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Equilibrium configurations of particles on a sphere: the case of logarithmic interactions

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Abstract. We consider a system of N particles which are confined to the surface of a sphere and which interact via a potential that depends logarithmically on their separation. The ground-state properties of this system are investigated for $N = 2$ to 65. Unlike the case of Coulomb interactions this system has ground-state configurations with zero dipole moment for *all* N. The thermal properties of a selected set of systems in the range $N = 2$ to 500 are determined by Monte Carlo simulation. The results are compared with analytical calculations in the small- and large-N limits.

1. Introduction

We re-visit an old problem in mathematical physics, which has been presented as having applications in a wide range of subject areas. The general problem is to find the minimum-energy configuration of a system of particles (or disclinations, molecules, pores or fuel depots) located on the surface of a sphere. The particles are subject to a repulsive pair interaction of the form $v(r) \propto r^{-n}$, with r the length of a chord connecting the two particles [1]. In the limit $n \to \infty$ the problem is commonly called the Tammes problem [2] after a Dutch botanist who was interested in the pattern of orifices in spherical pollen grains. The Tammes problem is equivalent to that of finding the largest radius of N non-overlapping circles on a sphere.

A related, but conceptually simpler problem was posed by Kepler almost 400 years ago. In that case the problem was to find the densest packing of spheres in a Euclidean space. In three dimensions 'mathematicians believe and physicists know' that the solution is one of the two closed packed lattices (hexagonal closed packed or face-centred cubic), while in two dimensions the solution is a triangular lattice [3, 4] . The reason the situation is more complicated in the curved space of a spherical surface is that it is not possible to cover the surface with a triangular lattice without defects. It is easy to understand that in the case of special numbers such as $N = 7, 11, 23$ there will be a great deal of frustration, and that complicated configurations will result [5]. However, it is surprising that in many cases when high-symmetry configurations are available, such as an inscribed Platonic solid, the high-symmetry configuration is often not the favoured solution [6]. This can be partially understood if one notes that the particles are most closely packed if the coordination number (number of nearest neighbours) is high. For example, in the case of the inscribed cube the average coordination number is 3. If, however, two opposing faces are rotated relative to each other by 45 degrees, the number of nearest neighbours can be increased to four (see figure 3).

Interest in the problem of N equal Coulomb charges on a sphere, $n = 1$, began with the J Thomson plum pudding model of the atom [7, 8]. Although the original motivation was quickly made obsolete by the advent of quantum mechanics, interest in the mathematical problem has continued. A practical motivation was provided by Hansen *et al* [9] who performed molecular dynamics simulations of ionic liquids on a sphere in order to avoid having to perform computationally intensive Ewald sums at each time step. The ground states for Coulomb charges on a sphere have recently been reviewed by Erber and Hockney [10]. The thermodynamic limit for charges on a sphere $N \to \infty$ has been studied by Corevaar [11].

Here, we address the case of logarithmic interactions, $n = 0$, on a sphere. Finite-temperature Monte Carlo simulations on this system have previously been carried out for $N = 104$, 160 and 256 by Caillol *et al* [12]. The corresponding problem in two-dimensional electrostatics of finding the equilibrium configurations of charges on a disk with a uniform neutralizing ('jellium') background has been studied by a number of authors (see, e.g., Thoquard and Clerouin [13] and de Leeuw and Perram [14]), and was recently re-discovered by Kogan *et al* [15].

The logarithmic potential is of interest when considering the thermodynamic limit of many particles on a large sphere. In this case it is tempting to describe the system in terms of disclinations distorting a triangular lattice with logarithmic interactions between nodes. Recently, Lubensky and Prost [16] examined the vortex defects in the hexatic phase of a liquid crystal confined to a closed surface with spherical topology. They determined that the longest-range interaction between the defects was logarithmic in the chord separating them.

