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LETTER TO THE EDITOR

Exact results for some Madelung-type constants in the finite-size scaling theory

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Abstract. A general formula is obtained from which the Madelung-type constant,

$$\mathcal{C}(d|\nu)=\int_0^\infty \mathrm{d}x\, x^{d/2-\nu-1}\left[\left(\sum_{l=-\infty}^{\infty}\mathrm{e}^{-xl^2}\right)^d-1-\left(\frac{\pi}{x}\right)^{d/2}\right]$$

that is extensively used in finite-size scaling theory is computed analytically for some particular cases of the parameters d and ν. By adjusting these parameters one can obtain different physical situations corresponding to different geometries and magnitudes of the interparticle interaction.

In the analytic investigation of the finite-size scaling theory of systems undergoing a phase transition, the Madelung-type constant [1],

$$\begin{aligned}\mathcal{C}(d|\nu)&=\int_0^\infty \mathrm{d}x\, x^{d/2-\nu-1}\left[\left(\sum_{l=-\infty}^{\infty}\mathrm{e}^{-xl^2}\right)^d-1-\left(\frac{\pi}{x}\right)^{d/2}\right]\\&=\lim_{\lambda\to 0}\left\{\sum_{\boldsymbol{l}}{}'\frac{\Gamma\left(\frac{1}{2}d-\nu,\lambda \boldsymbol{l}^2\right)}{\boldsymbol{l}^{d-2\nu}}-\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\mathrm{d}^d\boldsymbol{l}\,\frac{\Gamma\left(\frac{1}{2}d-\nu,\lambda \boldsymbol{l}^2\right)}{\boldsymbol{l}^{d-2\nu}}\right\}\qquad \frac{d}{2}>\nu>0\end{aligned}\tag{1}$$

where $\boldsymbol{l}\in\mathbb{Z}^d$ and $\Gamma(a,x)$ is the incomplete gamma function, plays a central role. By adjusting the parameters d and ν, one can obtain constants, describing different physical situations. These situations correspond to different geometries (hypercube, slab geometry and many others) and interparticle interaction in the system (short as well long range). The particular case $\mathcal{C}(4|1)$, corresponding to the short-range forces, has been widely used in the asymptotic analysis of the finite-size properties of the $\mathcal{O}(n)$-symmetric φ^4 model using a renormalization group treatment of static [2–4] as well dynamic [5–7] critical phenomena. The constant $\mathcal{C}\,(d|\nu)$ for the long-range case has been obtained in the asymptotic analysis of finite-size effects of the spherical model of Berlin and Kac [1, 8–11] as well as the quantum φ^4 model [12] in the large-n limit. The same constant is obtained in the renormalization group treatment of the finite-size scaling in $\mathcal{O}(n)$-symmetric systems [13].

The constant $\mathcal{C}(4|1)$ is evaluated numerically with very good accuracy. It is found to be (see, e.g., [2])

$$\mathcal{C}(4|1)=-1.765\,084\,8012\ldots\pi=-5.545\,177\,444\ldots.\tag{2}$$

It is the aim of this letter to find a general formula for the analytic evaluation of the constant $\mathcal{C}(d|\nu)$ and subsequently to deduce a useful expression for some particular cases of the parameters d and ν. Let us note that the integral $\mathcal{C}(d|\nu)$ has the remarkable symmetry property

$$\pi^{\nu}\mathcal{C}\,(d|\nu) = \pi^{d/2-\nu}\mathcal{C}\left(d\,\middle|\,\tfrac{d}{2}-\nu\right) \tag{3}$$

which relates the values of $\mathcal{C}\,(d|\nu)$ for $\nu > \frac{d}{4}$ with those for $\nu < \frac{d}{4}$. Equation (3) is obtained as a consequence of using the Jacobi identity for the sum in the integrand.

Our key finding is that the Madelung-type constant can be expressed in terms of the analytic continuation, over $\nu < \frac{d}{2}$, of

$$\mathcal{C}(d|\nu) = \pi^{d/2-2\nu}\Gamma(\nu){\sum_{\boldsymbol{l}}}' \boldsymbol{l}^{-2\nu} \qquad \nu > \frac{d}{2} \tag{4}$$

where $\boldsymbol{l} \in \mathbb{Z}^d$ and the primed summation indicates that the term corresponding to $\boldsymbol{l} \neq 0$ is excluded. For some particular values of the dimension of the lattice, the d-fold sum can be expressed as a product of simple sums such as Dirichlet series [14].

