

Prediction of Deterministic Melting Regions of Two and Three Laser-cooled Ions in a Paul Trap

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Abstract

Through the use of detailed numerical simulations we predict the existence of a nontrivial region in the Paul trap parameter space (a, q) where stable, singly periodic orbits (crystals) do not exist. As ions are dragged into this region via an adiabatic change in control parameters, a deterministic melting transition is observed. A detailed map of this deterministic melting region is constructed for the 2 and 3 ion cases. As crystals are dragged into this region by an adiabatic change of control parameters, a melting transition will occur. This transition does not depend on external perturbations, such as laser noise or collisions with neutral atoms.

The equation of motion for n ions in the Paul trap [1, 2] is of the form $\dot{q} = f(q, t)$, where q gives the position of the system in $6n$ dimensional phase space. The Paul trap equation is periodic in time, i.e., $f(q, t + T) = f(q, t)$, where T is the period of the trap's r.f. driving field. It is reasonable to assume that the periodicity of the driving force determines the behavior of the system in a fundamental way. In order to observe the interesting physics that results from the periodicity, it is not necessary to follow all the details of the motion through the full period of an r.f. cycle. A simple mapping will capture most of the essential physics. The mapping can be constructed by strobing the system at integer multiples of the fundamental driving period T . The behavior of such mappings has been studied extensively (see, e.g., [3] and references therein). For Hamiltonian systems the Liouville theorem [3] states that phase space volume is a constant of the motion. Thus a mapping created by strobing a Hamiltonian system will be volume conserving. If, however, a damping term is added to the equation of motion, e.g., to simulate laser cooling, then the phase space volume will contract exponentially. When there is a net contraction of a region in phase space, the phase space region converges onto an object called an attractor. These attractors may have dimensionality $0 \leq d < 6n$ and are embedded in the original $6n$ -dimensional phase space. They may even have a noninteger dimension, i.e., they may be fractals. Such fractal attractors are termed strange attractors.

Often in the case of periodically driven, damped systems, the type of attractor encountered is a periodic orbit whose period is a multiple of the period of the driving field. In these cases the utility of the stroboscopic mapping is revealed. In the mapping the orbit becomes a discrete set of

points. Much is known about nonlinear non-Hamiltonian mappings, especially concerning the behavior of these point sets. In general these points can undergo bifurcations, period doublings, and even order-chaos transitions as control parameters are varied. The simplest type of attractor found in such mappings is the fixed point, or 1-cycle, defined by $q(T) = q(0)$. It is this type of attractor that has been given a name, "crystal" [4], or Coulomb cluster [5], in the field of ion trapping. We will use the term "crystal" throughout this paper. Another type of attractor is the N th order fixed point ($N > 1$), or N -cycle, defined by $q(NT) = q(0)$. This type of attractor is characteristic of frequency locked motion and has been observed for various N values ($N > 1$) both numerically and experimentally in the two-ion Paul trap [6–8]. While motion on a high order fixed point may be quite complex (consider, e.g., $N = 10^6$), the strict determinism of classical mechanics prevents such motion from being chaotic. Thus higher order fixed points share many of the same properties as crystals, the absence of r.f. heating for example.

Like Hamiltonian chaos, non-Hamiltonian chaos is characterized by sensitive dependence on initial conditions. Such motion requires an attractor of the stroboscopic map to have a dimension greater than 0 (the dimension of an N -cycle). Most interesting of these situations would be chaotic motion on a strange attractor. To the best of our knowledge no conclusive evidence for the existence of a strange attractor in the Paul trap has ever been presented. The presence of stable cloud states in the Paul trap [4, 5, 7–10] strongly suggests that such attractors do exist, and many studies have reported results indicating that they are indeed chaotic [7–10]. Still, whether "cloud attractors" are of truly fractal structure, or merely N -cycles or other complicated regular attractors, has not yet been rigorously tested.

When a fixed point attractor exists, it is common for many systems that this attractor can be driven into chaos via an adiabatic change of control parameters. There are many scenarios for how this transition occurs. Most of them require a fixed point to undergo one or more bifurcations before the onset of chaos. Since non-Hamiltonian chaos does not require the presence of random noise or external perturbations, a transition from a stable fixed point to a chaotic situation may properly be termed a deterministic order-chaos scenario. Similarly, when chaos sets in, we call

this a deterministic order-chaos transition. In the Paul trap transitions from a crystal to a cloud state have been observed [4,7-10]. However all such transitions have involved the presence of noise or perturbations. In analogy to the order-chaos transition, we term a transition from a crystalline to a cloud state in the absence of noise or perturbations, a deterministic melting transition. This has to be contrasted with an order-chaos transition induced by external perturbations, such as collisions with rest-gas atoms, or externally induced rapid changes in the phase or the amplitude of the driving field [11]. We call a transition induced by an external perturbation a disruption (of the crystal). The central point of this paper is to prove the existence of a deterministic melting transition for the two- and three-ion Paul trap.