In this paper, we determine the ground states and low-temperature thermodynamics of a discrete number N of particles with logarithmic pair potentials, where the particles are confined to a spherical surface embedded in three dimensions. In section 2 we show that the logarithmic interaction yields ground-state configurations with zero net dipole moment for any N, in contrast to the Coulomb case where a number of ground-state configurations exhibit a net dipole moment [10]. We also determine the asymptotic form of the ground state for large N and compare with the ground-state energy for $N = 2$ to 65 from simulations. In addition we classify the ground-state configurations according to their chirality and properties of the moment of inertia tensor.

In section 3, we investigate the thermodynamics of a selected set of systems in the range $N = 2$ to 500 at low temperature via Monte Carlo simulation. We determine the heat capacities of these systems and extrapolate their mean energies to zero temperature. A summary is given in section 4.

2. Ground-state properties

We investigate a system in which the potential energy of N particles, confined to a spherical surface, is written as

$$H = -\sum_{i>j} \ln\left(\frac{r_{ij}}{L}\right) = -\tfrac{1}{2}\sum_{i>j} \ln[2(1 - \hat{r}_i \cdot \hat{r}_j)] + \frac{N(N-1)}{2} \ln\left(\frac{L}{R}\right) \qquad (1)$$

where r_{ij} is the chord between particles i and j, L is an arbitrary length needed to make the logarithm dimensionless, and R is the radius of the sphere. In what follows we choose $L = R$. The sum is performed over all particle pairs. The surface is taken to have unit radius, so the maximum value of r_{ij} is 2.

Contrary to the Coulomb case where several lowest-energy configurations exhibit a dipole moment [10], none of the ground-state configurations with the logarithmic potential have a dipole moment. To see this, we first note that the force on the ith particle due to all the others must be directed radially for any equilibrium configuration (otherwise the charge would move along the surface),

$$\sum_{j\neq i} \frac{\hat{r}_i - \hat{r}_j}{(\hat{r}_i - \hat{r}_j)^2} = f_i \hat{r}_i \,. \tag{2}$$

If we multiply both sides of (2) with $\hat{r}_i$, we see that $f_i = \frac{1}{2}(N-1)$ is the same for all i. By summing (2) over i, and using the fact that $\hat{r}_i - \hat{r}_j$ is antisymmetric in i and j, we find that the dipole moment must vanish. The logarithmic interaction appears to be unique in this respect.

We can obtain analytically two limits for the results for the ground-state energy. First, for $N = 2$, the partition function Z can be determined exactly:

$$\ln Z = \ln 4\pi + \beta \ln 2 - \ln\left(\frac{\beta}{2} + 1\right) \tag{3}$$

where β is the inverse temperature. From the partition function, we find $E_2 = -\ln 2$ for the ground-state energy, and $C/N = 0.5$ for the specific heat.

At large N, a mean-field model can be used to evaluate the energy. The average interaction energy of a single particle as a result of its interaction with $N-1$ other particles is

$$\epsilon = -\tfrac{1}{2}\int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \; p(\theta,\pi) \ln[2(1-\cos\theta)] \sin\theta \tag{4}$$

where $p(\theta,\phi)$ is the probability of finding a particle at polar angle θ and azimuthal angle ϕ, given that there is a particle at the north pole ($\theta = 0$). The ground-state energy of the system is then given by $E = \frac{1}{2}\epsilon N$. We can get an estimate of the ground-state energy by making the approximation

$$p(\theta,\phi) \approx \begin{cases} 0 & \theta < \theta_0 \\ N/4\pi & \pi > \theta > \theta_0 \,. \end{cases} \tag{5}$$

We determine θ_0 by requiring that

$$\int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \; p(\theta,\pi) = N - 1 \tag{6}$$

which gives $\theta_0 = \sqrt{4/N}$. Substituting into the expression for the energy gives

$$E \approx -N^2\left(\tfrac{1}{2}\ln 2 - \tfrac{1}{4}\right) - \tfrac{N}{4}\ln N + N\left(\tfrac{1}{2}\ln 2 - \tfrac{1}{4}\right). \tag{7}$$

