dimensional, Two-Component Plasma at $\gamma = 2$

The grand partition function Ξ_2 for this system has recently been evaluated exactly.[9] To stop collapse at small distances the positive charges were confined to equally spaced lines in the periodic direction (here the y direction) with x coordinate nL/M_2, $n = 1,\ldots, M_2$, while the negative charges were confined to the lines with x coordinate $(n-\phi_2)L/M_2$, where $0 < \phi_2 < 1$. (Note: the x and y directions have been interchanged here with respect to the coordinates used in ref. 9; consequently, L and W are also interchanged). With the domain thus defined and ξ denoting the fugacity, the exact evaluation of the grand partition function is[9]

$$\Xi_2 = \prod_{\rho=-\infty}^{\infty} \prod_{\alpha=1}^{M_2} \left[1 + (2\pi\xi)^2 \frac{e^{-Z_\rho(1-2\phi_2)}}{2(\cosh Z_\rho - \cos\theta_\alpha)}\right] \tag{3.9}$$

where

$$Z_\rho = \pi a_2(2\rho - 1)/W, \qquad a_2 = L/M_2 \tag{3.10}$$

and the θ_α are the solutions of an equation, given explicitly in ref. 9, which has its solutions uniformly distributed on $[0, \pi]$.

In the limit L, $M_2 \to \infty$, a_2 constant, we obtain a strip of width W with periodic boundary conditions. From the general formalism of statistical mechanics we know that for large systems

$$kT \log \Xi = \mu \langle N \rangle - F \tag{3.11}$$

where F is the total free energy, μ is the chemical potential, and $\langle N \rangle$ is the average number of particles. Thus the strip free energy kTf_W is given by

$$f_W = \mu \langle N \rangle / LkT - \lim_{L \to \infty} \frac{1}{L} \log \Xi \tag{3.12}$$

From (3.9) and the fact that the θ_α are uniform in the interval $[0, \pi]$ we have the exact result

$$\lim_{L \to \infty} \frac{1}{L} \log \Xi_2 = \frac{1}{\pi a_2} \sum_{\rho = -\infty}^{\infty} \int_0^\pi d\theta \log \left[1 + (2\pi\xi)^2 \frac{e^{-Z_\rho(1-2\phi_2)}}{2(\cosh Z_\rho - \cos\theta)} \right] \tag{3.13}$$

To verify (1.6), we thus require the large-W expansion of (3.13). This task can be accomplished by writing the right-hand side of (3.13) as

$$\frac{1}{\pi a_2} \lim_{N \to \infty} \left\{ I(N, L) - \sum_{\rho = -N}^{N} \int_0^\pi d\theta \log[2(\cosh Z_\rho - \cos\theta)] \right\} \tag{3.14}$$

where

$$I(N, L) = \sum_{\rho = -N}^{N} \int_0^\pi d\theta \log[2(\cosh Z_\rho - \cos\theta) + (2\pi\xi)^2 e^{-Z_\rho(1-2\phi_2)}] \tag{3.15}$$

for the sum $I(N, L)$ can be analyzed using a slight variant of the Euler–Maclaurin formula, while the summand in the final term of (3.14) is easily evaluated according to the formula

$$\int_0^\pi d\theta \log(2\cosh Z_\rho - 2\cos\theta) = \pi |Z_\rho| \tag{3.16}$$

The variation of the Euler–Maclaurin formula required is specified by the following result.

Theorem 1. Let $f(Z)$ be analytic in the strip $a \leqslant \text{Re}(Z) \leqslant N$ and assume that $f(Z)$ is real for Z real. Then

$$\sum_{\rho=a+1}^{N} f\left(\rho-\frac{1}{2}\right)=\int_a^N dt\, f(t)+2\int_0^\infty dt\,\frac{\text{Im}\, f(a+it)}{1+e^{2\pi t}}$$
$$-2\int_0^\infty dt\,\frac{\text{Im}\, f(N+it)}{1+e^{2\pi t}} \tag{3.17}$$

This result can be proved, using contour integration, in the same way as the usual Euler–Maclaurin formula, which transforms

$$\sum_{\rho=a}^{N-1} f(\rho) \tag{3.18}$$

(see, e.g., ref. 10 for this derivation).

