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LETTER TO THE EDITOR

Electrostatic energy minimisation by simulated annealing

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Abstract. We have determined the minimum energy configuration of N point charges confined to the interior of a circle. The minimisation problem in the multi-dimensional configuration space is solved by a technique based on the simulated-annealing method. We observe striking effects, which could lead to a better understanding of phenomena such as crystallisation, symmetry breaking, commensurate-incommensurate transitions, etc. Moreover, an experimental verification of our results appears to be possible.

Recently, the question of the equilibrium configuration of N equal charges confined to the interior of a circle was raised (Berezin 1985). It was found that the minimum (potential) energy configuration for $N = 12$ consists of one charge in the centre of the circle and $N-1$ charges on the vertices of an inscribed regular polygon, rather than N equally spaced charges along the circumference. Moreover, for all $N < 12$ it is this latter configuration which has the lower energy, so that we suggest calling $N = 12$ a 'magic number'. It is obvious that when more charges are added, some of them will be expelled to an inner position, so that two ring-like structures develop. Furthermore, there is no reason why this process should not continue, so that we expect more magic numbers, where charges are expelled from the inner ring to form a second inner ring, etc. In this letter we show preliminary results which have been obtained using a new algorithm.

From a computational point of view, the problem of determining the minimum energy configuration is a very complex one since one has to find the absolute minimum of the potential energy surface in the $2N$-dimensional configuration space. There is a certain similarity to the problem of determining the ground state of a cluster of identical atoms interacting via two-body forces. We have recently shown that the computational complexity of this latter problem (or rather a discretised version of it) belongs to the class NP (Wille and Vennik 1985). This means that there is no known algorithm which solves the problem in polynomial time and therefore it is considered intractable. Of course, for sufficiently small N, one can use a classical search technique to find all local minima and then decide, by simple enumeration, which one is the global minimum. Such search techniques are usually based on a gradient method (Powell 1982), in which, having started from a random initial configuration, one takes steps in the directions determined by the line of steepest descent after every step. This process continues until a (local) minimum is found. Such techniques have been applied quite successfully to the cluster problem (Hoare and McInnes 1983) but as the number

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of atoms increases, the algorithm soon becomes too time consuming, partly because the number of local minima increases very quickly. Obviously, what is needed is an algorithm that avoids getting trapped in local minima and, in the context of the cluster problem, we have suggested (Wille and Vennik 1985) using a continuous version of the simulated-annealing method proposed by Kirkpatrick *et al* (1983). This method has been applied successfully to discrete optimisation problems (Kirkpatrick *et al* 1983, Bonomi and Lutton 1984) as well as to continuous ones (Vanderbilt and Louie 1984). In our case, the physical system is slowly annealed into the minimum energy configuration by allowing it to escape from local minima with a temperature-dependent probability. As suggested by Kirkpatrick *et al* (1983), the presence of a minimum can be detected by looking at peaks in the specific heat. When the system is freezing into such a minimum careful annealing is needed.

Consider the potential energy to be minimised as $E(\mathbf{r}_1, \ldots, \mathbf{r}_N)$, $\mathbf{r}_i = (r_i, \theta_i)$, defined over the $2N$-dimensional configuration space. The simulated-annealing method uses the Metropolis prescription (Metropolis *et al* 1953) to decide whether or not to accept a random step $\Delta\mathbf{r}_i$, $i = 1, \ldots, N$, where the associated energy change is

$$\Delta E = E(\mathbf{r}_1, \ldots, \mathbf{r}_i + \Delta\mathbf{r}_i, \ldots, \mathbf{r}_N) - E(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N). \tag{1}$$

If ΔE is negative the step is accepted, whereas if ΔE is positive it is accepted with a probability

$$p = \exp(-\Delta E / T). \tag{2}$$

In the process of annealing, the system is started in a random configuration at a sufficiently high temperature T and is then slowly cooled. Several iterations are performed at each temperature, each iteration consisting of N attempted steps, one for each charge. The specific heat at a given temperature is defined as

$$C(T) = T^{-2}(\langle E^2 \rangle - \langle E \rangle^2), \tag{3}$$

where the brackets indicate an average over all attempted steps. Sophisticated schemes to implement the procedure for continuous problems have been developed by Vanderbilt and Louie (1984), but we have not used these in the calculations presented in this letter.

We now discuss our results for the minimum energy configuration of N equal point charges interacting via Coulomb forces and confined to the interior of a circle by an infinitely hard wall, the minimisation problem being solved by means of the simulated-annealing method. Obviously, neither the magnitude q of the charges nor the radius R of the circle do matter, since we can express all energies in units of q^2/R. As a first result we find that for $N = 12$ the ground state consists of one charge in the centre and 11 along the circumference. More extra charges are put on the circumference up to $N = 16$. From there on, the effect of additional charges is shown in figure 1, from $N = 16$ (a) to $N = 23$ (h). In the sequence (b)-(e), the inner triangle is squeezed together and when $N - 3$ is not a multiple of 3, it is slightly distorted from an equilateral shape since the two numbers are incommensurate. Further calculations have not yet been performed, except for $N = 50$ (see figure 2). In this case we find two additional rings containing respectively 11 and 5 charges inside the inscribed polygon, which contains 34 charges. These results were quite insensitive to the details of the annealing procedure. One merely has to take care that the configuration space is explored in