If a more accurate form is used instead of (5), equation (7) would be modified. However, since there will still be an average particle density $N/4\pi$ and an angle of closest approach $\theta_0 \sim 1/\sqrt{N}$, the terms in (7) proportional to N^2 and $N \ln N$ will not be affected. If we rescale our unit of length (make $R \neq L$) we add a term $[N(N-1)/2]\ln L/R$ in the expression for the energy. We can therefore choose the energy term proportional to N^2 to be zero. We believe the term proportional to $N \ln N$ to be exact and this term will pre-empt the system from having a proper thermodynamic limit.

We expect to be able to fit the ground-state energy for large N to a formula of the form

$$E = -N^2\left(\tfrac{1}{2}\ln 2 - \tfrac{1}{4}\right) - \frac{N}{4}\ln N + l_1 N + l_2 + \cdots \tag{8}$$

where l_1 and l_2 are fitting parameters.

Table 1. Absolute value of ground-state energies, and type of configuration for $N = 2$ to 65. N_D = biaxial, C = chiral, N_- = uniaxial disc-like, I = isotropic, N_+ = uniaxial rod-like.

N	Energy		N	Energy		N	Energy	
1	0		2	0.693 147 180 56	N_+	3	1.647 918 433 00	N_-
4	2.942 487 759 04	I	5	4.420 507 155 24	N_+	6	6.238 324 625 04	I
7	8.182 477 864 44	N_-	8	10.428 017 781 5	N_-	9	12.887 752 725 8	N_-
10	15.563 123 389 0	N_+	11	18.420 479 720 8	N_D	12	21.606 145 230 4	I
13	24.866 721 875 5	N_D	14	28.407 813 009 2	N_-	15	32.147 876 283 8	N_+C
16	36.106 152 162 0	IC	17	40.273 066 961 2	N_+	18	44.650 287 259 2	N_-
19	49.198 891 565 8	N_D	20	54.011 129 974 6	N_-	21	59.000 912 135 1	N_D
22	64.206 007 761 7	I	23	69.578 382 592 5	N_-C	24	75.213 984 788 6	IC
25	80.997 509 990 2	N_D	26	87.009 423 057 0	N_DC	27	93.251 986 400 0	N_-
28	99.658 609 384 1	IC	29	106.254 571 171	N_DC	30	113.089 255 497	N_DC
31	120.110 346 640	N_-	32	127.378 867 615	I	33	134.747 820 824	N_D
34	142.375 852 271	N_DC	35	150.192 058 511	N_DC	36	158.224 068 426	N_DC
37	166.450 697 524	N_+	38	174.880 197 152	N_-	39	183.509 225 712	N_-
40	192.337 689 917	I	41	201.359 206 648	N_+	42	210.584 511 558	N_-
43	220.003 477 052	N_D	44	229.641 801 488	I	45	239.453 698 253	N_-C
46	249.452 540 709	IC	47	259.661 759 853	N_D	48	270.117 949 959	IC
49	280.701 903 118	N_+C	50	291.528 600 658	N_+	51	302.533 673 455	N_+C
52	313.732 371 935	N_-C	53	325.138 234 695	N_D	54	336.745 464 397	N_DC
55	348.541 796 281	N_DC	56	360.545 899 244	N_DC	57	372.741 200 618	N_-C
58	385.132 829 792	N_DC	59	397.728 149 661	N_DC	60	410.533 162 793	N_+C
61	423.507 635 991	N_DC	62	436.703 979 238	N_-C	63	450.081 239 177	N_+C
64	463.654 432 987	N_DC	65	477.426 426 069	N_DC			

