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Energies and spacings of point charges on a sphere

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Received 6 August 1991

Abstract. Numerical methods are in general required for the determination of the stable configurations of N point charges on a sphere. The stable configurations for N up to 50 have previously been ascertained and we extend the calculations here for values up to 101. We report for the first time some remarkable global features of these configurations. We show that the minimum energy accurately follows a simple half-integral power law in $1/N$ over the full range we have investigated. This power law is explicable in terms of the idealization of mapping a planar Wigner lattice onto the surface of the unit sphere; the pair distribution functions of the larger- N configurations indicate predominant hexagonal coordination. The coefficients of the observed power law are closely straddled by values calculated on the basis of hexagonal and square Wigner lattices. This highly accurate description of the energy permits us to remark on the detailed deviations of the individual structures from the general trend. For $N < 30$, we note that structures with N prime are relatively less stable, while structures with N equal to 6, 12, 32, 44, 48 and 60 seem more stable.

1. Introduction

The stable (least energy) configurations of N point charges on a sphere and on a disk are of wide-ranging interest, in areas as diverse as botany, chemistry, mathematics and condensed matter physics [1-7]. Although it might seem at first sight that straightforward geometrical considerations would lead to a full description of the configurations, this is not so and numerical procedures must be invoked to establish the stable configurations [1]. Thus, Weinrach *et al* [2], have recently used a Monte Carlo procedure to infer the symmetries of the stable configurations of N equal charges on a sphere, up to $N = 50$, in the process correcting some earlier geometrically-inspired results based on regular polyhedra.

For larger values of N , because of the multiplicity of configurations having almost the same low value of energy, it becomes increasingly difficult to identify with certainty the configuration that has the true minimum in energy. A criterion, by which one can judge the likelihood that a candidate computer-generated configuration is the stable configuration, would be a useful asset. Further, when the stable energies are surveyed as a function of N , there are certain values of N , such as 2, 4, ... which stand out as having energies below the 'norm', rendering these structures more favourable in some sense. Likewise, for values of N such as 3, 5, ... the stable energies are above the 'norm' and these could therefore be regarded as less favourable. This notion of favourability needs to be formulated in a more concrete fashion that provides for a quantitative measure of relative stability and from which a deeper understanding of structures adopted may be obtained.

In this paper we provide a simple analytical formula which represents, to a high degree of accuracy, the stable configurational energies for N from 1 to beyond 100. This formula is initially introduced as an empirical fit to the data. Subsequently we show that it can be formally derived from considerations of the arrangement of the point charges in the form of a distorted Bravais lattice on the surface of the sphere. The parameters of the empirical fit lie within narrow bounds established on purely theoretical grounds.

2. Empirical fit to data

To supplement data which is already available in the literature, we have implemented a Monte Carlo optimization routine, similar to the prescription of Weinrach *et al* [2], in TurboBASIC and FORTRAN, and have calculated the energies of all the numerically stable potential energy minimal structures up to $N = 42$ and then for many values of N up to 101. The potential energy is calculated as the sum of interaction energies of equal point charges on a unit sphere:

$$W = \sum_{i>j} q_i q_j / d_{ij} \quad (1)$$

where the charges q_i are taken as unit and d_{ij} is the Euclidean distance between the charges. As has already been observed [2], the region of the minimum is easily attained but convergence to the true minimum is not assured. Our implementation is accurate to within about 1° of relative separation of the charged points on the sphere surface, which is good enough for our purposes. In addition, Dr Bennett [2] has provided us with his calculated values of W for most of N to 50, and $N = 60$.

Table 1 contains the minimum calculated energies $W(N)$, found or supplied to us, and the reported symmetries of those configurations [2], for unit point charges on a sphere. Figure 1 shows a graph of $W(N)$ versus N for N up to 101. It is striking how close the configuration energies lie to a smooth curve. On the scale that has been used, scatter in the energies can barely be discerned. Also plotted for comparison are the curves of $W_c(N) = N^2/2$ versus N and of $W_r(N) = N(N-1)/2$ versus N . $W_c(N)$ represents the energy of a continuous charge of magnitude N uniformly spread over the unit sphere, while $W_r(N)$ is the average configurational energy of N point charges randomly distributed over the unit sphere, which fact we have confirmed in computations. The curves for both these classical formulae lie well above that of $W(N)$. The failure of $W_r(N)$ as an estimator of $W(N)$ is due to the fact that it takes no account of the correlations between the positions of the particles. A characteristic of stable configurations is that nearest-neighbour distances tend to be comparable in magnitude and close contacts between the charges are avoided whereas, with random configurations, there is no limit to how close neighbouring charges can come to one another, which pushes up the configurational energies.