To show that the Madelung-type constant (1) is equivalent to the sum given in equation (4), we start from the generalized d-dimensional Jacobi identity:

$$\sum_{\boldsymbol{l}} \exp\left(-u\boldsymbol{l}^2\right) = \left(\frac{\pi}{u}\right)^{d/2} \sum_{\boldsymbol{l}} \left(-\frac{\pi^2\boldsymbol{l}^2}{u}\right) \qquad \boldsymbol{l} \in \mathbb{Z}^d. \tag{5}$$

Following [15], we multiply both sides of equation (5) by $u^{d/2-\nu-1}$ and integrate over u. Whence, we get the key identity (valid for $\nu \neq 0, \frac{d}{2}$)

$$\mathcal{C}(d|\nu) = -\frac{u^{d/2-\nu}}{d/2-\nu} + {\sum_{\boldsymbol{l}}}' \frac{\Gamma\left(d/2-\nu, u\boldsymbol{l}^2\right)}{\boldsymbol{l}^{d-2\nu}} - \frac{\pi^{d/2}}{\nu u^{\nu}} + \pi^{d/2-2\nu}{\sum_{\boldsymbol{l}}}' \frac{\Gamma\left(\nu, \pi^2\boldsymbol{l}^2/u\right)}{\boldsymbol{l}^{2\nu}}. \tag{6}$$

The right-hand side $\mathcal{C}(d|\nu)$ of identity (6) is a constant of integration independent of u. Consequently, the right-hand side should also be u independent. By adjusting the parameter u one obtains different expressions for the constant $\mathcal{C}(d|\nu)$. All of these expressions are equivalent in the sense that they give the same 'numerical' value for fixed d and ν. In particular, we find it is useful to obtain simple expressions for the constant $\mathcal{C}(d|\nu)$ corresponding to the limiting cases $u \to \infty$ and $u \to 0$. With the aid of the asymptotic behaviour of the incomplete gamma function [16]

$$\Gamma(a,x) = \begin{cases} x^{a-1}\mathrm{e}^{-x}\left[1 - \dfrac{a-1}{x} + \mathcal{O}\left(\dfrac{1}{x^2}\right)\right] & x \gg 1 \\ \Gamma(a) - \dfrac{x^a}{a}\mathrm{e}^{-x}\left[1 + \dfrac{x}{a+1} + \mathcal{O}\left(x^2\right)\right] & x \ll 1 \end{cases} \tag{7}$$

it is possible to evaluate the right-hand side of (6) and one obtains (1) (valid for $0 < \nu < \frac{d}{2}$) in the limit $u \to 0$, and (4) (valid for $\nu > \frac{d}{2}$) in the limit $u \to \infty$. It is not difficult to see that the results (1) and (4) are valid in two different intervals and so they complement each other.

On the other hand, the sum in the right-hand side of equation (4) can be expressed in terms of the Epstein zeta function [17]

$$\mathcal{Z}\begin{vmatrix}0\\0\end{vmatrix}(d,\nu) = {\sum_{\boldsymbol{l}}}' \boldsymbol{l}^{-2\nu} \qquad \boldsymbol{l} \in \mathbb{Z}^d \qquad \nu > \frac{d}{2} \tag{8}$$

which can be regarded as the generalized d-dimensional analogue of the Riemann zeta function $\zeta(\nu)$. In the case under consideration the Epstein zeta function has a simple pole at $\nu = \frac{d}{2}$ and may be analytically continued in the interval $\nu < \frac{d}{2}$. Note that, from the functional equation for the Epstein function [17], one can check easily that $\mathcal{C}\,(d|\nu)$, defined in (4), obeys the symmetry property (3).

Using the results of [14, 15], for the Epstein zeta function (8), we get simple expressions for $\mathcal{C}(d|\nu)$ for certain values of d.

(a) For the simplest one-dimensional case, $d = 1$, we obtain

$$\mathcal{C}(1|\nu) = 2\pi^{1/2-2\nu}\Gamma(\nu)\zeta(2\nu) \qquad \nu \neq 0, \tfrac{1}{2}. \tag{9}$$

As a particular case, we give here the value of the constant $\mathcal{C}(1|\frac{1}{4}) = 2\Gamma(\frac{1}{4})\zeta(\frac{1}{2}) = -10.589\,351\ldots$, corresponding to the short-range case with $\nu = \frac{1}{4}$.