To determine the ground-state properties numerically, we start an initial configuration with the particles randomly distributed on the spherical surface. We then calculate for each particle the force from all the other particles, and displace each particle a distance which is proportional to the force. This moves the particles off the surface of the sphere, so we project the particles back to the surface. The process is repeated and the energy E and dipole moment $d = \sum_i r$ is monitored. The process is stopped when the dipole moment is zero within a tolerance ($< 10^{-14}$), and the energy has stabilized to 15 significant figures. The calculated ground-state energies are listed in table 1. The calculated ground-state energies are also compared to the asymptotic formula (8) in figure 1, with fitted values of l_1 and l_2 given in the figure caption. We see that when $N \geqslant 60$ the scatter has been reduced to less than 1 part in 10^{-4}. The same argument which was used to obtain (8) can also be used to obtain an asymptotic formula for $n = 1$ (Coulomb case) [10], of the form

$$E = \tfrac{1}{2}N^2 + c_1 N^{3/2} - c_2 N + \cdots . \tag{9}$$

A plot of the scatter when (9) is fitted to the data of [10] is shown in figure 2. We see that the two figures are remarkably similar, although the ground-state configurations are, in fact, different for the two potentials (except for $N \leqslant 6$, $N = 12$, and somewhat surprisingly $N = 32$ see (figure 3)).

While ground-state configurations with the logarithmic interaction cannot exhibit a dipole moment they can exhibit *chirality*. Given a set of N points, one can generate a second set by doing an inversion about any point in space. The original set is chiral if the inverted set cannot be made identical to the first by a series of rotations (we do not need to worry about translations since all equilibrium configurations with logarithmic interactions

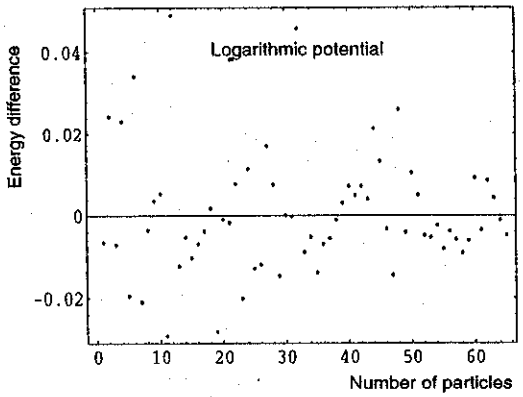

Figure 1. Scatter plot of the difference between $-N^2(\frac{1}{2}\ln 2 - \frac{1}{4}) - \frac{1}{4}N\ln N + 0.0260N - 0.116$ and the ground-state energies $E(N)$ of table 1 for the logarithmic potential.

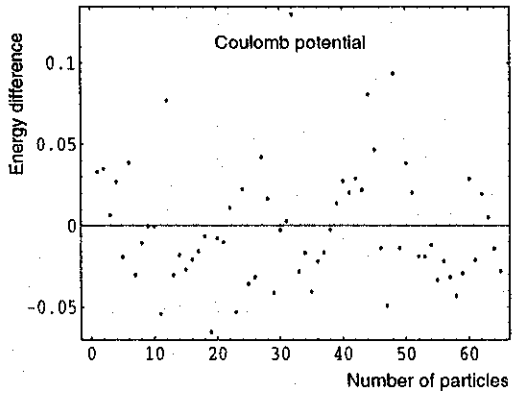

Figure 2. Scatter plot of the difference between $N^2/2 + 0.553N^{1.5} - 0.013N - 0.07$ and the ground-state energies of Erber and Hockney [10] using the Coulomb potential.

sets can be made identical by a set of rotations is as follows.

(1) From the coordinates of the original set construct the inverted set $r_i = -r_i$ for all i.
(2) Take the first two points of the original set and perform rotations about the origin until the chord joining the two points is in a 'standard position' parallel to the x-axis with the midpoint on the positive z-axis (see figure 3).
(3) Calculate the length of the chord and find the set of pairs of the inverted set which are separated by this length within a tolerance.
(4) Put the chords generated from all the pairs in the standard position.
(5) Test if the two sets are identical within a tolerance.

The low-N configurations for which the ground state is chiral are listed in table 1. We find for $N \leqslant 65$ that if the ground state with the logarithmic potential is chiral, it will be chiral with the Coulomb potential. If it is not, it will not be chiral with the Coulomb potential either, although the configurations are mostly different.