In the limit $N \rightarrow \infty$ the discrete charge distributions become effectively continuous so that both $W_r(N)/W_c(N) \rightarrow 1$ and $W(N)/W_c(N) \rightarrow 1$. In order to display the correct asymptotic behaviour, a power series representation of $W(N)$ will therefore take the form

$$W(N) = \frac{N^2}{2} (1 + p(N)) \quad (2)$$

Table 1. Energies and symmetries of point charges on a sphere.

<i>N</i>	Pt Grp ^a	<i>W</i> ^b	<i>W</i> ^c _{est}	<i>N</i>	Pt Grp	<i>W</i>	<i>W</i> _{est}
1	C ₁	0.000	-0.003	38	C _s	593.049 ^b	593.127
2	D _{∞h}	0.500	0.508	39	D _{3h}	626.389 ^b	626.499
3	D _{3h}	1.732 ^b	1.718	40	T _d	660.675 ^b	660.804
4	T _d	3.674 ^b	3.685	41	D _{3h}	695.917 ^b	696.044
5	D _{3h}	6.475 ^b	6.443	42	D _{5h}	732.078 ^b	732.219
6	O _h	9.985 ^b	10.014	43	C _s	769.191 ^b	769.331
7	D _{5h}	14.453 ^b	14.415	44	O _h	807.174 ^b	807.379
8	D _{4d}	19.675 ^b	19.659	45	D ₃	846.188 ^b	846.365
9	D _{3h}	25.760 ^b	25.756	46	C ₂	886.172 ^b	886.289
10	D _{4d}	32.717 ^b	32.715	47	C _s	927.062 ^b	927.152
11	C _{2v}	40.596	40.542	48	O	968.714 ^b	968.955
12	I _h	49.165 ^b	49.245	49	C ₁	1011.557 ^b	1011.698
13	C _{2v}	58.853 ^b	58.827	50	D _{6d}	1055.183 ^b	1055.383
14	D _{6d}	69.306 ^b	69.295	51		1100.037	1100.008
15	D ₃	80.670 ^b	80.652	52		1145.681	1145.576
16	T	92.912 ^b	92.901	53		1192.151	1192.086
17	D _{5h}	106.050 ^b	106.048				
18	C _{4v}	120.084	120.093	59		1490.952	1490.971
19	C _{2v}	135.089 ^b	135.041	60		1543.804	1544.094
20	D _{3h}	150.881	150.894	61		1598.293	1598.164
21	C _{2v}	167.641	167.655				
22	T _d	185.287	185.325	69		2064.916	2064.847
23	D ₃	203.930 ^b	203.907	70		2127.686	2127.455
24	O	223.347 ^b	223.402	71		2191.256	2191.012
25	C _s	243.813 ^b	243.813				
26	C ₂	265.133 ^b	265.141	79		2734.017	2733.736
27	D _{5h}	287.303 ^b	287.388	80		2806.022	2805.863
28	T	310.491 ^b	310.555	81		2879.435	2878.945
29	D ₃	334.627	334.643	82		2953.274	2952.980
30	C ₂	359.604 ^b	359.655	83		3028.419	3027.970
31	C _{3v}	385.531 ^b	385.592	84		3104.487	3103.915
32	I _h	412.245	412.454	85		3181.172	3180.814
33	C _s	440.195	440.243				
34	D ₂	468.904	468.960	90		3580.051	3579.642
35	C ₂	498.551	498.605	99		4358.055	4357.805
36	D ₂	529.122 ^b	529.181	100		4449.055	4449.057
37	C ₂	560.622	560.688	101		4541.035	4541.267

^a Point Group, as reported by Weinrach *et al* [2].

^b The lowest potential energy of *N* unit point charges on a sphere, obtained by a Monte Carlo procedure. Those labelled^b were supplied by Bennett [2], while the remainder were calculated by ourselves.

