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ORIGINAL PAPER

# Electrostatic energy of polygonal charge distributions

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**Abstract** An asymptotic series for the electrostatic energy $\mathcal{E}_1(N)$ of an N-gonal charge distribution, i.e., a set of unit charges occupying vertices of a regular N-gon with a unit circumradius, is derived. Application of Padé approximants to truncations of this expansion produces compact approximate formulae capable of estimating $\mathcal{E}_1(N)$ with great accuracy. A closed-form expression for the energy of electrostatic interaction of two polygonal charge distributions is obtained from the respective Fourier series. The availability of this expression allows for a rapid calculation of the relevant energy with computational effort independent of the numbers of particles involved.

**Keywords** Polygonal charge distribution · Electron–electron repulsion

## 1 Introduction

Systems of classical particles with isotropic pairwise interactions confined by isotropic external potentials are well known to exhibit intricate patterns of particle positions at equilibrium geometries. These patterns are often very sensitive to the exact nature of both the interparticle and the confining potentials [1]. However, 2D assemblies of equicharged particles interacting with external potentials of cylindrical symmetry almost invariably involve either patterns of polygons inscribed on concentric rings or fragments of triangular lattices, the latter being more prevalent in species composed of larger numbers of particles [1–15]. Formation of polygonal patterns is observed in both experimental measurements and numerical studies of such diverse systems as electrons in quantum dots at the classical limit (the Wigner crystals) [2–7], ions in dusty plasmas [8–10], triboelectrically charged macroscopic objects [11], and vertices

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in mesoscopic superconducting disks [12,13]. These patterns persist upon inclusion of small-magnitude quantum and finite-temperature effects [2,6,15].

In many cases, the polygonal patterns of equicharged particles are either perfectly [11] or sufficiently regular [3,12–14] to permit formulation of simple mathematical models describing their geometries and energetics. Unfortunately, survey of the available literature reveals complete absence of rigorous analytical studies of such models. The first step towards bridging this unsatisfactory gap in knowledge requires detailed understanding of electrostatic energetics of polygonal charge distributions. In this paper, some results relevant to this subject are presented.

## 2 Theory

Consider an N-gonal charge distribution, i.e., a set of unit point charges occupying the vertices of a regular N-gon with a unit circumradius. The sum of electrostatic interaction energies of these charges constitutes the intraring energy $\mathcal{E}_1(N)$. Another situation of physical interest concerns interaction of two polygonal charge distributions consisting of $N_1$ and $N_2$ unit point charges occupying polygons with the circumradii $r_1$ and $r_2$, respectively. Such interaction gives rise to the interring energy $\mathcal{E}_{12}(N_1, N_2, r_1, r_2, \phi)$, where $\phi$ is the angle of rotation measuring the relative angular positions of the first vertices of the polygons in question, which are assumed to share a common center. Efficient computation of $\mathcal{E}_1(N)$ and $\mathcal{E}_{12}(N_1, N_2, r_1, r_2, \phi)$ that circumvents the need for single or double summations calls for two distinct mathematical approaches that are presented below.

### 2.1 The intraring energy

The explicit expression for $\mathcal{E}_1(N)$ reads

$$\begin{aligned}\mathcal{E}_1(N) &= \frac{N}{4}\sum_{k=1}^{N-1} sin^{-1}\frac{\pi k}{N}\\ &= \frac{N}{4}\sum_{k=1}^{N-1}\left(\frac{\pi k}{N}\right)^{-1}\left(1-\frac{k}{N}\right)^{-1} + \frac{N}{4}\sum_{k=1}^{N-1} G\left(\frac{\pi k}{N}\right), \end{aligned} \tag{1}$$

where

$$G(x) = sin^{-1} x - x^{-1}\left(1-\frac{x}{\pi}\right)^{-1}. \tag{2}$$

The first sum of the r.h.s. of Eq. (1) is readily evaluated as

$$\sum_{k=1}^{N-1}\left(\frac{\pi k}{N}\right)^{-1}\left(1-\frac{k}{N}\right)^{-1} = \frac{2N}{\pi}\,[\,\Psi(N)+\gamma\,], \tag{3}$$

where $\gamma$ is the Euler-Mascheroni constant and $\Psi(x)$ is the digamma function [16]. On the other hand, computation of the second sum involves the Euler-Maclaurin formula [17],

$$\sum_{k=1}^{N-1} G\left(\frac{\pi k}{N}\right) = \int_0^N G\left(\frac{\pi k}{N}\right) dk - \frac{1}{2}\left[ G(0) + G(\pi) \right] \\ + \sum_{j=1}^{\infty} \frac{B_{2j}}{(2j)!}\left(\frac{\pi}{N}\right)^{2j-1}\left[ G^{(2j-1)}(\pi) - G^{(2j-1)}(0) \right], \tag{4}$$

where $B_j$ is the $j$th Bernoulli number. When combined, Eqs. (1)–(4) yield

$$\mathcal{E}_1(N) = \frac{N^2}{2\pi}\left[ \Psi(N) + \gamma + ln\,\frac{2}{\pi} \right] + \frac{N}{4\pi} - \frac{\pi}{2}\sum_{j=1}^{\infty} \frac{B_{2j}}{(2j)!}\left(\frac{\pi}{N}\right)^{2j-2} G^{(2j-1)}(0). \tag{5}$$

