Stability of polygonal Coulomb crystals

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The stability of polygonal patterns composed of a set of N point charges in a potential well is studied. It is shown that a right polygon is stable for $N\leqslant 5$. A right polygon with additional charge in its center is stable for $N=5,\ldots,9$. [S1050-2947(99)09602-X]

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I. INTRODUCTION

In recent experiments on the confinement of cold ionic systems, it was observed that a set of trapped ions self-organizes to an intrinsically structured charged cloud [1]. With a small enough number of ions, these clouds take the form of rather symmetrical patterns; e.g., under certain conditions, ions can order into a right planar polygon [2].

As a rule, small ion clouds are observed in the quadrupole radio frequency Paul trap [3] with the (averaged) confining potential per particle

$$U_{\text{eff}}=\tfrac{1}{2}m\omega^2(x^2+y^2+\alpha z^2), \tag{1}$$

where m is the particle mass, ω is defined by the ponderomotive force intensity, and the parameter $\alpha>0$ describes the anisotropy of the trap.

To describe the equilibrium state of a cold cloud one has to find the minimum of the potential energy for a set of likely charged particles inside the potential well [Eq. (1)]. A complete analytical description was performed for a small number of particles, $N\leqslant 4$ only [4]. As for larger ensembles, numerical methods were successfully implemented [4,5].

Obviously, the structure of the cloud depends on the degree of anisotropy of the confining potential. There are two evident ultimate cases: as $\alpha\to 0$, the particles are aligned in a string, while as $\alpha\to\infty$ some planar structures are formed. Classification of these two-dimensional ''atoms'' resembling the Mendeleev table was proposed in Refs. [6,7]. It is of interest that nearly the same problem was studied by Kelvin [8] and Thomson [9] in the context of a vortex model of an atom.

In the present Brief Report we study the stability of the two simplest planar configurations of N charges in potential (1). These configurations are a right polygon in the xOy plane and the same polygon with an additional ion in its center. We evaluate the spectrum of linear oscillations and find the criteria for stability.

II. RIGHT POLYGON

Let N point particles with mass m and charge q be placed in potential (1). The classical equation of motion is

$$\frac{d^2\vec{r}_n}{dt^2}+\omega^2A\vec{r}_n=\frac{q^2}{m}\sum_{k=1}^{N}{}' \frac{\vec{r}_n-\vec{r}_k}{|\vec{r}_n-\vec{r}_k|^3}, \tag{2}$$

where $A=\text{diag}(1,1,\alpha)$ and $1\leqslant n\leqslant N$. The prime over the sum sign indicates that terms with $k=n$ are omitted.

This equation has a special class of solutions with all particles moving in the xOy plane. Let the projection of $\vec{r}$ on the xOy plane be $\vec{\rho}$. Introducing the complex variable $x+iy\equiv\zeta$ instead of $\vec{\rho}=(x,y)$, the corresponding equation of motion is of the form

$$\frac{d^2\zeta_n}{dt^2}+\omega^2\zeta_n=\frac{q^2}{m}\sum_{k=1}^{N}{}' \frac{\zeta_n-\zeta_k}{|\zeta_n-\zeta_k|^3}.$$

Although generally there are the solutions to this equation corresponding to a rotating polygon, the energy takes a minimal value for a stationary polygon. To obtain the equilibrium size of a stationary polygon we set $\zeta_n=R\eta^n$, where $\eta=\exp(2\pi i/N)$, which results in

$$\left(\frac{\omega}{\nu}\right)^2=\frac{1}{4}S_1(N). \tag{3}$$

Here $\nu^2\equiv q^2/mR^3$ is an analog of the plasma frequency, and we introduce a notation

$$S_l(N)=\sum_{k=1}^{N-1}\frac{\sin^2(\pi kl/N)}{\sin^3(\pi k/N)}$$

to denote some trigonometric sums in what follows.

To investigate the stability of the polygonal atom, we linearize Eq. (2) with respect to small perturbations, $\vec{r}_n=(\vec{\rho}_n,0)+(\delta\vec{\rho}_n,\delta z_n)$. Then the perturbations perpendicular to the polygon plane are governed by the equation

$$\frac{d^2}{dt^2}\delta z_n+\alpha\omega^2\delta z_n=\nu^2\sum_{k=1}^{N}{}' \frac{\delta z_n-\delta z_k}{|\eta^n-\eta^k|^3}.$$

The perturbation can be taken in the form $\delta z_n=\text{Re}\,z(t)\eta^{ln}$, where l is analogous to the azimuthal wave number and takes the values $0\leqslant l\leqslant N$. For one particular harmonic this yields the equation

$$\frac{d^2z}{dt^2}+\alpha\omega^2z=\frac{1}{4}\nu^2S_l(N)z.$$

Evidently, the right polygon is stable with respect to perpendicular deformations if there are only oscillating solutions to this equation, that is, $\alpha \geqslant S_l(N)/S_1(N)$. The stability can always be provided by increasing α. To obtain the lowest α providing stability for a given number of particles, N, it is necessary to check all possible l's. For example, if $N=3$ it must be $\alpha \geqslant 1$. The typical value $\alpha=4$ provides the stability for all $N \leqslant 9$.