To apply Theorem 1 to the summation (3.15), it is first necessary to study the argument of the logarithm in the summand as a function of complex Z_ρ and locate its zeros. This is straightforward, and we find that there exists a value a_0 such that

$$f(Z)=\int_0^\pi d\theta\, \log\{2(\cosh 2\pi a_2 Z/W-\cos\theta)+(2\pi\xi)^2\, e^{-2\pi(1-2\phi_2)\, a_2 Z/W}\} \tag{3.19}$$

is analytic for $|\text{Re}(Z)| \geqslant a_0$. Thus, we can apply Theorem 1 to transform

$$\frac{1}{\pi a_2}\lim_{N\to\infty}\sum_{\rho=a_0+1}^{N}\left[f\left(\rho-\frac{1}{2}\right)-\int_0^\pi d\theta\, \log(2\cosh Z_\rho-\cos\theta)\right] \tag{3.20}$$

with $f(Z)$ given by (3.19). A short calculation, which uses the result (3.16) and the evaluation

$$\int_0^\infty dt\,\frac{t}{1+e^t}=\frac{\pi^2}{12} \tag{3.21}$$

then gives that (3.20) is equal to

$$\frac{1}{\pi a_2}\left(\int_{a_0}^\infty ds\int_0^\pi d\theta\, g(s,\theta)+I_1-\frac{\pi^2 a_2}{12W}\right) \tag{3.22}$$

where

$$g(s,\theta)=1+\frac{(2\pi\xi)^2\, e^{-2\pi a_2 s(1-2\phi_2)/W}}{2(\cosh 2\pi a_2 s/W-\cos\theta)} \tag{3.23}$$

and

$$I_1 = 2\int_0^\infty dt\, \frac{\mathrm{Im}\, f(a_0 + it)}{1 + e^{2\pi t}} \tag{3.24}$$

A similar transformation applies to (3.20) with the ρ summation ranging from $-N+1$ to $-a_0$, which together with (3.22) gives that (3.14) can be rewritten as

$$\begin{aligned}\frac{1}{\pi a_2}\Bigg\{&\int_{-\infty}^{\infty} ds \int_0^\pi d\theta\, g(s,\theta) - \int_{-a}^{a} ds \int_0^\pi d\theta\, g(s,\theta)\\ &+ \sum_{\rho=-a_0+1}^{a_0} \left[f\left(\rho - \frac{1}{2}\right) - \int_0^\pi d\theta \log(2\cosh Z_\rho - 2\cos\theta)\right]\\ &+ I_1 - J_1 - \frac{\pi^2 a_2}{12W}\Bigg\}\end{aligned} \tag{3.25}$$

Here $g(s, \theta)$ is given by (3.23), $f(Z)$ by (3.19), I_1 is given by (3.24), and

$$J_1 = 2\int_0^\infty dt\, \frac{\mathrm{Im}\, f(-a_0 + it)}{1 + e^{2\pi t}} \tag{3.26}$$

It is straightforward to expand (3.25) in inverse powers of W. Again using (3.21) and also the simple summation

$$\sum_{\rho=-a+1}^{a} (\rho - 1/2)^2 = \tfrac{1}{6}a[(2a)^2 - 1] \tag{3.27}$$

we thus find that for large W

$$\lim_{L\to\infty} \frac{1}{L} \log \Xi_2 \sim \left[W p_\infty - \frac{\pi}{6W} + O\left(\frac{1}{W^3}\right)\right] \tag{3.28}$$

where

$$p_\infty = \frac{1}{2(\pi a_2)^2} \int_{-\infty}^{\infty} dt \int_0^\pi d\theta \log\left[1 + (2\pi\xi)^2 \frac{e^{-t(1-2\phi_2)}}{2(\cosh t - \cos\theta)}\right] \tag{3.29}$$

Substituting (3.28) in (3.12), we thus have

$$f_W \sim W(\rho\mu - p_\infty) + \frac{\pi}{6W} + O\left(\frac{1}{W^3}\right) \tag{3.30}$$

where ρ is the particle density. This is in precise agreement with (1.6) when $d = 2$.

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