However, since

$$G(x) = sin^{-1}x - x^{-1} + (x-\pi)^{-1} \\ = \sum_{j=1}^{\infty} \frac{(-1)^{j+1}\,2\,(2^{2j-1}-1)B_{2j}}{(2j)!}\,x^{2j-1} - \frac{1}{\pi}\sum_{j=0}^{\infty}\left(\frac{x}{\pi}\right)^{j}, \tag{6}$$

the derivatives of $G(x)$ that enter Eq. (5) are given by

$$G^{(2j-1)}(0) = \frac{(-1)^{j+1}\,(2^{2j-1}-1)B_{2j}}{j} - \frac{(2j-1)!}{\pi^{2j}}, \tag{7}$$

affording the expression

$$\mathcal{E}_1(N) = \frac{N^2}{2\pi}\left[ \Psi(N) + \gamma + ln\,\frac{2}{\pi} \right] \\ + \frac{N}{4\pi} + \sum_{j=1}^{\infty}\left[ \frac{B_{2j}}{4\pi j} + \frac{(-1)^{j}\,(2^{2j-1}-1)}{2j\,(2j)!}\,B_{2j}^2\,\pi^{2j-1} \right] N^{2-2j}. \tag{8}$$

The final substitution [16]

$$\Psi(N) = ln\,N - \frac{1}{2N} - \sum_{j=1}^{\infty} \frac{B_{2j}}{2j} N^{-2j} \tag{9}$$

yields the asymptotic series representation

$$\mathcal{E}_1(N) = \frac{N^2}{2\pi}\left(\gamma + ln\,\frac{2N}{\pi}\right) + \sum_{j=1}^{\infty} \frac{(-1)^j\,(2^{2j-1}-1)}{2j\,(2j)!} B_{2j}^2\,\pi^{2j-1}\,N^{2-2j}$$
$$= \frac{N^2}{2\pi}\left(\gamma + ln\,\frac{2N}{\pi}\right) + \left(-\frac{\pi}{144} + \frac{7\pi^3}{86400}N^{-2} + \cdots\right), \tag{10}$$

truncation of which produces quite accurate estimates of $\mathcal{E}_1(N)$ even for small values of N. The series (10) improves upon the asymptotics of $\frac{N^2}{2\pi}\,lnN$ obtained as a corollary from the Martinez-Finkelshtein theorem [18].

Further improvement in the accuracy of the closed-form approximations for $\mathcal{E}_1(N)$ is attained by retaining the leading terms of the r.h.s. of Eq. (10) up to the constant term and replacing the power series in $N^{-2}$ by Padé approximants with coefficients obtained by requesting that the approximate energies $\mathcal{E}_1(N)$ are exact for $1 \le N \le N_{max}$. In particular, the approximate expression,

$$\mathcal{E}_1(N) \approx \frac{N^2}{2\pi}\left(\gamma + ln\,\frac{2N}{\pi}\right) - \frac{\pi}{144} + \sum_{j=1}^{3} \frac{a_j}{b_j + N^2}, \tag{11}$$

corresponding to $N_{max} = 6$, where $a_1 = 1.5583690776957 \cdot 10^{-3}$, $a_2 = 8.9401249562521 \cdot 10^{-4}$, $a_3 = 5.9700243915101 \cdot 10^{-5}$, $b_1 = 1.6643500081388 \cdot 10^{-1}$, $b_2 = 8.9923320030262 \cdot 10^{-1}$, and $b_3 = 3.0403440002549$, reproduces the exact values of the intraring energies for $N > 6$ with the relative error of less than $7 \cdot 10^{-14}$.