The investigation of crystal-stability in the Paul trap involved two basic numerical "experiments". In one type of experiment the control parameters (a, q) were held fixed and the damping parameters γ was varied adiabatically, observing the behavior of the 1-cycle throughout the variation. This is called a cooling experiment. The other type, called a dragging experiment involves holding γ fixed and adiabatically varying a and q . Because the structure of the phase space is determined uniquely by the parameters ($a, q; \gamma$), this structure is independent of the path used to reach a specific set, and both experiments must give the same structure at ($a_0, q_0; \gamma_0$). This includes the phenomenon of bistability, or more generally, co-existence of phase-space structures, observed in the Paul trap [4, 9, 10]. First, we shall discuss the cooling experiment. This experiment is done for both two- and three-ion cases. In the two-ion case only the ρ and z components of the relative motion were studied because the center of mass coordinates satisfy simply decoupled Mathieu equations [12] whose dynamics is always regular and therefore not interesting. This results in four independent variables. In the three-ion case a separation into relative and center of mass variables is possible, but tedious. So the full three-dimensional motion was included. This results in 18 phase-space variables. Due to the large increase in the number of variables, the parameter space of the three-ion case was scanned with less resolution than the parameter space of the two-ion case.

The two-ion equations of motion are

$$\begin{aligned} \ddot{\rho} &= -[a + 2q \cos(2t)]\rho + \frac{\mu_x^2 \rho}{(\rho^2 + z^2)^{3/2}} - \gamma \dot{\rho} \\ \ddot{z} &= 2[a + 2q \cos(2t)]z + \frac{\mu_x^2 z}{(\rho^2 + z^2)^{3/2}} - \gamma \dot{z}, \end{aligned} \quad (1)$$

where

$$\mu_x^2 = a + q^2/2. \quad (2)$$

The three-ion equations of motion are

$$\ddot{q}_i = -[a + 2q \cos(2t)]Kq_i + \mu_x^2 \sum_{j \neq i} \frac{q_i - q_j}{|q_i - q_j|^3} - \gamma \dot{q}_i \quad (3)$$

$i = 1, 2, 3,$

where

$$K = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \quad (4)$$

Throughout the experiments, eqs (1) and (3) were integrated using a fourth-order Runge-Kutta procedure [13].

It was discovered that for any a and q values within the Mathieu stability diagram, a crystal could be formed, provided γ was chosen high enough. The γ value at which the crystal is to be studied is γ_{\min} , with the intention that the $\gamma_{\min} \rightarrow 0$ limit would be effectively reached. By stepping γ_{\min} upwards, a γ_{\max} was found where crystallization occurred. Then, γ was reduced from γ_{\max} to γ_{\min} over M oscillations of the driving term according to

$$\gamma(t) = \frac{1}{2}(\gamma_{\max} - \gamma_{\min})[1 + \cos(t/M)] + \gamma_{\min}. \quad (5)$$

Equation (5) was chosen, because γ and $\dot{\gamma}$ are continuous. This is necessary, because it was observed that discontinuities in γ and $\dot{\gamma}$ were sometimes sufficient to perturb the crystal strongly enough to prevent rapid re-crystallization.

If, at ($a, q; \gamma_{\min}$) stable crystals do not exist, crystals formed at ($a, q; \gamma_{\max}$) will melt at some point during the experiment. Thus, by looking at the motion after γ_{\min} is reached, one can determine whether the crystal survived. Since the location of the crystal depends weakly on γ , changing γ adiabatically introduces tiny perturbations on the crystal. This is sufficient to test the stability of the crystal. For a stable crystal, the damping force will restore a crystal. But if the crystal becomes unstable, these tiny perturbations will be amplified and melting will occur. Following eq. (5), the crystal was integrated at γ_{\min} for M more cycles to give sufficient time for re-crystallization to occur. The final experiment was done for $M = 1000$. Tests with $M = 5000$ were performed, showing no significant change over the $M = 1000$ results. For M much smaller than 1000 the adiabatic condition is violated. Disruption is observed.

Various γ_{\min} values were studied, with the hope of learning something about $\gamma_{\min} \rightarrow 0$ limiting behavior. For larger values of γ_{\min} ($10^{-1}, 10^{-2}, 10^{-3}$) noticeable changes in (a, q) melting values occurred with each change in γ_{\min} . For $\gamma_{\min} < 10^{-3}$ no significant changes in the data were observed. Thus for our final experiments, $\gamma_{\min} = 10^{-3}$ was chosen as sufficient to observe $\gamma_{\min} \rightarrow 0$ limiting behavior.