Another way of describing the configurations is through the traceless part of the moment of inertia tensor

$$Q_{\alpha,\beta} = \frac{1}{2N}\sum_{i=1}^{N}(3r_{i,\alpha}r_{i,\beta} - \delta_{\alpha\beta})\,. \tag{10}$$

In accordance with liquid-crystal terminology we write $q, -\frac{1}{2}(q-p), -\frac{1}{2}(p+q)$ for the eigenvalues of Q (where q is the eigenvalue which is largest in magnitude). If p and q

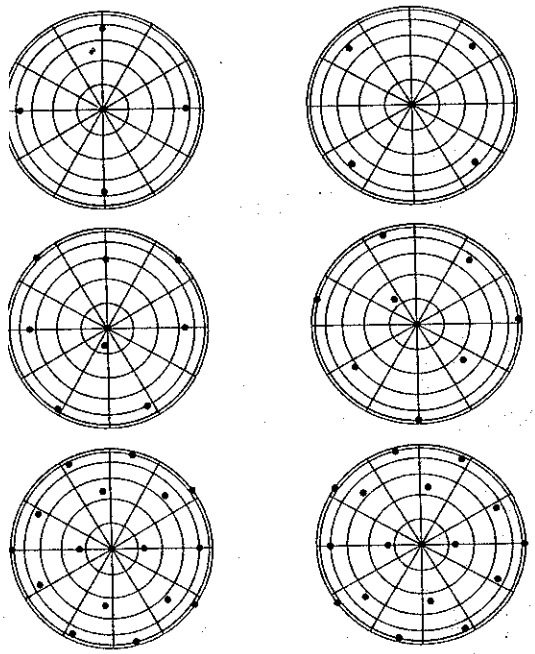

Figure 3. Polar plots of the ground-state configurations for $N = 8$ (top), $N = 16$ (middle) and $N = 32$ (bottom). Parallels are separated by 15°. All configurations are in one of the 'standard positions' used in the chirality tests. Left and right columns are projections of the upper and lower hemisphere on the equatorial plane. The $N = 16$ configuration is *chiral*. Note the inversion symmetry of the $N = 32$ ground state.

are both zero we refer to the configuration as isotropic (I), if $q > 0$, $p = 0$ it is uniaxial rod-like nematic (N_+), if $q < 0$, $p = 0$ it is uniaxial disk-like and we call it (N_-), while if p and q are both non-zero it is biaxial with notation (N_D). The classification of the ground-state configurations in this scheme is listed in the table.

For $N = 47$ the biaxiality was found to be quite weak. The ground states with the Coulomb potential have the same classification *except*

$N = 29$, which is (N_D) with the logarithmic and (N_-) with the Coulomb potential,
$N = 52$ which is (N_-) with the logarithmic and (N_+) with the Coulomb potential.

For a number of N-values there are more than one stable configuration, the lowest of these in energy being the ground state. Suppose we have started up the system with either the logarithmic or Coulomb potential, and happened to reach the ground state. Then in *almost* all cases, if we switch from one potential to another, and keep the step size small enough, we will evolve into a ground state of the other potential. The exception is $N = 56$, where the ground state of one potential evolves into a metastable configuration for the other, and vice versa. Of course, we cannot be sure that we have the true ground state in all cases. We reproduce the results of [10] for the Coulomb potential in almost all cases. The exceptions are $N = 36$ where we find a slightly different ground-state energy $E = 529.122\,408\,38$ and a dipole moment $< 10^{-8}$, and $N = 38$ and 44, where we find that the dipole moment is zero.

3. The case of non-zero temperature

Monte Carlo computer simulations allow us to calculate the mean energies of N-particle systems at non-zero temperature and to determine the ground-state energies via extrapolation to zero temperature. Because the extrapolations require simulation at several non-zero temperatures for a given N, the method is not as computationally efficient as the approach

used in the previous section for finding ground states. Hence, the Monte Carlo simulations are focused on a limited range of N where finite-temperature properties are of interest.

