Reply to "Comment on 'Thomson rings in a disk' "

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We demonstrate that our model [Phys. Rev. E **91**, 032312 (2015)] serves as a useful tool to trace the evolution of equilibrium configurations of one-component charged particles confined in a disk. Our approach reduces significantly the computational effort in minimizing the energy of equilibrium configurations, and it demonstrates a remarkable agreement with the values provided by molecular-dynamics calculations. We show that the Comment misrepresents our paper and fails to provide plausible arguments against the formation hexagonal structure for $n \geqslant 200$ in molecular-dynamics calculations.

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In our recent publication [1], we developed a semianalytical approach that allows us to determine equilibrium configurations for an arbitrary, but finite, number of charged particles confined in a disk geometry. In the Comment [2] by Amore, it was found that the minimum energy configuration of $N = 395$ charges confined in a disk and interacting via the Coulomb potential has a lower energy than the result of our molecular-dynamics (MD) calculations [1]. Based only on this result, Ref. [2] concluded that, *"... the formation of a hexagonal core and valence circular rings for the centered configurations, predicted by the model of Ref. [1], 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. In light of these findings, the validity of the model of Ref. [1] must be questioned, particularly for $N \gtrsim 200$."*

Hereafter, for the sake of convenience, we will refer to our model as the circular model (CM). We agree with the author that his possible global MD minimum is better than our estimate for the particular case $N = 395$. However, this is not enough to conclude that the CM cannot help to reduce substantially the computational effort in MD or simulated annealing (SA) calculations for the following reasons:

(i) From the Monte Carlo and MD calculations, even for a relatively small number of charged particles, it follows that the amount of stable configurations grows very rapidly with the number of particles. Sometimes, metastable states with lower (or higher) symmetry are found with much higher probability than the true ground state. This fact was confirmed by the author who *"generated 3001 configurations..."* to get just one instance of the improved $E_{\rm MIN} = 110\,664.44$ new tentative ground state, with our prediction for the particle number at the boundary ring: *"... $N_p = 147$ charges are disposed on the border of the disk, in agreement with Ref. [1]."* Evidently, in contrast its claim, the Comment has confirmed the usefulness of the CM.

Indeed, the particle number on the boundary ring N_p is one of the key elements for any calculation, since once it is defined, it is necessary to simulate less various configurations (with a number of charges $N - N_p$). We recall that $N_p \gg N_{p-1} > N_{p-2} > \cdots > 1$, where p is a number of rings and N is the total number of charges.

In fact, external ring occupations are extremely well predicted with some occasional ± 1 mismatch by means of the expression $N_p(N) = (2.795N^{2/3} - 3.184)$, where $p \simeq [\sqrt{N}/2]$ [1]. It is noteworthy that these expressions are obtained from the systematic CM results.

(ii) In our publication [1], in order to obtain our estimate of the MD ground state $E_{\rm MD}$, we generated only 100 configurations with the boundary ring $N_{p=9} = 147$ charges, where the internal charges were randomly distributed. As a result, we have obtained $E_{\rm CM} = 110\,667.6 > E_{\rm MD} = 110\,665.1 > E_{\rm MIN} = 110\,664.44$. Note, however, that the disagreement between the author's new result and our model prediction $E_{\rm CM}$ is still less than $3\times10^{-3}\%$ (as we stated in our paper, it is $2\times10^{-3}\%$). Moreover, the occupations for the external (approximately circular) shells are quite accurately predicted within CM for any N. In the case of $N = 395$ we have obtained (147,65,50,40), while the analysis of the MD ground state in Ref. [2] yields (147,66,51,40). This comparison suggests that the effectiveness of the CM prediction might be improved if the second ring, the nearest neighbor to the boundary one, should be taken into account.

(iii) To prove the usefulness of this idea, we consider initial configurations characterized by external occupations: N_9=147 (Set 1); $N_9 = 147, N_8 = 65$ (Set 2); $N_9 = 147, N_8 = 66$ (Set 3). In all cases, we have generated 2000 configurations, where N_9 particles were initially set on the boundary at $R_1 = 1$, and for two other sets N_8 particles have been distributed at $R_2 = 0.96$. That value was chosen to take into account monopole oscillations around the equilibrium configuration. The remaining particles were distributed randomly.

For the Set 1 (Fig. 1, top panel), we found the lowest state $E_{\rm MD} = 110\,664.52 > E_{\rm MIN} = 110\,664.44$, which occurs just once. In the middle panel (Set 2) we use two boundary shells $N_9 = 147$, $N_8 = 65$, predicted by the CM partition, and we obtain a slightly lower state. However, the ground state is not reached yet.