^c Estimate of *W* from equation (2) (see text).

where

$$p(N) = a/N^\alpha + b/N^\beta + \dots \quad 0 < \alpha < \beta < \dots \quad (3)$$

Since *p(N)* is undefined for negative *N*, *p(N)* need not be analytic at the limit *N* → ∞ and the exponents α, β, ... are not required to be integers. For sufficiently large *N*, *b/N^β* and subsequent terms in the expansion become negligible in comparison with the first term and can be neglected. Treating α and *a* as adjustable parameters and fitting (3) to the data points *W*(80) = 2806.022 and *W*(70) = 2127.686 one obtains

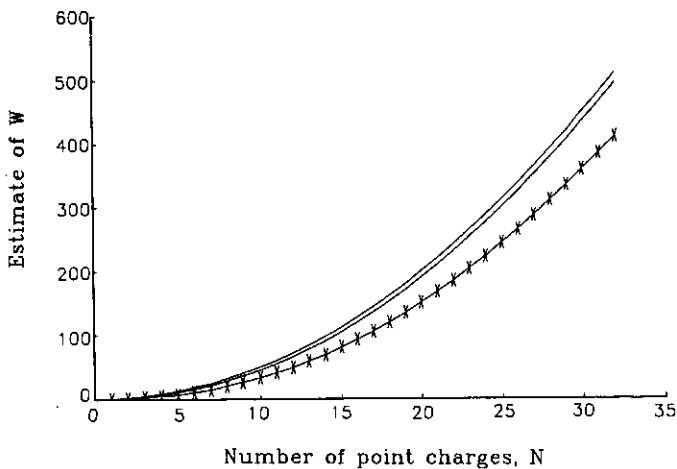


Figure 1. Dependence of the Monte Carlo minimum energies $W(N)$ (indicated by crosses), the energy of a continuous charge $W_c(N)$ (uppermost curve) and the average energy of randomly distributed charges $W_r(N)$ (central curve) on N .

$\alpha = 0.496$ and $a = -1.084$, leaving little doubt that α should be $1/2$. With these values of the parameters, equation (3) fits the data for $W(N)$ accurately down to about $N = 30$. For smaller values of N , the term b/N^β has to be included in the expansion to maintain the quality of the fit. The correction required of this term is relatively small and β and b cannot therefore be as accurately determined as α and a . The value of β is found to lie close to $3/2$ and $b \approx 0.10$. By taking $p(N)$ to be of the form

$$p(N) = a/N^{1/2} + b/N^{3/2} \tag{4}$$

and simultaneously varying a and b in a weighted nonlinear least squares analysis using $1/N^2$ as the weight [8], an optimized fit to the $W(N)$ data is obtained with

$$a = -1.1028 \quad \text{and} \quad b = +0.096.$$

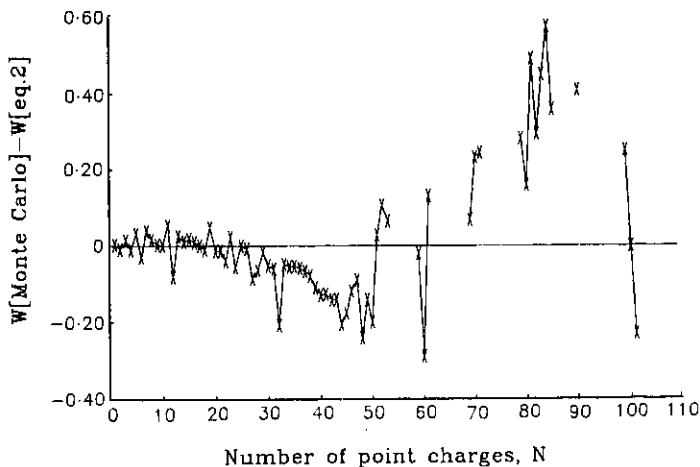


Figure 2. Difference between the configurational energies $W(N)$ as calculated by the Monte Carlo procedure and obtained from equations (2) and (4). Note the expanded energy scale.

We do not provide the standard deviations of these parameters since the scatter in the data is not random but appears to have a large systematic component, as we discuss later. The agreement between equation (4) and the data, as shown in table 1, is extremely good all the way down to $N = 1$. In figure 1 the data and equation (4) are so close as to be indistinguishable. Most data values lie within 0.1 of the fitted relation and several lie within 0.01. For the larger values of N the fractional differences between the data and equation (4) are of the order 0.02% or less. The deviations of the $W(N)$ data from equation (4) are shown in figure 2 in an expanded scale, where the systematic nature of the deviations can be seen.

