Genetic Algorithm Energy Minimization for Point Charges on a Sphere

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Abstract

We demonstrate that a new approach for optimizing atomic structures is very effective for attacking the Thomson problem of finding the lowest energy configuration of N point charges on a unit sphere. Our approach uses a genetic algorithm, combined with a "cut and paste" scheme of mating, that efficiently explores the different low energy structures.[1] Not only have we reproduced the known results[2–5] for $10 \leq N \leq 132$, this approach has allowed us to extend the calculation for all $N \leq 200$. This has allowed us to identify series of "magic" numbers, where the lowest energy structures are particularly stable. Most of these structures are icosahedral, but we also find new low-energy structures that deviate from icosahedral symmetry.

02.70.-c, 36.40.Mr, 61.46.+w, 82.20.Wt

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A recurring problem in computational physics and chemistry is the minimization of a structure with respect to atomic positions. One difficulty is the development of an accurate model of atomic interactions in the material. However, even once such a model is chosen, optimization is often difficult, due to the many competing structures that may be locally stable. This is especially true for non-crystalline structures, such as atomic clusters and defect structures (such as grain boundaries or surfaces).[6] While accurate models of materials are becoming increasingly available, and the computational time to calculate energies is rapidly decreasing, there have been relatively few developments in the optimization process. Most efforts focus on using some form of steepest descent or conjugate gradient relaxation, or Monte Carlo or molecular dynamic simulations (including simulated annealing approaches).

In this paper, we use a recently developed technique[1] to study the long-standing Thomson problem of finding the lowest energy configuration of N point charges on a unit sphere. The problem we consider here originated with Thomson's "plum pudding" model of the atomic nucleus. This minimization problem has been attempted by simulated annealing,[8–11] Monte Carlo approaches,[2,12] and symmetry considerations,[13] yet none of these techniques have proven as reliable as the simplest method: a repeated random search with a steepest descent relaxation.[3,4] Thus, this problem is an ideal benchmark of new global optimization algorithms.

The energy of N point charges constrained to lie on the surface of a unit sphere is

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{1}$$

Even for small N, there are multiple possible stable structures; for $N \lesssim 20$, simulated annealing suffices to locate the global minimum.[8–10] However, this will not suffice once the number of local minima is large. The difficulty is that the number of metastable structures grows exponentially[3,4] with N, and these approaches do not explore different minima sufficiently rapidly once N becomes large ($N > 70$). For $N \sim 100 - 110$, there are $\sim 50 - 90$ metastable states;[4] this grows to ~ 8000 for $N \sim 200$. Furthermore, for many of the structures, the basin of attraction (or "catchment region") containing the global minimum is small compared with those of other minima.[4]

These difficulties are a generic feature of many systems, including the related problem of determining structures of atomic clusters.[1,6,7] Often, there are techniques to provide local optimization, such as steepest descent or conjugate gradient algorithms. Monte Carlo simulations[2] and simulated annealing[8–10] are typically used to explore nearby minima, in an effort to improve upon the current minimum. The difficulty is that these techniques for "hopping" from one minimum to the next are time consuming, and if there are many local minima, with large barriers separating them, then these techniques are not practical. The Thomson problem is a good example of such a problem. Finding a local minimum from a random structure is straightforward, but exploring many different minima is not.

We have used a genetic algorithm[15] (GA) to tackle this problem. The idea is simple: starting with a small set of initial geometries, a number of "children" – structures that derive their properties from two of the initial geometries – are generated. From this "population," the lowest energy ("most fit") structures are chosen to replace the initial geometries. Repeating this process leads to lower energy structures. In general, there may be other search

criteria; these may be accounted for directly by constructing a "fitness" function that reflects the different criteria of interest, and optimizing this function by selection.[15] GA's have been applied to problems in a number of fields, but there have been few successful applications to the physical sciences.[16–19]

One of the difficulties in the type of problem that we are considering is that the evaluation of the energy is time consuming, especially for problems using more accurate models of materials. For most current applications of GAs, the computational effort in calculating the fitness is very small. Therefore, we can not afford to use traditional approaches, which might require calculating the energies of thousands of structures, most of which would not be competitive.[17,18]

Our approach is successful because of a novel mating algorithm[1] that allows for efficient exploration of different minima, while preserving the important properties of the parent structures. Unlike most applications of genetic algorithms,[15,17–19] our algorithm is not based upon an artificial "genetic sequence:" most implementations represent the parameters of the problem symbolically as a string of numbers or characters, and then perform "mating" and "mutation" operations on a set of strings. Such an approach is inefficient for structural optimization, as many resulting structures are clearly unphysical. Instead of working with an artificial genetic sequence, we work directly with the structure itself. A new candidate structure is generated from two randomly chosen halves of two parent structures, subject to the constraint that the correct number of particles is maintained. Each candidate is then fully relaxed, using a conjugate gradient technique. By breaking with the traditional GA approaches, we are able to generate new structures that may retain the important structural features of the parents, while still being able to explore different local minima in the solution landscape. This approach has been successful for finding fullerene structures,[1] encouraging us to attempt this problem.