The systematic analysis of the CM results leads us to conclude that the second shell occupation is fitted by the formula $N_{p-1}(N) = (1.351N^{2/3} - 6.566)$, which yields $N_8 = 66$. Considering the initial configuration with $N_9 = 147$, $N_8 = 66$ (Set 3) with randomly distributed internal charges (Fig. 1, bottom panel), we obtain that the ground state $E_{\rm MIN}$

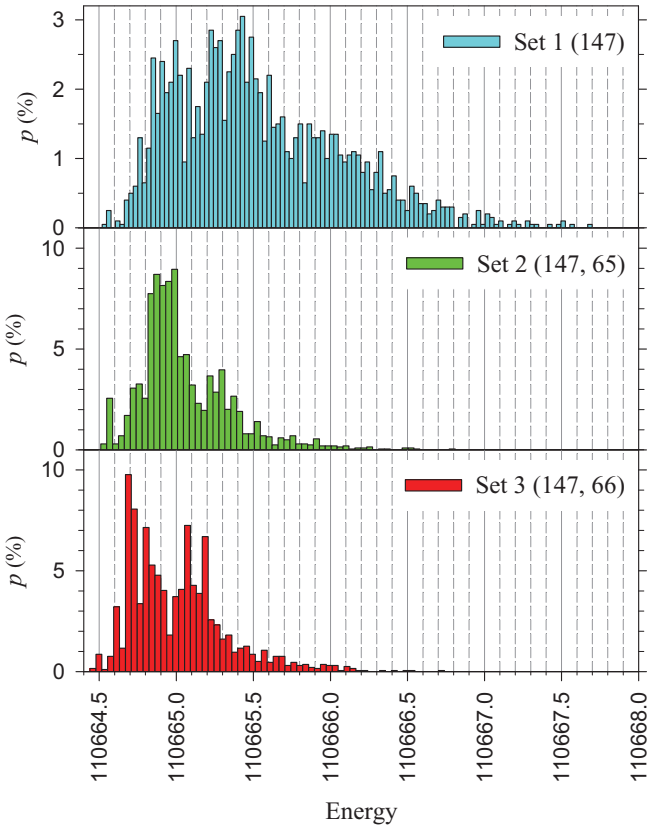

FIG. 1. Histograms for energy states of $N = 395$ charges in the disk geometry obtained by means of the MD method for different initialization procedures.

occurs three times (0.15%). In other words, with this initialization it appears once every 666 generated configurations. Note that Ref. [2] has generated 3001 configurations to obtain just one realization of the possible ground state.

(iv) We recall that for infinite systems, the hexagonal lattice has the lowest energy of all two-dimensional Wigner Bravais crystals [3]. Evidently, the decrease of system size places primary emphasis upon system boundaries (see, for example, the discussion in Refs. [4,5]). Therefore, one needs to understand how the Wigner crystallization may settle down, in particular in a disk geometry as a function of the number of interacting charged particles. In Ref. [6], we compare our results corresponding to the MD and the semianalytical approach for $161 \leqslant N \leqslant 260$ charges. These results demonstrate a remarkable agreement between two approaches, and they make it clear how the centered hexagonal lattice (CHL) evolves with the increase of charge particle number. Therefore, we strongly believe that the results obtained by means of our method can be successfully used to feed SA or MD calculations with sensible initial configurations, reducing significantly the amount of scanning normally needed to visit the global energy minima.

(v) The systematic manifestation of the CHL with the increase of particle number $N \geqslant 200$ in our CM and MD results can be interpreted as the onset of the hexagonal crystallization in the disk geometry. There is not, however, any manifestation of a phase transition, typical for infinite systems. In a finite system, a crossover takes place from the CHL to ring localization with the approach to the disk boundary. This ring organization is clearly seen at the boundary in Fig. 2 of Ref. [2] presented by the author (two clear rings).

In our paper, we have compared the MD configuration with the prediction of the CM for the CHL at $N = 395$. In fact, in our MD calculations the clean CHL takes place at $N = 381$ with the configuration **143**,**64**,**49**,39,30,19,**18**,**12**,**6**,**1** and the minimal energy $E = 102\,764.53$. The valence configurations with $N_7 = 49$, $N_8 = 64$, $N_9 = 143$ form a well-defined ring structure.

The increase of the particle number disintegrates slowly the CHL in the disk geometry, while the hexagonal lattice still exists. Nevertheless, with each new shell, as soon as a new particle appears at the center it gives rise to the CHL again. Since we deal with a finite system restricted by circular geometry, the boundary affects the plain symmetrical configurations, giving rise to defects.

In conclusion, we disagree with the main outcome of the author's Comment [2] formulated in his Summary. To argue against our model and the corresponding conclusions, there must be a systematic and thorough analysis of the system with increasing particle number, but not only in one particular case. In fact, we have demonstrated that the CM predictions for external rings (N_p, N_{p-1}) enable us to reduce substantially the scanning efforts needed to reach the ground state in the MD.

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