3. Theoretical model

To simplify the calculation of the configurational energy, we will suppose that, in addition to the N point charges, there is a uniform continuous compensating charge $-N$ placed on the sphere. From symmetry considerations, this continuous charge can have no effect on the stable arrangement of the point charges, serving only to reduce the total energy. The self-energy of this continuous charge is $N^2/2$ and the interaction energy between the continuous and the point charges is $-N^2$. When these are combined with (2) for the energy of the point charges, the total energy becomes

$$W'(N) = \frac{N^2}{2} p(N). \quad (5)$$

The energetically most favourable arrangement of point charges in an infinite plane is the form of a hexagonal Wigner lattice. The energies of the other two-dimensional Bravais lattices have been calculated and they lie somewhat higher in energy [9]. It might be expected therefore that the stable arrangement of point charges on a sphere, when N is large and the lattice spacing correspondingly small, will closely resemble a hexagonal lattice over much of the surface. Hexagonal coordination cannot be maintained indefinitely on a sphere without gross distortions developing, and variations in coordination are required from place to place to take up the strain [10]. This global characterization is corroborated by the pair distribution functions (PDFs) of the larger- N stable configurations. For our purposes we define the PDF $\Omega(d)$ such that $2\pi d \Omega(d) \Delta d$ is the number of pair separations d_{ij} in the interval Δd around the value d . As an example, figure 3 shows $\Omega(d)$ for the $N = 100$ stable configuration. Peaks occur very close to the first four hexagonal lattice nearest-neighbour distances $l_1 = l = 0.381$, $l_2 = \sqrt{3}l = 0.660$, $l_3 = 2l = 0.762$ and $l_4 = \sqrt{7}l = 1.008$, where l is obtained from equation (6) below. The first peak of $\Omega(d)$ is skewed slightly to smaller values of d , indicating a small proportion of points with less than 6-fold coordination. In conclusion, therefore, the energy of a stable configuration is expected to be greater than that of a comparable hexagonal lattice, but not by a large margin. Since there is likely to be a small proportion of points with 4-fold coordination, the energy of the square lattice can be taken as a plausible upper bound for the configurational energy.

The theory of two-dimensional Wigner lattices has received considerable attention because of its relevance to the ordering of electrons on the free surface of liquid helium [11]. It has also been suggested that electrons and holes in semiconductor inversion layers [12] and quantum-well structures [13] undergo Wigner crystallization at low densities and temperatures. Our treatment below contains the novel feature that it treats a Wigner lattice which has been projected onto a sphere, which gives rise to a

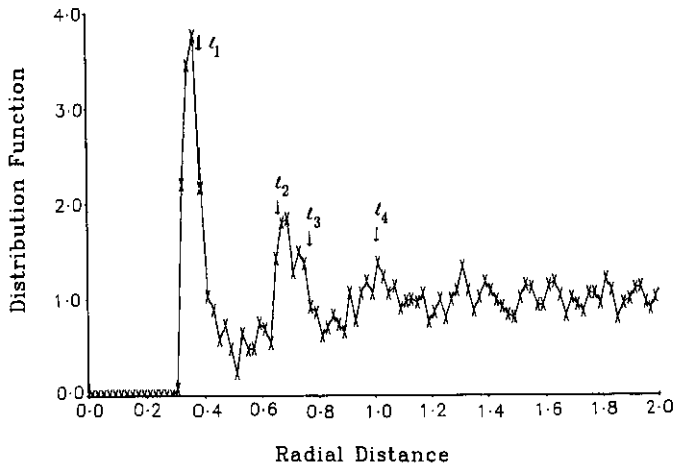


Figure 3. Pair distribution function $\Omega(d)$ for the $N=100$ stable configuration. The first four hexagonal nearest neighbour distances l_1, l_2, l_3 and l_4 are shown.

strain energy term. Because of the presence of the compensating continuous charge, the Wigner-Seitz cell of each lattice point is electrically neutral and the intercellular interactions consequently fall off rapidly with distance, r . When N is large, lattice defects are sparse and most cells are surrounded for some distance by a regular lattice. A reasonably accurate first estimate of the configurational energy can therefore be obtained by assuming, for calculational purposes, a perfect lattice.