In the work presented here, we began with four random geometries. By generating children from each pair of initial geometries, we construct sixteen more candidate structures. (Note that a cluster may "mate" with itself, by aligning any two randomly chosen halves of the structure.) From the twenty structures, we select the best four candidates, choosing only structures whose energies differ by more than $\Delta E = 10^{-6}$ to ensure that one structure does not dominate the entire population.

For $10 \leq N \leq 132$, and also for $N = 192$ and $N = 212$, we found the same minimum energies as given in Refs. 4 and 5. Most strikingly, for $N \leq 132$, we were almost always able to find the lowest energy structures within 5 generations. With these successes, we went on to search for the lowest energy structures for $133 \leq N \leq 200$. The values for $110 \leq N \leq 200$ are shown in Table I. We ran these for 10 generations, considering a total of 200 structures. Note that our technique does not guarantee that the lowest energy will be found, although we believe that in most cases the final structure was the global minimum. We fitted the lowest energies to the form[12,4]

$$E(N) = \frac{N^2}{2}\left(1 - aN^{-1/2} + bN^{-3/2}\right). \tag{2}$$

The fitted values were $a = 1.10461 \pm 0.00001$ and $b = 0.137 \pm 0.001$, in reasonable agreement with the fit of Erber[4] and the calculations of Glasser.[12]

In fig. 1, we show the difference between the fitted energy and the actual value for the lowest energy structure obtained using our approach. Note that there are a series of "magic" numbers, with particularly low ground-state energies (relative to the trend given in Eq. 2), for N = 12, 32, 72, 122, 132, 137, 146, 182, and 187. In this series, the structures for N = 12, 32, 72, 122, 132 and 192 have icosahedral symmetry. The icosahedral structures for N =212, 272, 282 and 312 also have very low energies.[5] Icosahedral structures have been predicted to have the lowest energy,[11] but for N = 42, 92 and 162, the icosahedral structures have high energies relative to the trend in Eq. 2.

For most of the lowest energy structures we found, the atoms tend to arrange themselves in a triangular configuration, with twelve points that have five near neighbors, and the rest having six neighbors (see fig. 2). With this type of configuration, the application of Euler's formula predicts that the number of faces will be $F = 2N - 4$. This prediction is confirmed for most of the lowest energy structures, with some exceptions (see Ref. 4). (The exceptions demonstrate that not all structures can be uniquely decomposed into triangles – on some structures, there are rectangular faces. This counter-intuitive result illustrates the difficulties in making general statements concerning this problem.) The five-fold coordinated points tend to separate themselves – suggesting that the icosahedral structures would be particularly stable, with each of the five-fold coordinated points located along a line of five-fold rotational symmetry.

The striking result is that this technique can find the lowest energy configurations, both for the high-symmetry icosahedral structures and also for structures with lower symmetry. The structures for N = 137, 182, and 187 are distorted icosahedral structures, with D_5 symmetry. The N = 146 structure, shown in fig. 2, has D_2 symmetry, much lower than the symmetries of the other magic numbers. Unlike many of the structures, in which the five-fold coordinated charges form equilateral triangles, the five-fold coordinated points are not in an icosahedral arrangement. Instead, the lines connecting five-fold coordinated atoms along the shortest distance between them produce two interlocking "C" structures. To our knowledge, no other similar structure has been predicted as being particularly favorable. We believe that there will be other magic numbers with similar structures at larger N, and are currently exploring this.

It may seem surprising that such a simple approach works where more complicated schemes have not. We believe that there are two principal features of our technique that are important. First, we try many different geometries in parallel rather than exploring phase space in a single series of geometries. Simulated annealing or other techniques may explore several different local minima with a reasonable computational effort, but for problems with many minima, these approaches becomes impractical. This is why a simple random search is more successful than these approaches. Second, unlike a random search or more traditional approaches to genetic algorithms, our technique of generating new structures preserves much of the previous structural optimization that has occurred. The two halves remain reasonably intact, while "healing" occurs near the joining region. Thus, while we rapidly explore other minima, we do so with a bias toward the types of low energy structures that have already been obtained.