The simulation is performed using the traditional Metropolis algorithm. A system of N particles is initialized with the particles randomly placed on the surface of a sphere with unit radius. The particles are subject to the Hamiltonian (1). The kinetic energy does not appear in the Hamiltonian since we are interested only in equilibrium properties, and the potential is independent of momentum. Each particle is described by its polar coordinates θ, ϕ. On each particle in turn, a trial move is made by changing $\cos\theta$ and ϕ randomly within a range $\pm\delta s$ and $\pm 2\pi\delta s$, respectively. The change in energy associated with the attempted move is determined from the Hamiltonian, and the move is conditionally accepted according to the Boltzmann weight $e^{-\beta H}$, where β is the inverse temperature. The choice $\delta s = 0.01$ provides a reasonable acceptance rate for the moves. Because the procedure produces configurations which are highly correlated, not every configuration in the simulation is used to construct ensemble averages. Rather, configurations are 'saved' only $\delta s^{-2} = 10^4$ sweeps over the positions, where each particle receives one trial move per sweep. Typically 100 configurations are used for constructing ensemble averages at each N, β combination. The exceptions are $N = 2$ (300), 3 (200), 200 (40) and 500 (20), where the number in parentheses indicates the number of configurations, separated by 10^4 sweeps, used at each β.

Each ensemble is used to determine a value for $\epsilon = \langle H \rangle / N$. It is observed that ϵ rises linearly with temperature $1/\beta$ for β in the range 1000 to 300. This linear behaviour allows us to determine the heat capacity C at low temperatures and to obtain the ground-state energy by extrapolation. The absolute statistical accuracy of our calculation for ϵ is about 10^{-4}. The statistical uncertanties in heat capacity per particle C/N are about 3%.

Table 2. Ground-state energy ϵ_{gs} and specific heat C/Nk_B obtained by linear fits to ϵ as a function of $1/\beta$ in the range β =1000 to 300.

N	$\epsilon_{gs} = \lim_{1/\beta \to 0} \langle H \rangle / N$	C/Nk_B
2	− 0.346 53± 0.000 06	0.48± 0.03
3	− 0.549 28± 0.000 05	0.46± 0.02
4	− 0.735 77± 0.000 08	0.71± 0.04
5	− 0.884 15± 0.000 06	0.73± 0.03
6	− 1.039 77± 0.000 10	0.75± 0.04
7	− 1.168 91± 0.000 06	0.74± 0.03
8	− 1.303 26± 0.000 08	0.68± 0.04
50	− 5.830 67± 0.000 05	1.05± 0.02
100	− 10.833 83± 0.000 02	1.05± 0.01
200	− 20.665 01± 0.000 02	1.07± 0.01
500	− 49.866 61± 0.000 04	1.02± 0.02

A summary of the Monte Carlo results is shown in table 2. Within the statistical accurac the extrapolated ground-state energies agree with the results of section 2. The Monte Carl ground-state energies were used in the fitting procedure of the previous section to determin l_1 and l_2 of (8). The low-temperature heat capacity per particle increases from $\frac{1}{2}$ at $N =$ (as can be computed from (3)) to a value close to 1 for large N. This large-N behaviour expected if the particles are in Hooke's-law potentials.

4. Conclusions

We have investigated the properties of a system of particles located on the surface of a sphere and interacting with a potential which varies logarithmically with the chord separating the particles. One striking difference between the logarithmic and other potentials is that the ground states have zero dipole moment for all N in the former case. Except for a few special cases, the ground-state configurations will be distinct from those calculated with the Coulomb or a short-range potential. Nevertheless, the configurations with different potentials are similar in many respects. Because of the long range of the logarithmic interaction the ground-state energy does not have a proper thermodynamic limit, but the heat capacity is proportional to N and at low temperatures the system behaves as if connected with Hookean springs.

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