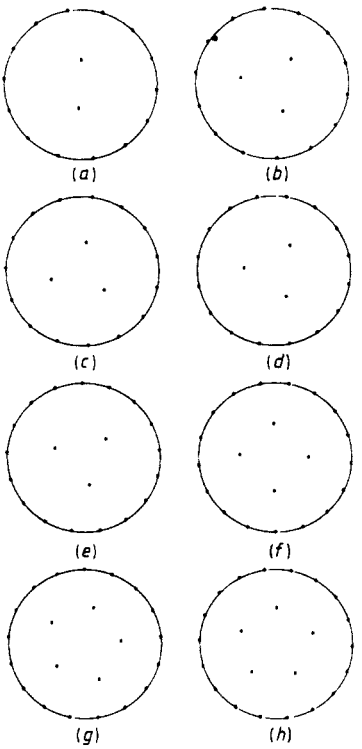

Figure 1. Ground-state configuration of N charges confined to a circular region. $N = (a)16$, $(b)17$, $(c)18$, $(d)19$, $(e)20$, $(f)21$, $(g)22$, $(h)23$.

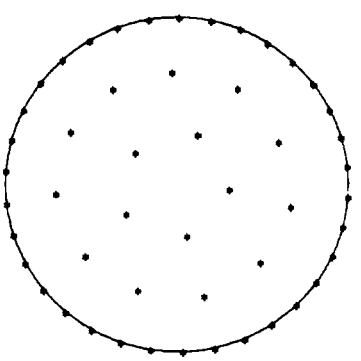

Figure 2. Ground-state configuration of 50 charges confined to a circle.

sufficient detail at high temperatures and that the annealing proceeds slowly enough. We used 100 iterations at every temperature and then reduced the temperature by a factor of 0.9. In order to show how the cooling proceeds (for $N = 16$) we have plotted $C(T)$, defined in (3), against $\ln(T)$, in the lower curve of figure 3 and E (divided by a factor of 10) against $\ln(T)$ in the upper curve. We note that $C(T)$ is very spiky indeed when the system freezes into a minimum, but that there are still quite large peaks at low temperatures when the system hardly changes in energy. These peaks

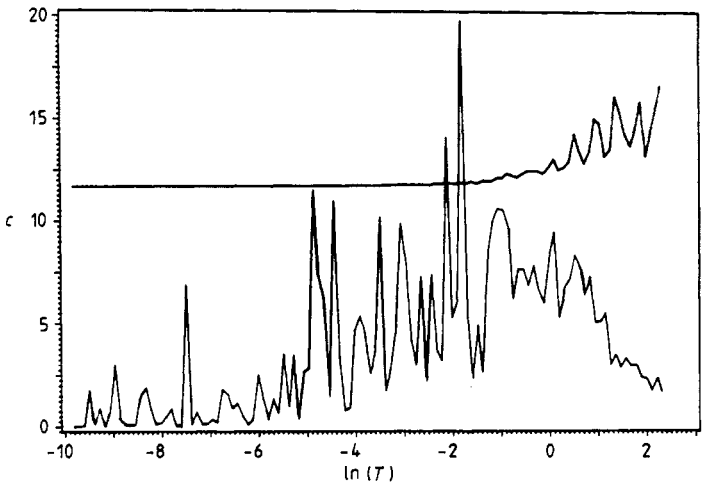

Figure 3. The cooling procedure for $N = 16$. Lower curve—specific heat against $\ln(T)$; upper curve—total energy (divided by 10) against $\ln(T)$.

are due to very small changes in energy at these low temperatures, so that $C(T)$ defined in (3) is relatively large. These minute energy differences have a negligible effect on the geometries depicted in figures 1-2. We conclude that some care is needed in using the specific heat to monitor the cooling process, at least if one is mainly interested in the ground-state geometry.

The results presented here appear interesting in their own right and also show the power of the simulated-annealing method. We believe that this method will prove to be a powerful tool in the solution of many continuous optimisation problems, which arise quite often in physics. In future work, we intend to investigate the electrostatic problem in more detail by extending our calculations to more N values. Furthermore, the influence of the boundary conditions should be studied: one could for example confine the system to a polygonal box where the number of sides is incommensurate with that of the inscribed polygons found in the circular case. Obviously this will lead to commensurate-incommensurate structures. Also the influence of charged boundaries or external fields can be investigated. The method is obviously not restricted to Coulomb forces and one could equally well study dipole-type or van der Waals forces.

Finally we would like to mention the possibility of an experimental verification of our results. A two-dimensional system, similar to the one discussed here, has been constructed by Blonder (1985). It consists of small metallic spheres which can move freely along the bottom plate of a plane parallel capacitor. Application of a high voltage charges the balls, which leads to effects similar to the ones described here. In the cell built by Blonder (1985) the balls interact via dipole-dipole forces and the walls carry a uniform charge distribution, but it is highly plausible that the model system considered in this letter can be built using the same techniques. Alternatively, we intend to extend our calculations, so that a direct comparison with Blonder's (1985) experiment will be possible.

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