Let us turn to perturbations in the xOy plane. It is convenient to write the equation for the perturbations in a complex form:

$$\frac{d^2}{dt^2}\delta\zeta_n+\omega^2\delta\zeta_n+\frac{q^2}{2m}\sum_{k=1}^{N}{}' \left\{\frac{\delta\zeta_n-\delta\zeta_k}{|\zeta_n-\zeta_k|^3}+\frac{3(\zeta_n-\zeta_k)^2}{|\zeta_n-\zeta_k|^5}\overline{(\delta\zeta_n-\delta\zeta_k)}\right\}=0.$$

Since the latter equation contains both ζ_n and $\overline{\zeta_n}$, two harmonics should be taken into account. Substituting

$$\zeta_n+\delta\zeta_n=\eta^n(R+w_n), \quad w_n=u(t)\eta^{ln}+\overline{v}(t)\eta^{-ln},$$

where $0 \leqslant l \leqslant N/2$, we obtain a set of coupled equations:

$$\begin{bmatrix} \frac{d^2}{dt^2}+\omega^2+\frac{\nu^2}{2}\sum_k{}' \frac{1-\eta^{(l+1)k}}{|1-\eta^k|^3} & \frac{3\nu^2}{2}\sum_k{}' \frac{(1-\eta^k)^2(1-\eta^{(l-1)k})}{|1-\eta^k|^5} \\ \frac{3\nu^2}{2}\sum_k{}' \frac{(1-\eta^{-k})^2(1-\eta^{(l+1)k})}{|1-\eta^k|^5} & \frac{d^2}{dt^2}+\omega^2+\frac{\nu^2}{2}\sum_k{}' \frac{1-\eta^{(l-1)k}}{|1-\eta^k|^3} \end{bmatrix}\begin{pmatrix} u \\ v \end{pmatrix}=0.$$

All sums here can be expressed in terms of $S_l(N)$. By doing this and looking for the solution in the form of $u,v \sim \exp(-i\nu\Gamma t)$, we obtain the dispersion relation

$$\begin{vmatrix} -\Gamma^2+\frac{1}{4}(S_1(N)+\frac{1}{2}S_{l+1}(N)) & \frac{3}{8}(S_1(N)-S_l(N)) \\ \frac{3}{8}(S_1(N)-S_l(N)) & -\Gamma^2+\frac{1}{4}(S_1(N)+\frac{1}{2}S_{l-1}(N)) \end{vmatrix}=0,$$

resulting in two real values for Γ^2. To ensure the stability of the polygon all eigenfrequencies should be real, that is provided that

$$(S_1(N)+\tfrac{1}{2}S_{l+1}(N))(S_1(N)+\tfrac{1}{2}S_{l-1}(N)) \geqslant \tfrac{9}{4}(S_1(N)-S_l(N))^2,$$

where the inequality has to be held for all $l: 0 \leqslant l \leqslant N/2$. The numerical calculations show that the N-gon is stable if and only if $N \leqslant 5$.

III. POLYGON WITH CENTRAL PARTICLE

This section deals with another equilibrium pattern: a polygon with an additional particle in its center. Let the radius vector of an additional particle be $\vec{r}_0$. The equations of motion in this situation are given by Eq. (2) but the sum is taken over $k=0,\ldots,N$. One can easily verify that the stationary solution of the form $\zeta_0=0, \quad \zeta_n=\eta^n R, \quad 1 \leqslant n \leqslant N$ exists if the following restrictions hold:

$$\sum_{k=1}^{N}\eta^k=0, \quad \left(\frac{\omega}{\nu}\right)^2=1+\frac{1}{4}S_1(N).$$

The first restriction results in $N \geqslant 2$, and the second is similar to Eq (3).

To explore the stability it is convenient to exclude the center-of-mass motion by imposing the constraint $\vec{r}_0+\vec{r}_1+\cdots+\vec{r}_N \equiv 0$; that is, the coordinates of the central particle are expressed in terms of the coordinates of the peripheral particles. The perturbations parallel to the $\hat{z}$ axis are now governed by the equation

$$\frac{d^2}{dt^2}\delta z_n+\alpha\omega^2\delta z_n=\nu^2(\delta z_n-\delta z_0)+\nu^2\sum_{k=1}^{N}{}' \frac{\delta z_n-\delta z_k}{|\eta^n-\eta^k|^3}.$$

As in Sec. II, we take the perturbation in the form $\delta z_n=\mathrm{Re}\{z(t)\eta^{ln}\}$. Taking into account that the displacement of the central ion is

$$\delta z_0=-\mathrm{Re}\left\{z(t)\sum_{k=1}^{N}\eta^{ln}\right\}=-\mathrm{Re}\{N\delta_{l,0}z(t)\eta^{ln}\},$$

we finally obtain the equation for the amplitude of the oscillations, $z(t)$,

$$\frac{d^2z}{dt^2}+\alpha\omega^2 z=\nu^2\left\{1+N\delta_{l,0}+\sum_{k=1}^{N-1}\frac{1-\eta^{kl}}{|1-\eta^k|^3}\right\}z.$$

The stability in the $\hat{z}$ direction is provided if

$$\alpha \geqslant \frac{1+N\delta_{l,0}+\frac{1}{4}S_l(N)}{1+\frac{1}{4}S_1(N)}.$$

The result is very close to the previous one, and the instability is always suppressed by α increasing.