### 2.2 The interring energy

The explicit expression for $\mathcal{E}_{12}(N_1, N_2, r_1, r_2, \phi)$, reads

$$\mathcal{E}_{12}(N_1, N_2, r_1, r_2, \phi) = \sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\left[ r_1^2 + r_2^2 - 2r_1r_2\,cos\left(\frac{2\pi i}{N_1} - \frac{2\pi j}{N_2} + \phi\right)\right]^{-1/2}. \tag{12}$$

In terms of dimensionless parameters, Eq. (12) can be rewritten as

$$\mathcal{E}_{12}(N_1, N_2, r_1, r_2, \phi) = N_1N_2\,(2\sqrt{r_1r_2})^{-1}\,\mathcal{F}\left(N_1, N_2, \left(\frac{r_1 - r_2}{2\sqrt{r_1r_2}}\right)^2, \phi\right), \tag{13}$$

where

$$\mathcal{F}(N_1, N_2, a, \phi) = (N_1N_2)^{-1}\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\left[ a + sin^2\left(\frac{\pi i}{N_1} - \frac{\pi j}{N_2} + \frac{\phi}{2}\right)\right]^{-1/2}. \tag{14}$$

The limiting behavior

$$\lim_{N_1\to\infty,\, N_2\to\infty} \mathcal{F}(N_1, N_2, a, \phi) = \frac{2}{\pi}\,\frac{1}{\sqrt{a}}\,K\left(-\frac{1}{a}\right), \tag{15}$$

where $K(x)$ is the complete elliptic integral of the first kind [16], can be readily demonstrated by replacing the double summation in Eq. (14) with the respective integration. It is equivalent to the previously derived [4] more complicated expression involving the hypergeometric function ${}_2F_1$.

After some manipulations, application of the Laplace expansion [19] to Eq. (12) yields

$$\begin{aligned}
&\mathcal{F}(N_1, N_2, a, \phi)\\
&= \frac{2}{\pi}\,\frac{1}{\sqrt{a}}\,K\left(-\frac{1}{a}\right) + \frac{4}{\sqrt{\pi}}\sum_{m=1}^{\infty}\left(\sqrt{a+1}-\sqrt{a}\right)^{-(2mL+1)}\\
&\quad\times\frac{\Gamma\left(mL+\frac{1}{2}\right)}{\Gamma\left(mL+1\right)}\,{}_2F_1\left(\frac{1}{2}, mL+\frac{1}{2}, mL+1, \left(\sqrt{a+1}+\sqrt{a}\right)^{-4}\right) cos\, mL\phi\\
&= \frac{2}{\pi}\,\frac{1}{\sqrt{a}}\,K\left(-\frac{1}{a}\right) + \frac{4}{\sqrt{\pi}}\sum_{m=1}^{\infty}\left(\frac{1}{4a+2}\right)^{mL+1/2}\frac{\Gamma\left(mL+\frac{1}{2}\right)}{\Gamma\left(mL+1\right)}\\
&\quad\times{}_2F_1\left(\frac{2mL+1}{4}, \frac{2mL+3}{4}, mL+1, \frac{1}{(2a+1)^2}\right) cos\, mL\phi,
\end{aligned} \tag{16}$$

where $L \equiv L(N_1, N_2)$ is the least common multiple of $N_1$ and $N_2$, and the identity [16]

$$\begin{aligned}
&{}_2F_1\left(\frac{1}{2}, m+\frac{1}{2}, m+1, z\right)\\
&\quad= (z+1)^{-(m+1/2)}\,{}_2F_1\left(\frac{2m+1}{4}, \frac{2m+3}{4}, m+1, \frac{4z}{(z+1)^2}\right)
\end{aligned} \tag{17}$$

has been used. Although the summation over $m$ in Eq. (16) cannot be carried out explicitly, application of the well-known integral representation of ${}_2F_1$ [16] produces

$$\begin{aligned}
&\mathcal{F}(N_1, N_2, a, \phi)\\
&= \frac{2}{\pi}\,\frac{1}{\sqrt{a}}\,K\left(-\frac{1}{a}\right) + \frac{2}{\pi}\sum_{m=1}^{\infty} cos\, mL\phi \int_0^1 \left(\frac{(1-t)\,t}{(2a+1)^2-t}\right)^{(2mL+1)/4}\frac{dt}{(1-t)\sqrt{t}}\\
&= \frac{2}{\pi}\,\frac{1}{\sqrt{a}}\,K\left(-\frac{1}{a}\right)\\
&\quad+\frac{2}{\pi}\int_0^{(\sqrt{1+a}-\sqrt{a})^4}\frac{-z^L+z^{L/2}\,cos\, L\phi}{1+z^L-2\,z^{L/2}\,cos\, L\phi}\,\frac{z^{-3/4}\,dz}{\sqrt{1-2\,(2a+1)\,\sqrt{z}+z}}.
\end{aligned} \tag{18}$$