For the two-ion case the experiment was done on a grid of (a, q) values with $\Delta a = \Delta q = 0.001$. The black regions in Fig. 1 show the set of (a, q) values where melting occurred. Two distinct melting regions were revealed, an inner melting region and an outer melting region. They are separated by a channel where stable two-ion crystals were observed. A small region containing portions of the outer region, the inner region, and the channel was examined with $\Delta a = \Delta q = 10^{-4}$. No new fine structure was revealed. The data presented in Fig. 1 represents a substantial improvement in resolution over the data shown in [6].

The three ion case was done with $\Delta a = \Delta q = 0.0025$. The resulting three-ion melting regions are shown in Fig. 2.

For both the two-ion case and the three-ion case, the melting experiments were repeated for $\Delta a = \Delta q = 0.01$ with the integration step size of the Runge-Kutta procedure halved and M doubled. No changes in the results were observed. As computer run-time considerations are important for numerical experiments, as large an integration step size as is reasonable is preferred. The final experiments were done using 25 integration steps per r.f. cycle. This number is quite small, and would be insufficient for accurately simulating ion dynamics in general, in particular the dynamics of

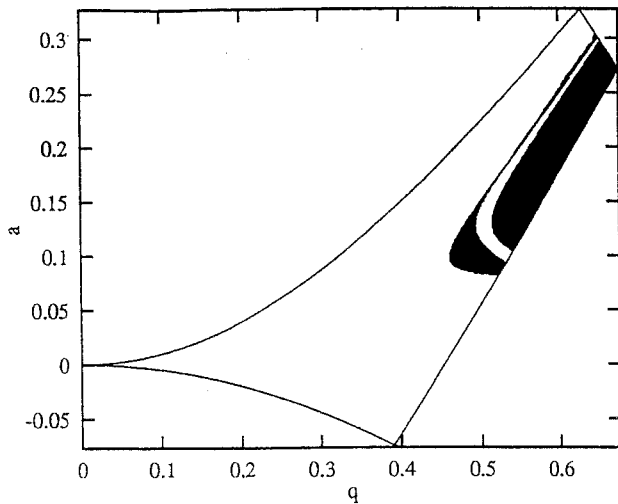


Fig. 1. The deterministic melting region for the two-ion case. The black regions indicate where melting occurred in the numerical cooling experiment with $\gamma_{\min} = 10^{-3}$ on a grid $\Delta a = \Delta q = 10^{-3}$. The outline of this region is verified by dragging experiments.

an ion cloud. However, due to the regularity of the motion around a stable periodic orbit as well as the presence of damping, numerical integration in these regions is very robust. Tests with a much higher number of steps revealed that 25 steps were sufficient to model crystalline motion.

One possible source of errors in Figs 1 and 2 is the following. Suppose that the crystal does indeed become unstable at $\gamma_{\max} > \gamma_{\text{melt}} > \gamma_{\min}$, but becomes stable again at some $\gamma_{\text{melt}} > \gamma_{\text{stable}} > \gamma_{\min}$. Once the crystal has melted, it will not reform at γ_{stable} on the time scale of the experiment, due to a hysteresis phenomenon. Thus it is possible that stable crystals do exist in small regions within or along segments of the border of the melting regions of Figs 1 and 2. In order to test these possibilities one would also like to reach $(a, q; \gamma_{\min})$ along some other path in parameter space. This is where the dragging experiment comes in. Typically dragging experiments involved integrating eq. (1) over 10^6

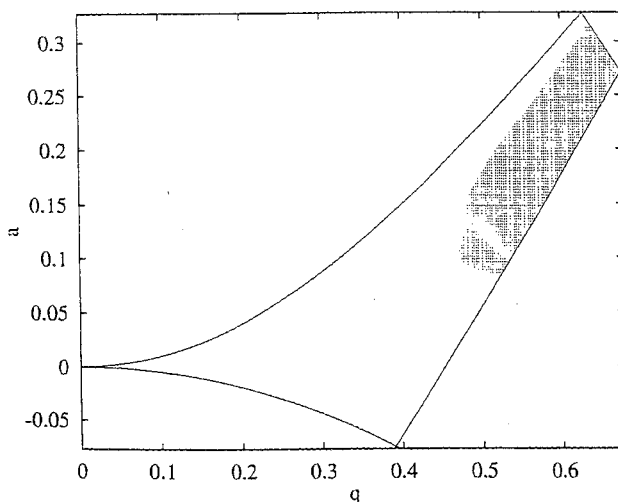


Fig. 2. The deterministic melting region for the three-ion case with $\gamma_{\min} = 10^{-3}$, and $\Delta a = \Delta q = 2.5 \times 10^{-3}$.

