

Comment on “Thomson rings in a disk”

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We have found that the minimum energy configuration of $N = 395$ charges confined in a disk and interacting via the Coulomb potential, reported by Cerkaški *et al.* [*Phys. Rev. E* **91**, 032312 (2015)], is not a global minimum of the total electrostatic energy. We have identified a large number of configurations with lower energy, where defects are present close to the center of the disk; thus, the formation of a hexagonal core and valence circular rings for the centered configurations, predicted by the model of the above-mentioned reference, is not supported by numerical evidence, and the configurations obtained with this model cannot be used as a guide for the numerical calculations, as claimed by the authors.

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In a recent paper (Ref. [1]), Cerkaški *et al.* studied the problem of a finite number of equal charges, interacting via the Coulomb potential and confined inside a disk. This problem has been previously studied by several authors in a series of papers [2–8], and it can be regarded as a generalization of the well-known Thomson problem [9] (finding the configurations of minimum energy of N equal charges on the surface of a sphere). Despite the apparent simplicity, both problems provide a serious computational challenge of increasing difficulty with N : in particular, the number of local minima of the total electrostatic energy grows very fast with N (for the case of the Thomson problem, see, for example, the discussion in Ref. [10]). As a result, the identification of the global minimum of a system of N charges typically requires extensive numerical calculations: in the absence of a formal criterion to establish whether a given configuration of equilibrium is a global minimum, one has to repeat the numerical calculations several times, keeping N fixed, and regard the configuration with the lowest energy among those obtained as a probable candidate for a global minimum.

For the case of the disk, Erkoc and Oymak [5,6] have observed the tendency, for systems with a modest number of charges ($N \leq 109$), to accommodate the charges on concentric rings, empirically deducing the rules for the distribution of charges on the disk (incidentally, most of the energies reported by these authors [6] do not correspond to global minima). The analysis performed by Cerkaški *et al.* in Ref. [1] is a refinement of the work of Erkoc and Oymak [5,6], and it relies on the hypothesis that charges are arranged on concentric rings for configurations of minimum energy. In this way, the original problem is reduced to the much simpler problem of calculating the electrostatic energy due to p rings, each carrying an appropriate number of charges uniformly distributed over the ring; the equilibrium configuration in this case is obtained by solving a system of two equations [their Eqs. (16) and (17)].

To test their model, the authors performed numerical [molecular-dynamics (MD)] calculations for systems up to $N = 400$ charges. Based on this analysis, they concluded that their approach allows one “to determine with high accuracy the equilibrium configurations of a few hundred charged particles.” In particular, for $N \gtrsim 200$ their approach “predicts the formation of the hexagonal core and valence circular rings for the centered configurations,” with “an increasing

sequence of rings, starting from the center, matching the regular hexagonal pattern.” For the case of $N = 395$, discussed at length in Ref. [1], the authors observed the formation of a hexagonal structure with rings {1,6,12,18,24}. Figure 2(b) of Ref. [1], which reports a comparison between the model and the numerical MD calculations for $N = 395$ charges, displays excellent agreement between the two, with only a small mismatch just outside the hexagonal structure (the green region in the figure is used to highlight the hexagonal structure). The energy reported by the authors for this configuration, which is expected to be a global minimum of the total energy, is $\mathcal{E}_{\text{MD}} = 110\,665.1$ compared to the energy $\mathcal{E}_{\text{av}} = 110\,667.6$ obtained with their model, with an error of just $2 \times 10^{-3}\%$.

For the purpose of verifying the results of Ref. [1], we have carried out extensive numerical calculations, in particular for the case of 395 charges. The approach that we have implemented allows one to generate configurations with the desired number of charges on the border: in this way, we have verified that the lower energies occur when $N_p = 147$ charges are disposed on the border of the disk, in agreement with Ref. [1]. We have thus generated 3001 configurations with $N_p = 147$, starting from initial configurations where the internal charges are randomly distributed, and we have found that 824 of them have energy lower than the value reported in Ref. [1], $\mathcal{E} < \mathcal{E}_{\text{MD}} = 110\,665.1$. The lowest energy among those that we have calculated (possibly a global minimum) is $\mathcal{E}_{\text{MIN}} = 110\,664.44$. The histogram in Fig. 1 illustrates these points. Interestingly, we have also found that even the configuration with the highest energy has an energy slightly lower than the value predicted by the model of Ref. [1], $\mathcal{E} = 110\,667.576 < \mathcal{E}_{\text{av}}$ (see Fig. 1).