To investigate more dangerous perturbations in the xOy plane we use the substitution $\zeta_n+\delta\zeta_n=\eta^n(R+w_n)$ for $1\leqslant n\leqslant N$ and $\delta\zeta_0=w_0$, resulting in

$$\frac{d^2w_n}{dt^2}+\omega^2w_n=-\frac{\nu^2}{2}\{(w_n-\eta^{-n}w_0)+3\overline{(w_n-\eta^{-n}w_0)}\}-\frac{\nu^2}{2}\sum_{k=1}^{N}{}'\left\{\frac{w_n-\eta^{k-n}w_k}{|1-\eta^{k-n}|^3}+3\frac{(1-\eta^{k-n})^2}{|1-\eta^{k-n}|^5}\overline{(w_n-\eta^{k-n}w_k)}\right\}.$$

Looking for the solution in the form of $w_n=u(t)\,\eta^{ln}+\overline{v(t)}\,\eta^{-ln}$, and excluding the central particle

$$\eta^{-n}w_0=-N\{\delta_{l,N-1}u\,\eta^{ln}+\delta_{l,1}\overline{v}\,\eta^{-ln}\},$$

yields the set

$$\begin{bmatrix}\dfrac{d^2}{dt^2}+\nu^2a & \nu^2c_1\\ \nu^2c_2 & \dfrac{d^2}{dt^2}+\nu^2b\end{bmatrix}\begin{pmatrix}u\\ v\end{pmatrix}=0,$$

where

$$a=\tfrac{1}{2}(3+N\delta_{l,N-1}+\tfrac{1}{2}S_1(N)+\tfrac{1}{4}S_{l+1}(N)),$$

$$b=\tfrac{1}{2}(3+N\delta_{l,1}+\tfrac{1}{2}S_1(N)+\tfrac{1}{4}S_{l-1}(N)),$$

$$c_1=\tfrac{3}{2}(1+N\delta_{l,1}+\tfrac{1}{4}S_1(N)-\tfrac{1}{4}S_l(N)),$$

$$c_2=\tfrac{3}{2}(1+N\delta_{l,N-1}+\tfrac{1}{4}S_1(N)-\tfrac{1}{4}S_l(N)).$$

The eigenfrequencies of this equation are real if $ab\geqslant c_1c_2$. The numeric investigation of the latter inequality show that configurations with $4\leqslant N\leqslant 8$ (i.e., from five to nine particles) are stable. If $N=2$ or 3 or $N>8$, a polygon with the additional particle in the center is broken by the perturbations.

IV. CONCLUSION

To conclude, let us list our discoveries. A set of point charges in the potential well [Eq. (1)] in the form of a right polygon is stable only if a number of particles $N\leqslant 5$. Another configuration consisting of N charges in the corners of a right polygon plus an additional charge in the center is stable if $4\leqslant N\leqslant 8$, that is, polygonal configurations can be observed for no more than nine particles.

Of course, an investigation of small perturbations is an incomplete alternative to a full nonlinear stability analysis. To clear this subject let us compare our results with recently reported Monte Carlo studies [6,7]. First, linearly unstable configurations were never observed in computer simulations. Second, in most cases the stable configurations were truly the ground states, but there are two exceptions.

(a) The linear analysis allows five particles to form both a pentagon as well as a square with the central ion. However, the potential energy of the square configuration is a little larger, so it must be unstable under finite perturbations.

(b) Similarly, the octagon with the central particle is broken by finite perturbations, and the real ground state is somewhat like a heptagon with two central particles. This is the way the second circle shell begins to form. According to Refs. [5–7], the general planar equilibrium is a system of concentric quasicircles.

Although we considered the stability of the stationary polygon only, our approach is applicable to a rotating one as well. In this case, the dispersion relation depends on the rotation frequency. Rather cumbersome analysis shows that the main conclusion remains the same: the polygon is stable for $N\leqslant 5$. Also, the influence of the external magnetic field can be taken into account with the same conclusion. This allows us to extend our results in another direction.

The problem of a rotating polygon stability in the Paul trap can be shown to be closely related to the polygon stability in the Penning trap, which is one of the widely used confinement devices based on a combination of electrostatic and magnetostatic fields (see Ref. [1] and references cited therein). According to Ref. [10] no more than a pentagon can be observed in the Penning trap.

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