3.1. Hexagonal lattice

For the stable configuration of N point charges on a unit sphere, each of these charges and its cell of compensating negative charge occupy, on average, an area of $4\pi/N$. Assuming a structure resembling a plane hexagonal lattice of lattice spacing l , the cell area is $l^2\sqrt{3}/2$ and so

$$l = \left(\frac{8\pi}{\sqrt{3}N} \right)^{1/2}. \quad (6)$$

Let r and ψ be polar coordinates of a point in the plane, with the origin taken to coincide with one of the point charges. Dimensionless Cartesian coordinates normalized to the lattice spacing are

$$X = \frac{r}{l} \cos \psi \quad (7)$$

$$Y = \frac{r}{l} \sin \psi.$$

We project this lattice onto the unit sphere with the mapping

$$\begin{aligned} \psi &\Leftrightarrow \varphi \\ r &\Leftrightarrow 2 \sin \frac{\theta}{2} \end{aligned} \quad (8)$$

where φ and θ are the polar angular coordinates of the sphere. This mapping satisfies the area-conserving condition $r dr d\psi = \sin \theta d\theta d\varphi$. The Euclidean distance between two points

$$\mathbf{R}_i = (\sin \theta_i \cos \varphi_i, \sin \theta_i \sin \varphi_i, \cos \theta_i) \tag{9}$$

and

$$\mathbf{R}_j = (\sin \theta_j \cos \varphi_j, \sin \theta_j \sin \varphi_j, \cos \theta_j). \tag{10}$$

on the sphere is given by

$$d_{ij} = |\mathbf{R}_i - \mathbf{R}_j| = \{2 - 2 \sin \theta_i \sin \theta_j \cos(\varphi_i - \varphi_j) - 2 \cos \theta_i \cos \theta_j\}^{1/2}. \tag{11}$$

If one of the points, say \mathbf{R}_i , is at the origin (the pole of the sphere), then $\theta_i = 0$ and

$$d_{ij} = (2 - 2 \cos \theta_j)^{1/2} = 2 \sin(\theta_j/2) = r_j. \tag{12}$$

This shows that distances from the origin are unaffected by the projection, although distances between points neither of which is at the origin are, in general, altered.

For small θ , $\sin \theta \approx \theta - \theta^3/6$, and $\theta = 2 \sin^{-1}(r/2) \approx r + r^3/24$ and so, from equation (7)

$$\sin \theta \approx r - r^3/8 = l(X^2 + Y^2)^{1/2} - \frac{l^3}{8}(X^2 + Y^2)^{3/2} \tag{13}$$

and

$$\cos \theta \approx 1 - r^2/2 = 1 - \frac{l^2}{2}(X^2 + Y^2). \tag{14}$$

Using these approximations, it follows from (11) that

$$1/d_{ij} = 1/(lf^{1/2}) + lg/(2f^{3/2}) \tag{15}$$

where

$$f = (X_i - X_j)^2 + (Y_i - Y_j)^2 \tag{16}$$

and

$$g = \frac{1}{4}\{2(X_i^2 + Y_i^2)(X_j^2 + Y_j^2) - (X_i X_j + Y_i Y_j)(X_i^2 + Y_i^2 + X_j^2 + Y_j^2)\}. \tag{17}$$

When one of the pair of points is at the origin, g clearly vanishes.

The contribution of the cell at the origin to the total energy of the lattice can be written

$$w = \mathcal{S}1/d_{ij} \tag{18}$$

where \mathcal{S} denotes a sum over discrete charges and integration over continuous charges, using X and Y as integration variables. The sum combines contributions from the self-interaction of the continuous charge in the first cell, the interaction of this continuous charge with the point charge in that cell, and one half of the interaction energy of the charges in the first cell with the discrete and continuous charges in all the other cells. Considerable cancellation occurs between negative and positive contributions to the interaction energy between different cells, particularly when they are far apart, and rapid convergence is attained.