In Fig. 2 we display the configuration with the lowest energy among those calculated (a hexagonal grid is also plotted to facilitate the identification of a centered hexagonal structure) [11]; note that the color of the vertices, representing the charges, depends on the number of nearest neighbors. Studying this figure, we observe the presence of defects very close to the center of the disk, and of a single, slightly deformed, hexagonal cell (the yellow region), centered at the origin, in sharp contrast with the numerical and theoretical observations of Ref. [1]. Additionally, we have also found that similar behaviors are also observed for the configurations with slightly higher energy.

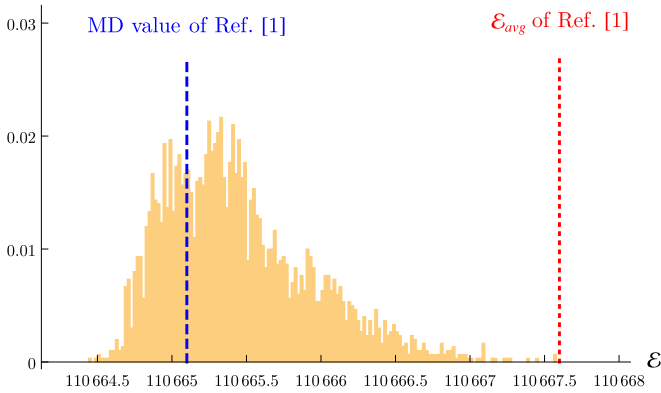


FIG. 1. Histogram for the energies of the configurations with 395 charges with $N_p = 147$.

We summarize our main findings as follows:

(i) The occurrence of defects, even very close to the center of the disk, may help to lower the total energy while disrupting the hexagonal structure.

(ii) All the configurations with $N_p = 147$ that we have calculated have energy lower than the theoretical value obtained in Ref. [1], and about 27% of them have energy lower than the numerical MD value of Ref. [1].

(iii) The use of the model of Ref. [1] as a guide for the numerical MD calculation (which is also claimed to cut the CPU times by a factor 10^3), as suggested by the authors, is definitely unjustified. Using this approach, we may expect that the solutions will not only correspond to local minima of the energy, but that they will also be strongly biased (i.e., the more symmetric structures could be favored).

(iv) The number of configurations grows very fast with N , thus requiring an efficient numerical approach: our program allows us to generate configurations with a desired number of charges on the border. We have found that in this way the performance is drastically improved.

In light of these findings, the validity of the model of Ref. [1] must be questioned, particularly for $N \gtrsim 200$; it also appears

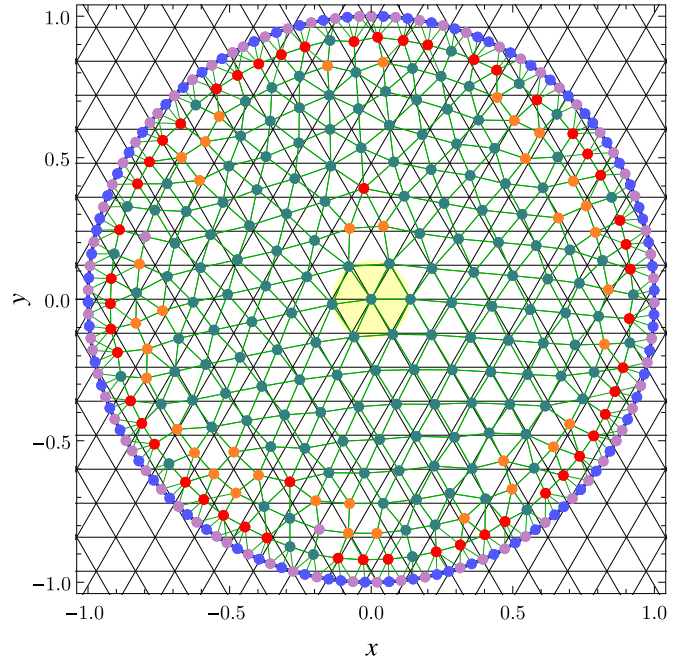


FIG. 2. Numerical solution corresponding to a configuration of 395 charges with energy $\mathcal{E} = 110664.44$.

clear that the numerical calculation of Ref. [1], which has failed to identify a very large number of configurations with energy lower than that reported by the authors, is inadequate (about 27% of the configurations that we have calculated have lower energy than that of Ref. [1]). We are not sure whether this problem has been triggered by using the output of the model as a guide for the numerical calculation, or if the program used by the authors produced a small number of configurations with $N_p = 147$.

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