With the help of the representation (18), the dependence of $\mathcal{F}(N_1, N_2, a, \phi)$ on $\phi$ is readily analyzed. In particular, it turns out that, as expected on physical grounds [compare Eq. (12)], $\mathcal{F}(N_1, N_2, a, \phi)$ possesses a period of $\frac{2\pi}{L}$ with respect to $\phi$, the maxima of

$$\mathcal{F}_{max}(N_1, N_2, a) = \frac{2}{\pi}\frac{1}{\sqrt{a}}K\left(-\frac{1}{a}\right) + \frac{2}{\pi}\int\limits_0^{(\sqrt{1+a}-\sqrt{a})^4} \frac{z^{L/2-3/4}}{1-z^{L/2}}\frac{dz}{\sqrt{1-2\,(2a+1)\sqrt{z}+z}} \tag{19}$$

occurring only at $\phi = 0,\ \frac{2\pi}{L}, \ldots$, and the minima of

$$\mathcal{F}_{min}(N_1, N_2, a) = \frac{2}{\pi}\frac{1}{\sqrt{a}}K\left(-\frac{1}{a}\right) - \frac{2}{\pi}\int\limits_0^{(\sqrt{1+a}-\sqrt{a})^4} \frac{z^{L/2-3/4}}{1+z^{L/2}}\frac{dz}{\sqrt{1-2(2a+1)\sqrt{z}+z}} \tag{20}$$

occurring only at $\phi = \frac{\pi}{L},\ \frac{3\pi}{L}, \ldots$. The respective second-order derivatives with respect to $\phi$ equal

$$\mathcal{F}''_{max}(N_1, N_2, a) = -\frac{2}{\pi}L^2\int\limits_0^{(\sqrt{1+a}-\sqrt{a})^4} \frac{1+z^{L/2}}{(1-z^{L/2})^3}\frac{z^{L/2-3/4}\,dz}{\sqrt{1-2\,(2a+1)\sqrt{z}+z}} \tag{21}$$

and

$$\mathcal{F}''_{min}(N_1, N_2, a) = \frac{2}{\pi}L^2\int\limits_0^{(\sqrt{1+a}-\sqrt{a})^4} \frac{1-z^{L/2}}{(1+z^{L/2})^3}\frac{z^{L/2-3/4}\,dz}{\sqrt{1-2\,(2a+1)\sqrt{z}+z}}. \tag{22}$$

The representation (18) is not well-suited for numerical computations of $\mathcal{F}(N_1, N_2, a, \phi)$. However, employment of an alternative formula,

$$\mathcal{F}(N_1, N_2, a, \phi) = \frac{2}{\pi}\frac{1}{\sqrt{a}}K\left(-\frac{1}{a}\right) + \frac{4}{\pi}\int\limits_0^{(1/2)\,ln(1+a^{-1})} \left.\frac{-z^{L-1/4}+z^{L/2-1/4}\cos L\phi}{1+z^L-2\,z^{L/2}\cos L\phi}\right|_{z=[\,e^{-u}-1+a(e^u+e^{-u}-2)\,]^2} du, \tag{23}$$

in conjunction with trapezoidal quadrature produces accurate results with relatively small numbers of the quadrature points.

## 3 Discussion and conclusions

It is instructive to compare the asymptotic series (10) for the energy of the optimal distribution of equicharged particles on a circle with a unit radius with its 3D counterpart (known as the solution of the Thomson problem [20]). Unlike in the latter case, where the energy scales like the squared number of particles at the limit of $N \to \infty$, the leading term in Eq. (10) contains a logarithmic contribution. However, the 2D case is amenable to exact asymptotic analysis, whereas neither the general solution of the Thomson problem nor the exact asymptotics of the corresponding energy beyond the first two leading terms are currently known [21].

The availability of the Fourier expansion (16) for the dependence of the interaction energy of two polygonal charge distributions on their relative angular positions allows for detailed analysis of rotational barriers that play a crucial role in melting of Wigner crystals due to quantum and finite-temperature effects [2,14]. In particular, the availability of the expressions (19)–(22) makes it possible to readily estimate the magnitudes of rotational barriers and the Hessian eigenvalues describing the rotational motion. For example, combining these expressions at the limit of $a \to \infty$ immediately reproduces several of the approximate equations presented in Ref. [14] and permits derivation of the leading corrections to them. Similarly, the failure of the model introduced in Ref. [3] to accurately estimate energies of 2D Coulomb crystals is readily accounted for by the strong deviation of the angle-independent term in the r.h.s. of Eq. (13) combined with Eq. (16) from its $r_1 \to 0$ limit. From the practical standpoint, it is important to mention that employing numerical quadrature in evaluation of the integral that enters Eq. (23) produces a fast algorithm for the computation of $\mathcal{E}_{12}(N_1, N_2, r_1, r_2, \phi)$ with computational cost independent of the numbers of particles involved.

In light of these observations, we believe that the present results are slated to stimulate and aid future formulations and detailed analyses of simple geometrical models that accurately describe self-assemblies of equicharged particles.

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