The total lattice energy for N cells is given by $W' = Nw$, and from equation (5) it follows that

$$p(N) = 2W'/N^2 = (2/N)\mathcal{P}1/d_{ij}. \quad (19)$$

Using equations (6) and (15) to substitute for l and d_{ij} one arrives at the result

$$p(N) = a/N^{1/2} + b/N^{3/2} \quad (20)$$

where

$$a = \left(\frac{\sqrt{3}}{2\pi}\right)^{1/2} \mathcal{P}1/f^{1/2} \quad (21)$$

and

$$b = \left(\frac{8\pi}{\sqrt{3}}\right)^{1/2} \mathcal{P}g/f^{3/2}. \quad (22)$$

This establishes a theoretical basis for the functional form of $p(N)$ that was found to fit the data on the configurational energies. The first term, $a/N^{1/2}$, is associated with the energy of the plane lattice and the second term, $b/N^{3/2}$, derives from the increase in energy of the lattice due to distortional effects when it is projected onto the spherical surface. In the evaluation of a , because the individual cells are neutral and have no dipole moment, the intercellular interactions show a $1/r^5$ decrease in magnitude with distance, characteristic of quadrupole-quadrupole interaction, and convergence is rapid. In the evaluation of b there are no contributions from the central point charge, and the intercellular contributions decrease as $1/r^3$. Numerical integration and summation over the various contributions to a and b yield

$$a = -1.1061 \quad \text{and} \quad b = +0.104.$$

The value of a is consistent with the energy of the hexagonal Wigner lattice calculated by Bonsall and Maradudin [9] using the Ewald method and in agreement with equation 3.14 of Gann *et al* [14]. The value for b is a new result.

3.2. Square lattice

For a square lattice of N point charges projected onto a unit sphere, the lattice spacing is $l = (4\pi/N)^{1/2}$ and a and b are given by

$$a = (1/\pi)^{1/2} \mathcal{P}1/f^{1/2} \quad (23)$$

and

$$b = 2\pi^{1/2} \mathcal{P}g/f^{3/2}. \quad (24)$$

Numerical evaluation of the integrals and summation yield

$$a = -1.1002 \quad \text{and} \quad b = +0.084.$$

The value of a is consistent with the lattice energy calculated by Bonsall and Maradudin [9]. the value for b is a new result.

4. Discussion and conclusions

We have been able to derive a simple expression for the minimum energy of N equal charges on the surface of a sphere, which involves a series expansion in half-integer

powers of $1/N$. We have established limiting values for the first two coefficients in the expansion, based on the idealizations of the point charges lying on either a hexagonal or square lattice projected onto a sphere; the values of the coefficients so evaluated neatly straddle the values obtained by a nonlinear least squares fit on the data derived by numerical procedures. This appears to be the first general consideration of the energetics of point charges on a sphere, as opposed to discussion of the structures of such systems.

These results, and the excellent fit of our expression to the data, suggest that we have captured the essential physics of the problem in our model. In that case, it becomes worthwhile to consider some of the residual deviations of the data from the model. Since the data becomes less reliable at larger values of N , where repetitions of the numerical procedure have to be done sparingly as they are very costly in computer time (more than three hours per simulation on an IBM 3083J mainframe computer for $N = 100$), we will concentrate on the energies for $N \leq 35$. The energy differences from our fitted formula for $1 \leq N \leq 35$ is shown with a highly expanded scale in figure 4.

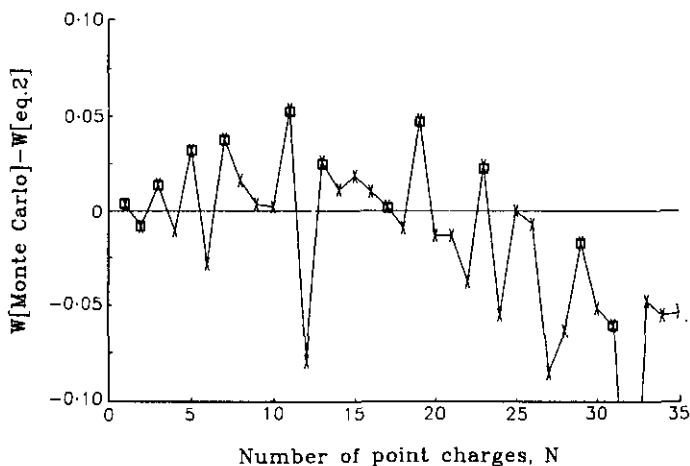


Figure 4. Difference between the Monte Carlo and fitted configurational energies for $N \leq 35$. Note the considerably expanded energy scale. □: N prime.

