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Discrete transformations in the Thomson Problem

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A B S T R A C T

A significantly lower upper limit to minimum energy solutions of the electrostatic Thomson Problem is reported. A point charge is introduced to the origin of each N-charge solution. This raises the total energy by N as an upper limit to each $(N+1)$-charge solution. Minimization of energy to $U(N+1)$ is well fit with $-0.5518(3/2)\sqrt{N}+1/2$ for up to $N=500$. The energy distribution due to this displacement exhibits correspondences with shell-filling behavior in atomic systems. This work may aid development of more efficient and innovative numerical search algorithms to obtain N-charge configurations having global energy minima and yield new insights to atomic structure.

1. Introduction

The Thomson Problem has drawn considerable interest since the mid-1900s [1] having found use in modeling fullerenes [2,3], drug encapsulants [4], spherical viruses [5], and crystalline order on curved surfaces [6]. In the past few decades several computational algorithms have yielded precise numerical solutions for many-N electron systems [7–18]. The Thomson Problem has emerged as a benchmark for global optimization algorithms [16,17] though its general solution remains unknown [19].

Numerical solutions of the Thomson Problem are those for which the total Coulomb repulsion energy,

$$U(N) = \sum_{i<j}^{N} \frac{1}{|r_i - r_j|}, \tag{1}$$

is a minimum for each N-charge system with r_i and r_j constrained to the surface of a unit sphere.

The initial condition of some minimization algorithms is the random distribution of N point charges on the unit sphere. This sets a relatively distant upper energy limit, $U_r(N) = N(N-1)/2$ [8], from which numerous iterations progress toward a global minimum for each N-charge system. The distribution of numerical solutions has been fit with empirical functions including $U(N) = N^2/2 + aN^{3/2}$ [7] and $U(N) = N^2/2 + aN^{3/2} + bN^{1/2}$ [8]. The quadratic term is ascribed to energy stored within a continuous charged shell of unit radius having total charge, N. With this interpretation, the half-integer terms may correspond to self-energies of N uniformly charged disks that are removed to yield the final minimized energy of discrete charges. If the $N^2/2$ term is associated with the random distribution of point charges, the half-integer terms may be related to correlation energies of surface Coulomb equilibrium states [7]. These ascriptions of energy terms to physical entities have guided the development of fairly useful minimization algorithms.

Here, the discrete derivative of $N^2/2$ is shown to correspond to the introduction of a single point charge, q_0, at the origin of a given N-charge solution, and the discrete derivative of the remaining half-integer term(s) accounts for energy needed to displace q_0 to the unit sphere. This yields each subsequent $(N+1)$-charge solution of the Thomson Problem. In this manner, the upper limit of each minimized $(N+1)$ energy solution is given by $U(N)+N$. This represents a well-defined charge configuration with a significantly lower energy than random charge distributions and may be useful as initial conditions in relatively more efficient energy minimization algorithms.

Notably, the distribution of energy solutions of the Thomson Problem is "systematic" [8] and not random. Here, having ignored the linear term in the discrete derivative, the remaining "systematic" distribution of energy associated with the displacement of q_0 to the surface of the unit sphere demonstrably exhibits features uniquely correspondent with numerous shell-filling features throughout the periodic table of natural atomic systems [20–22].

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Hence, introduction of q_0 to the Thomson Problem represents an intriguingly fresh perspective of this extensively useful mathematical model and the classical underpinnings of atomic structure.

Numerical solutions of the Thomson Problem for up to 500 charges used in this communication have been obtained from a continually updated database maintained by Syracuse University [23].

2. Discrete derivatives

Two upper energy bounds of some interest are those associated with a continuous charge shell [8] consisting of infinite-many N charges such that

$$U_\infty(N) = \frac{N^2}{2} \tag{2}$$

and the random distribution of N discrete point charges across the surface of the unit sphere

$$U_r(N) = \frac{N}{2}(N-1) = \frac{N^2}{2} - \frac{N}{2}. \tag{3}$$

Plots of Eqs. (2) and (3) are shown in Fig. 1 together with a few numerical solutions (open circles) of the Thomson Problem for illustration.

The minimized global potential energy solutions for up to $N = 65$ point charges were previously fit using, [7]

$$f_1(N) = \frac{N^2}{2} + aN^{3/2} \tag{4}$$

in which $a = -0.5510$, and for up to $N \sim 100$ using [8]

$$f_2(N) = \frac{N^2}{2} + aN^{3/2} + bN^{1/2}. \tag{5}$$

These smooth, continuous fit functions are generally unrepresentative of the absolute minimum energy configurations of discrete charges due to a variety of issues. Among them, discrete charges cannot be infinitesimally subdivided so all points, $f(N)$, for non-integer N have no physical significance without imposing additional arguments. If these intermediate values of $f(N)$ should have physical usefulness, for instance if an effective fractional charge on the unit sphere surface is admitted as a discrete charge approaches or leaves the surface, $f(N)$ should have local minima at integer values of N. Though these fit functions, Eqs. (4) and (5) have no local minima at integer values of N, they are coarsely instructive.