We believe that these results are an important test of our optimization technique, as this is the first systematic approach that reliably reproduces all of the known low-energy structures. Our mating algorithm is easily implemented, computationally efficient, and

capable of finding unusual structures. We are currently applying similar techniques to more realistic atomic models, including Lennard-Jones and embedded atom clusters, and are exploring ways of optimizing our approach. GA's have been previously proven useful in many areas, but have not been as popular or successful in the physical sciences.[16–19] We believe that successes such as ours will allow the strengths of GA's to become an effective tool in the physical sciences.

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TABLES

TABLE I.

N	E_1	N	E_1	N	E_1
111	5515.29321459	141	9016.61534919	171	13386.35593072
112	5618.04488233	142	9148.27157999	172	13547.01810880
113	5721.82497803	143	9280.83985119	173	13708.63524304
114	5826.52157216	144	9414.37179446	174	13871.18709230
115	5932.18128578	145	9548.92883723	175	14034.78130694
116	6038.81559358	146	9684.38182558	176	14199.35477565
117	6146.34244658	147	9820.93237838	177	14364.85051922
118	6254.87702779	148	9958.40600427	178	14531.30955293
119	6364.34731748	149	10096.85990740	179	14698.75459423
120	6474.75632498	150	10236.19643670	180	14867.09992753
121	6586.12194958	151	10376.57146928	181	15036.46723978
122	6698.37449926	152	10517.86759288	182	15206.73061091
123	6811.82722817	153	10660.08274824	183	15378.16657104
124	6926.16997419	154	10803.37242114	184	15550.42145032
125	7041.47326402	155	10947.57469228	185	15723.72007408
126	7157.66922487	156	11092.80311478	186	15897.89743705
127	7274.81950468	157	11238.90304116	187	16072.97518632
128	7393.00744307	158	11385.99018620	188	16249.25013148
129	7512.10731927	159	11534.02396096	189	16426.37193887
130	7632.16737891	160	11683.05480555	190	16604.44596500
131	7753.20516694	161	11833.08473947	191	16783.45221937
132	7875.04534280	162	11984.05033581	192	16963.33838646
133	7998.17921290	163	12136.01305322	193	17144.56474088
134	8122.08972119	164	12288.93010532	194	17326.61613647
135	8246.90948699	165	12442.80445137	195	17509.48930393
136	8372.74330254	166	12597.64907132	196	17693.46055212
137	8499.53449478	167	12753.46942975	197	17878.38274577
138	8627.40638988	168	12910.21267227	198	18064.28806296
139	8756.22705695	169	13068.00645113	199	18251.08249564
140	8885.98060904	170	13226.68107860	200	18438.84227198