r.f. cycles, while slowly changing a and q . Due to the long time scales involved, dragging experiments were performed only in the two-ion case. As soon as the point (a, q) entered the melting region predicted by the cooling experiment, melting was observed. This result is independent of the particular path chosen to reach the boundary of the melting region. Thus, although dragging experiments are able to rule out the existence of crystals along the boundaries of the melting regions displayed in Figs 1 and 2, they cannot rule out the existence of "crystalline patches" within the melting regions. The dragging method is ideally suited for laboratory experiments with laser cooled ions. Dragging experiments have been reported in the literature [8–10]. However, the chosen paths never intersected with the deterministic melting regions in Figs 1 and 2. This explains why the deterministic melting region has not been previously reported.

Figure 3 shows a typical dragging experiment. A crystal was formed at $(a, q) = (0.2, 0.5)$. Then q was increased at a rate of $\dot{q} = 5 \times 10^{-10}/\pi$ and dragged over 10^8 cycles towards the boundary of the outer sector of the deterministic melting region. This corresponds to a 10 seconds experiment in a Paul trap operated at 10 MHz. Fig. 3(a) shows $\hat{z} = z - \bar{z}$ as a function of q for q values close to the boundary of the melting region. Here \bar{z} is the average of z over eight consecutive r.f. cycles. This eliminates the slow variation of z with changing q . Thus $\hat{z} = 0$ indicates a crystalline state, while an erratic $\hat{z} \sim 1$ indicates a cloud state.

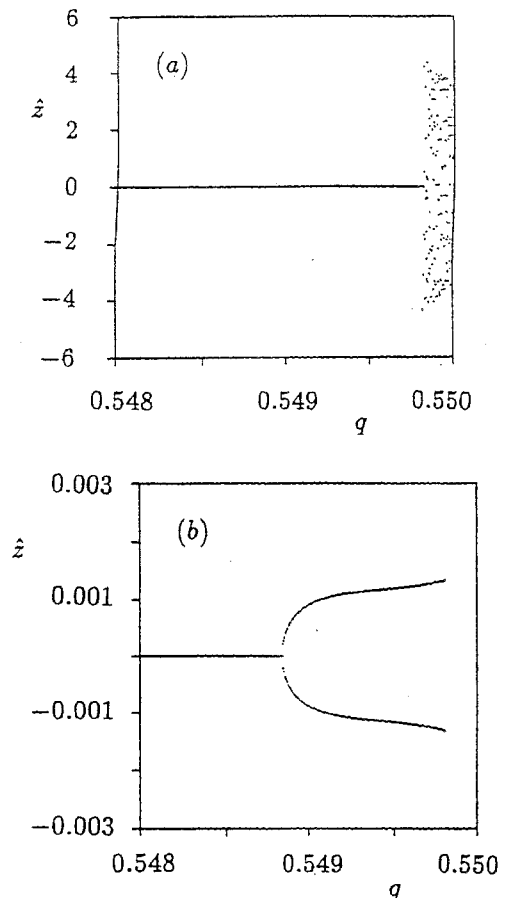


Fig. 3. A typical dragging experiment. (a) Melting transition occurs at $q \approx 0.5498$. (b) Magnification of (a), showing a period doubling bifurcation at $q \approx 0.5488$.

While it appears that the "cloud" state in Fig 3(a) damps out, in fact it eventually stabilizes at $\hat{z} \sim 1$. In this experiment the melting transition occurred at $q \approx 0.5498$. This agrees with the edge of the outer region in Fig. 1.

Figure 3(b) shows a magnification of Fig. 3(a). Clearly we see a period doubling bifurcation at $q \approx 0.5488$. Although the range $\Delta q = 2 \times 10^{-3}$ was covered in as many as 4×10^6 r.f. cycles, a second bifurcation did not appear. Thus, based on our current data, a period of doubling bifurcation is followed by a deterministic melting transition. While we are confident that a period doubling bifurcation does occur, further research may reveal a more complex scenario following the bifurcation and preceding the actual deterministic melting transition. Future work will concentrate on clarifying this scenario further, as well as investigating the scenario occurring as either one of the two melting regions is entered from the crystalline channel between the two parts of the melting region.

In conclusion, based on careful numerical calculations, we have advanced the understanding of the dynamical regimes of two and three ions in a Paul trap. In particular, we considerably increased the resolution of the deterministic melting region previously predicted to occur in the two-ion case [6]. In addition we provided evidence that an analogous melting region exists for three ions in a Paul trap. We

conjecture that a deterministic melting region exists for higher numbers of ions as well.

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