It is potentially more fruitful to design a fit function in accordance with the physical nature of electrostatic charge configurations. In particular, knowledge of $f(N)$ at integer values of N, given the discrete nature of point charges is paramount. Consider the discrete derivative of $f(N)$ at integer values of N,

$$\frac{\Delta f_i(N)}{\Delta N} = \frac{f(N+\Delta N) - f(N)}{\Delta N} \tag{6}$$

of Eq. (4), which yields, after binomial expansion of the half-integer term,

$$\Delta f_1(N) = \left(N + \frac{1}{2}\right) + \frac{a}{2}\left(3N^{\frac{1}{2}} + \frac{3}{4}N^{-\frac{1}{2}} - \frac{1}{8}N^{-\frac{3}{2}} + \cdots\right) \tag{7}$$

for $\Delta N = 1$. For comparison, the derivative of Eq. (5), with binomial expansion of the half-integer terms,

$$\Delta f_2(N) = \left(N + \frac{1}{2}\right) + \frac{1}{2}\left[3aN^{\frac{1}{2}} + \frac{7}{4}(a+b)N^{-\frac{1}{2}} + \frac{1}{8}(a-b)N^{-\frac{3}{2}} + \cdots\right] \tag{8}$$

for $\Delta N = 1$. The first set of parentheses in Eqs. (7) and (8) is the discrete derivative of $N^2/2$, the energy of a continuous charge shell, Eq. (2).

3. Discrete transformation energies

To understand the physical charge distribution represented by the discrete energy differences, Eqs. (7) and (8), consider an N-charge solution, such as that of [N] shown in Fig. 2 for which the total minimized electrostatic energy is $U(N)$ as shown in Fig. 1. The discrete energy changes needed to obtain the solution $U(N+1)$ in Fig. 1 may be obtained by introducing an $(N+1)$th point charge, q_0, to the origin denoted [N^+] in Fig. 2. Its contribution to the total

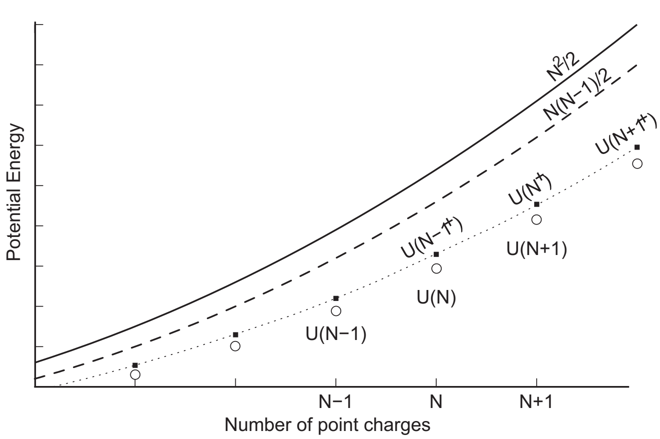

Fig. 1. The extreme upper energy limit of the Thomson Problem is given by $N^2/2$ for a continuous charge shell followed by $N(N-1)/2$, the energy associated with a random distribution of N point charges. Significantly lower, $U(N^+)$, the energy of a given N-charge solution of the Thomson Problem with one charge at its origin is readily obtained by $U(N) + N$, where $U(N)$ are solutions of the Thomson Problem.

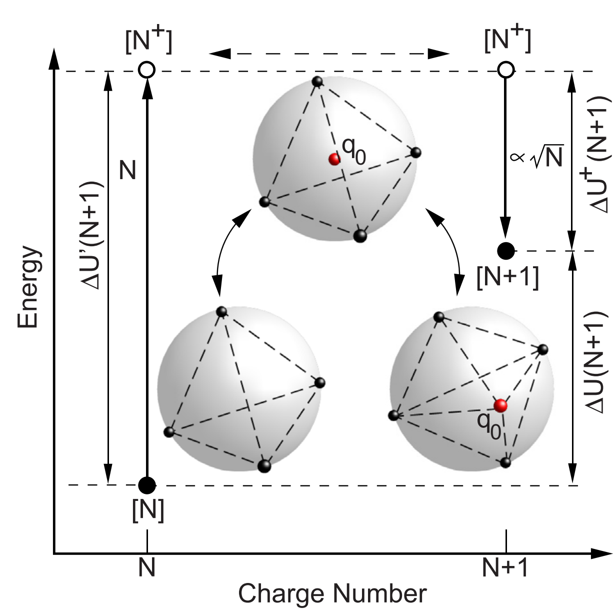

Fig. 2. A well-defined intermediate charge configuration, [N^+], with q_0 at the origin of [N] linearly increases the energy by N. Consequently, $U(N^+)$ is readily accessible. Displacement of q_0 to the unit sphere surface and global minimization of energy yields the new [N+1] solution with $\Delta U^+(N+1) \propto \sqrt{N}$.