FIGURES

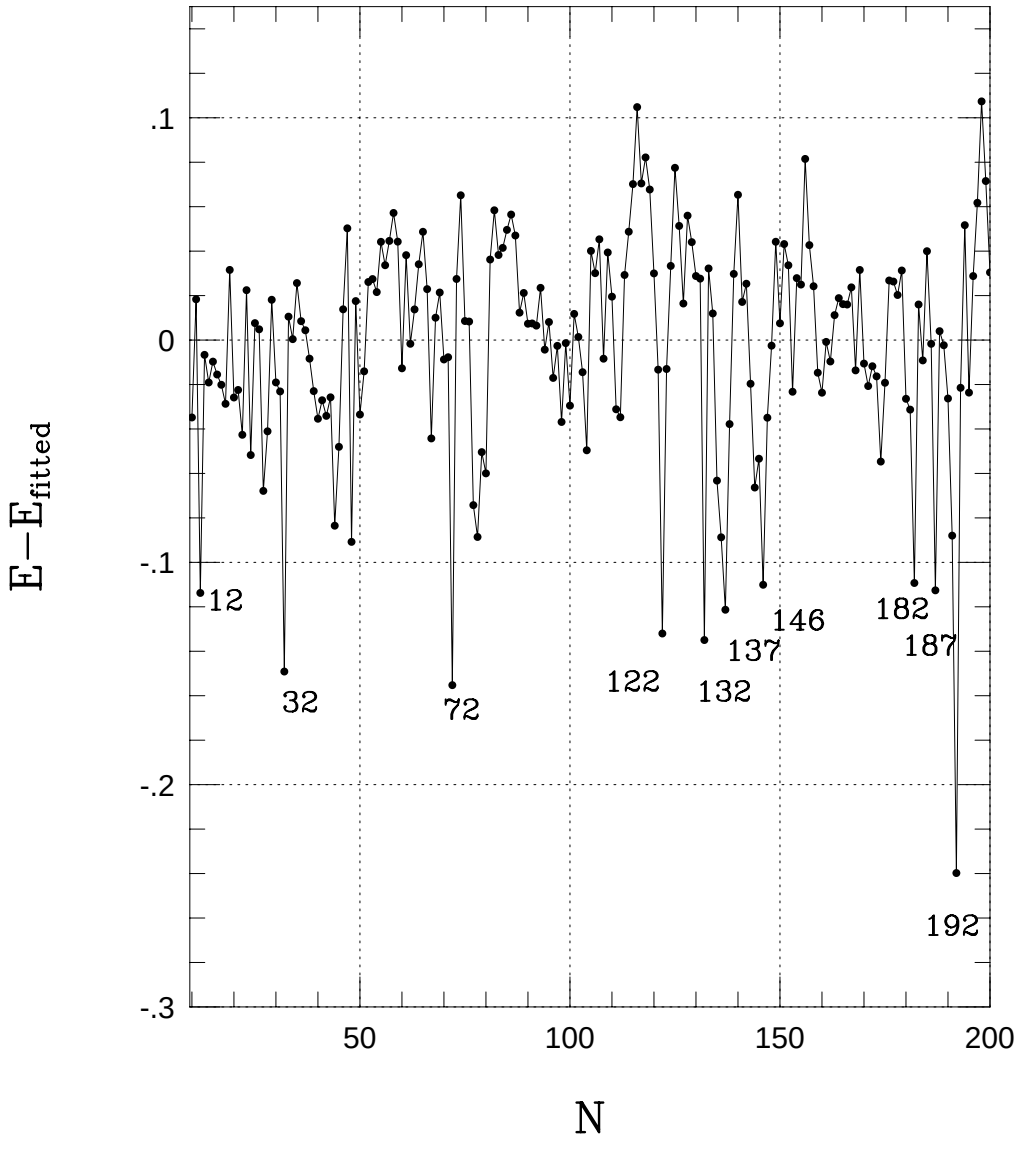

FIG. 1. We show the difference between the calculated lowest energy configuration and the fit to the form $\frac{1}{2}N^2(1 + aN^{-1/2} + bN^{-3/2})$. Note the "magic numbers" at N =12, 32, 72, 122, 132, 137, 146, 182, 187 and 192.

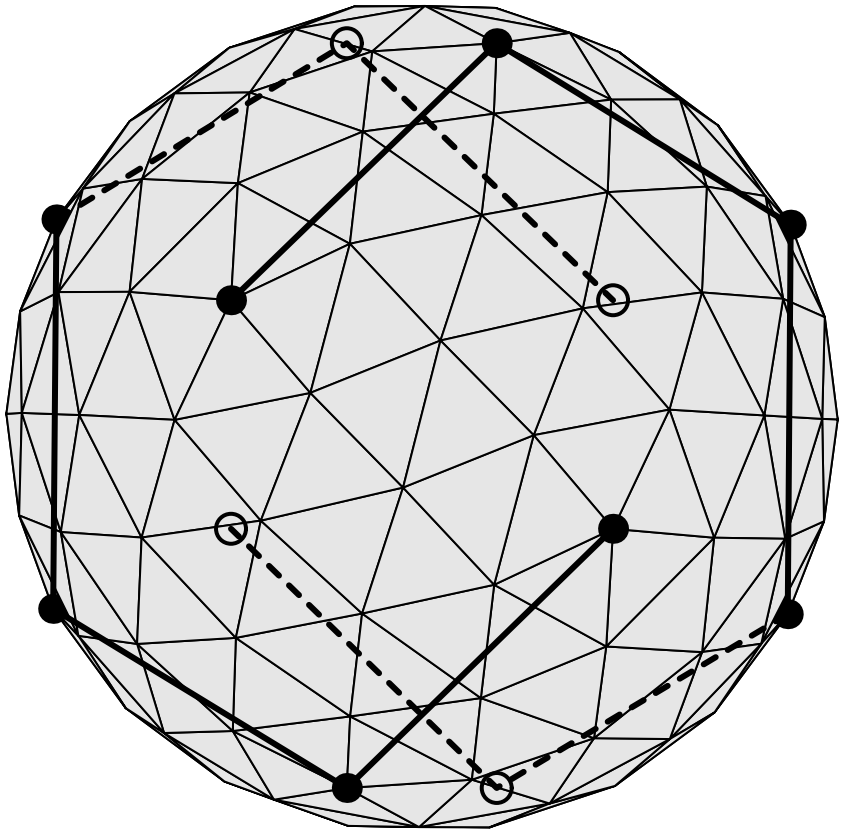

FIG. 2. This figure shows the lowest energy structure for $N = 146$, looking down one of the two-fold axes. We have emphasized the five-fold coordinated charges, and indicated the interlocking "C" structures formed by connecting the five-fold coordinated charges to their nearest neighbor.