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Ground-State Configurations of 2D Clusters of Classical Charged Particles

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The ground-state configurations of the classical point-charge particles were calculated using a new genetic-algorithm-based approach. The structures obtained confirmed the recent Monte Carlo findings, including the metastable states.

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1. Introduction

An increased interest in theoretical and experimental studies of two--dimensional (2D) confined clusters of classical particles follows from wide applicability of such theoretical 2D models to real physical systems [1]. The 2D clusters offer rich physics and can be accurately described.

For the classical Coulomb clusters, which are basically point-charged particles confined by a parabolic potential, geometrical structures consisting of well--separated shells have been found using Monte Carlo simulations [1, 2] (see also [3] for more references). Despite recent developments [4–6], some discrepancies between theoretical predictions and experimentally observed configurations [3] have remained.

We address the problem of the ground state configurations of the 2D classical Coulomb clusters as the optimization task. We have developed a genetic algorithm approach to find the global minimum of the potential energy which corresponds to the optimal geometrical structure.

2. Model and simulation technique

Here we briefly describe a genetic algorithm (GA) technique proposed to minimize the potential energy of the two-dimensional classical system consisting of N uniformly charged particles interacting through a repulsive Coulomb potential

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and trapped by a confining parabolic potential. The potential energy can be written in dimensionless units [7] as

$$U = \sum_{i=1}^{N} \left(r_i^2 + \sum_{j>i}^{N} \frac{q_i q_j}{|r_i - r_j|} \right), \tag{1}$$

where r_i and q_i denote the radial distance and the charge of a given particle. In this report we assume $q_i = 1$.

The genetic algorithm is a search procedure based on the process of natural evolution, following the principles of natural selection, crossover and survival. The method has been proposed and developed by Holland [8]. Due to complex specification of initial conditions, GA is useful for searching for the optimal solution in situations where other optimization techniques may fail. A major characteristics of genetic algorithms is that they work with a population and can explore concurrently different regions of the solution space.

In the GA optimization, any individual belonging to a given population is represented by a set of parameters (genes in chromosomes) which express a potential solution of the problem. Each individual is evaluated according to the fitness function which is related in our problem to the potential energy (1). The GA optimization starts with random potential solution of the problem. The number of solutions is represented by the size of the population. Individuals with higher evaluation scores (better fitted, due to a smaller total energy value U) are selected to generate a new population. Because of the genetic evolution, the individual (chromosome) with better fitness tends to yield a superior offspring, which means that it provides a better solution to the problem.

In the GA applications three genetic operations are distinguished: reproduction (selection), crossover and mutations. In the reproduction process, a new population is generated from the individuals according to the value of their fitness function. After that, the crossover follows. The individuals are paired, the chromosomes are split and an exchange of genes is performed. The progeny heritages some parent genes and the new chromosomes are close to those of their predecessors. The mutation is applied seldom and changes randomly one or more genes in a given chromosome. Both crossover and mutation are subject to the sampling procedure which leads to a crossover with much higher probability than to a mutation.

Our approach follows the idea of Holland [8]. We choose chromosomes as sets of all the independent planar variables x_i and y_i (each representing a gene), where $1 \leq i \leq N$, and search for a global minimum of the potential energy U. We scan the space of solutions, changing the number of chromosomes denoted by S (i.e. the size of the population), the number of iterations N_{s} (or a number of generations) as well as the probability of mutation p_{m} and crossover p_{c}. The numerical calculations are based on the flow-point coding. More details on the GA procedure, and genetic operations and implementation are given elsewhere [9].

In the final generation, the chromosome which reaches the highest value of the fitness function is assumed as the solution. Its genes determine the best coordinates of the particles in the 2D structure.

3. Results and discussion

Our selected results for the ground state configurations of the 2D Coulomb clusters are summarized in Table. They were obtained choosing the following

TABLE

Ground-state configurations for the systems with parabolic--confinement potential as a function of the number of particles N. The subsequent columns give the energies U/N, the shell structure following from the experiment and the GA, as well as the radii and width of the shells.

N	U/N	Experiment	GA	Radii	Width
9	4.0881163	1, 8	2, 7	0.432084927	0.0267664
				1.301830415	0.1638026
10	4.4849429	2, 8	2, 8	0.426483771	0.0000065
				1.348796692	0.1765400
12	5.2389364	3, 9	3, 9	0.559366761	0.0000360
				1.489745003	0.1465582
15	6.3075833	4, 11	5, 10	0.751081135	0.0003891
				1.694040557	0.0902504
16	6.6499026	5, 11	1, 5, 10	0.0000939	0
				0.91102125	0.0001456
				1.768245767	0.1406669
17	6.9829032	1, 5, 11	1, 6, 10	0.0003688	0
				0.969551951	0.0058029
				1.841763095	0.0795039
20	7.9496139	1, 6, 13	1, 7, 12	0.0012170	0
				1.018237413	0.0083781
				1.952229248	0.0735389
21	8.2658786	1, 7, 13	1, 7, 13	0.0013884	0
				1.0148676	0.0106270
				1.9732824	0.1374630

values of the GA parameters: $N_{\mathrm{s}} = 100000000$, $S = 200 \div 500$, $p_{\mathrm{c}} = 0.3 \div 0.7$, $p_{\mathrm{m}} = 0.02 \div 0.15$. We were mainly interested in the systems which display the ground-state configurations different from those observed experimentally [3]. The first column gives the size of the system. The second column contains the values of the minimal potential energy per particle. The next two columns describe the

shell structure of the ground-state configurations determined experimentally and those found from our calculations. The remaining columns present some details on the radii of the shells and their width.

Strong evidence for reliability of the recent Monte Carlo simulations [4] of the ground-state configurations of the classical Coulomb clusters has been provided using the powerful genetic algorithm. The ground state configurations and the ring structure found previously by the Monte Carlo simulations [1, 4, 7] have been confirmed by our GA approach as shown in Table. The estimates of the potential energy minima shown in Table confirm the previous findings [4] up to all decimal places quoted there. Furthermore, we have also confirmed the metastable configurations, increasing somewhat the probability of mutation p_{m} with respect to the value leading to the optimal solution. These metastable configurations correspond to the observed ones in [3] except for $N = 15$. In fact, for $N > 21$, there are more cases ($N = 22$, 28, 29, 30) where the experimental configurations (Table I in [3]) are not recovered neither by the ground-state nor by the metastable configurations computed in Table I of [4].

The remaining discrepancies between the theoretical and experimental configurations may be then attributed to the parabolic confinement potential chosen in the present study, to the form of the interacting potential or to the metastable configurations appearing in experiment. In view of the analysis presented in [3, 4] and our study, the latter seems unlikely so that other possibilities should be pursued, in particular the logarithmic potential [3].

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