(b) In the two-dimensional case, $d = 2$, we obtain

$$\mathcal{C}(2|\nu) = 4\pi^{1-2\nu}\Gamma(\nu)\zeta(\nu)\beta(\nu) \qquad \nu \neq 0, 1 \tag{10}$$

where $\beta(\nu)$ is the analytic continuation of the Dirichlet series:

$$\beta(\nu) = \sum_{l=0}^{\infty}(-1)^l(2l+1)^\nu \qquad \nu > 0.$$

Note here that in the particular case corresponding to a long-range potential with $\nu = \frac{1}{2}$, we get $\mathcal{C}(2|\frac{1}{2}) = 4\sqrt{\pi}\zeta(\frac{1}{2})\beta(\frac{1}{2}) = -6.913\,039\,577\ldots$.

(c) The constant $\mathcal{C}(d|\nu)$ in the four-dimensional case, $d = 4$, turns out to be

$$\mathcal{C}(4|\nu) = 8\left(1 - 4^{1-\nu}\right)\pi^{2(1-\nu)}\Gamma(\nu)\zeta(\nu-1)\zeta(\nu) \qquad \nu \neq 0, 2. \tag{11}$$

We are particularly interested in the value of the constant in the case of the short-range interaction corresponding to $\nu = 2$. We find it to be exactly [15]

$$\mathcal{C}(4|1) = -8\ln 2.$$

As we mentioned above this constant has been widely used in the analytic investigation of finite-size scaling and its relation to numerical analysis.

Now we turn our attention to the three-dimensional case. To our knowledge there have been no analytic expressions for it up to now. This interesting case has been investigated numerically in reference [17]. In order to evaluate numerically the constant $\mathcal{C}(d|\nu)$, here we propose the following general formula:

$$\mathcal{C}(d|\nu) = -\frac{u^{d/2-\nu}}{d/2-\nu} + \sum_{l}{}' \frac{\Gamma\left(d/2-\nu, ul^2\right)}{l^{d-2\nu}} - \frac{\pi^{d/2}}{\nu u^\nu} + \mathcal{O}\left(u^{\nu-1}\exp\left[-\frac{\pi^2}{u}\right]\right) \tag{12}$$

obtained from equation (6) for u small enough. Equation (12) is a generalization of a three-dimensional result obtained in [18]. Note that equation (12) is valid for arbitrary d and $\nu \neq 0, \frac{d}{2}$, which makes it suitable for numerical evaluations of the constant $\mathcal{C}(d|\nu)$, especially in the cases of three and five dimensions used in finite-size scaling.

The nature of the error term equation (12) is such that this formula is useful for numerical evaluations even when the parameter u is not too small. Since $\mathcal{C}(d|\nu)$ with concrete values of the parameters d and ν is related to finite-size properties of confined systems with different geometries and different types of interparticle interaction, we shall present some of the most useful values obtained numerically from equation (12).

In the case of short-range interaction two constants were used in the literature corresponding to different situations. For a three-dimensional system confined to a fully finite geometry we find the value $\mathcal{C}(3|\frac{1}{2}) = -8.913\,629\,17\ldots$ in perfect agreement with [4, 8, 18, 19]. For a system with a slab geometry, we obtain $\mathcal{C}(3|1) = -5.028\,978\,843\ldots$, coinciding with the value given in [2]. Another case of interest is that of a system with the long-range case $\nu = \frac{3}{4}$ and a cubic geometry. For this case we have $\mathcal{C}(3|\frac{3}{4}) = -5.909\,841\,5587\ldots$. Finally, we quote a result for the five-dimensional case: it is $\mathcal{C}(5|1) = -4.228709895\ldots$ in agreement with that of reference [4], where this constant was used in the investigation of the finite scaling in a five-dimensional system confined to a cubic geometry.

Numerical values of $\mathcal{C}(4\nu|\nu)/\Gamma(\frac{\nu}{4})$ for $\nu = \frac{1}{4},\ \frac{1}{2},\ \frac{3}{4}$ and the exact value for $\nu = 1$ were recently reported in [20].

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Note added in proof. After the completion of this paper, we learned that identity (6), in a particular form, was first used by Epstein in 1903. We are grateful to R M Ziff, who brought to our attention both this fact and the review article [21] on the ideal Bose–Einstein gas, where the same type of functions appear in the case of a finite volume.

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