The differences observed are small, but show some consistent patterns—with intriguing deviations. One observes an oscillating pattern of relative stability (low values of the difference) and relative instability (high values). The most striking point is that the principal relative instabilities appear for prime values of N for $1 \leq N \leq 30$, excepting $N = 2$ and 17 only, while the value for $N = 13$ is relatively small. Smaller relative instabilities may also occur when N is odd. The principal locally more stable energy values occur with high symmetry structures for N equal to $2, 4, 6$ and 12 . Other relative stabilities appear for N equal to $10, 18, 22, 24$ and 27 , also for fairly high symmetry. Beyond $N = 30$ the pattern is less clear. There are strong local stabilities for $N = 32$ and for $N = 60$, which latter may bear some relationship to the truncated icosahedron. This structure is generally recognized as being exceptionally stable, being represented in nature by the recently-discovered C_{60} molecule buckminsterfullerene [6]. (The other stable fullerene structures, C_{70} and C_{84} , are not described by our model as they do

not approximate to spherical in shape.) Thus, the following are observed to be most stable relative to their neighbours: $N = 6, 12, 32, 44, 48$ and 60 .

We offer here a tentative suggestion as to the lines an explanation of these observations might take, in the realization that there may well be some subtle underlying rules that have eluded us. Thus, there appears to be difficulty in organizing a good lattice on a sphere with a small and odd (or worse, prime) number of points, while numbers which permit high symmetry are stable. Clearly there remains much detail to be understood in this apparently simple problem, such as, for example, the large scale oscillation apparent in figure 2; we have only scratched the surface of its fascination.

We also suggest that it may be worthwhile to examine the energetics and spacing of points on a sphere with non-Coulombic interactions [1], for a better understanding of the structures that might be engendered [7, 15].

Acknowledgments

We wish to thank Dr D W Bennett for supplying us with his values of the Monte Carlo energies for most N up to 50, and $N = 60$, and the Foundation for Research Development for financial support.

Note added in proof. Subsequent to the submission of our paper, Erber and Hockney [15] have published a list of energies of N unit charges on a unit sphere, for $2 \leq N \leq 65$. Their results agree rather well with those we report here, with some of our results being lower in energy than theirs, and vice versa; the discrepancies do not exceed about 0.01. In addition, some of the gaps in our data are now filled in, and the data to $N \leq 65$ shows a smoother profile than in our figure 2. The best fit parameters for (4) for the lowest energy values for $2 \leq N \leq 65$ and a weighting of $1/N^2$ are

$$a = -1.1039 \quad b = +0.105.$$

Our energy values for $N > 65$ are, from these results, clearly upper bounds to the true values, having been insufficiently optimized.

References

- [1] Melnyk T W, Knop O and Smith W R 1977 *Can. J. Chem.* **55** 1745
- [2] Weinrach J B, Carter K L, Bennett D W and McDowell H K 1990 *J. Chem. Educ.* **67** 995
- [3] Munera H A 1986 *Nature* **320** 597
- [4] Webb S 1986 *Nature* **323** 20
- [5] Calinon R, Choquard Ph, Jamin E and Navet M 1980 *Ordering in Two Dimensions* ed S K Sinha (Amsterdam: North-Holland)
- [6] Zhang Q L, O'Brien S C, Heath J R, Liu Y, Curl R F, Kroto H W and Smalley R E 1986 *J. Phys. Chem.* **90** 525
- [7] Tarnai T 1991 *J. Mol. Biol.* **218** 485
Tarnai T and Gaspar Zs 1991 *Proc. R. Soc. A* **433** 257
- [8] Brink G 1991 *Library of Numerical Methods* (Johannesburg: Precision Engineering and Scientific Software)
- [9] Bonsall L and Maradudin A A 1977 *Phys. Rev. B* **15** 1959
- [10] Coxeter H S M 1973 *Regular Polytopes* 3rd edn (New York: Dover)
- [11] Grimes C C and Adams G 1979 *Phys. Rev. Lett.* **42** 795
- [12] Chaplik A V 1972 *Zh. Eksp. Teor. Fiz.* **62** 746 (Engl. Transl. 1972 *Sov. Phys.-JETP* **35** 395)
- [13] Swierkowski L, Neilson D and Szymanski J 1991 *Phys. Rev. Lett.* **67** 240
- [14] Gann R C, Chakravarty S and Chester G V 1979 *Phys. Rev. B* **20** 326
- [15] Erber T and Hockney G M 1991 *J. Phys. A: Math. Gen.* **24** L1369