

Self-bunching induced by negative effective mass instability in an electrostatic ion beam trap

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Abstract

We demonstrate that the synchronization effect, which has been observed when a bunch of ions oscillates between two mirrors in an electrostatic ion beam trap, can be explained as a negative effective mass instability. We derive simple necessary conditions for the existence of a regime in which this dispersionless behaviour occurs and demonstrate that, in this regime, the ion trap can be used as a high resolution mass spectrometer.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In a recent experiment, Pedersen *et al* [1, 2] demonstrated that, when a bunch of interacting (charged) particles oscillates between two electrostatic mirrors, its size can be kept constant, in spite of the fact that not all the ions have the same velocity, not all of them move on the same trajectory and the Coulomb repulsion between them is non-negligible. This counter-intuitive effect, which was called motion synchronization by Pedersen *et al* [1, 2], but which we term self-bunching in this work, was tentatively explained as due to the interaction between the particles and some kinematical effects due to the special geometry of the trap.

In a typical experiment, an ion bunch, with kinetic energy of the order of several kiloelectronvolts, made of singly charged ions, is injected into an electrostatic ion beam trap [3–5]. The trap is made of two identical electrostatic mirrors composed of several cylindrically symmetric electrodes. The potential of each of these electrodes can be changed independently, so that various trapping potentials are possible. The distance between the innermost grounded electrodes of each mirror is 227 mm, so that the region between the mirrors is practically field-free. The number of ions in a bunch varies between 10^4 and 10^6 , corresponding to typical densities of between 5×10^3 and $5 \times 10^5 \text{ cm}^{-3}$. The typical oscillation time of the ions in the trap is a few microseconds. The bunch size and intensity is detected via a capacitive pickup electrode which produces a signal whose width is proportional to the bunch length.

When such a bunch is introduced into the trap, its bunch length usually increases rapidly, because of the reasons mentioned above, and reaches the trap size in a few hundred oscillations. However, under certain conditions which are related to the specific shape of the electrical

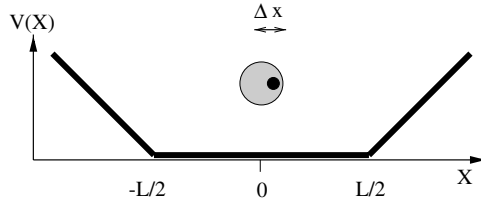


Figure 1. The one-dimensional potential used for the model. The charged particle (black dot) is located inside the homogeneously charged (same sign as for the particle) sphere, and both move in the potential well. The relative distance between the centre of the sphere and the test particle at the centre of the trap is Δx .

potential of the trap (as produced by the trapping electrodes), it has been observed that the bunch length can be stabilized to a finite value, which is much smaller than the trap length. A systematic study of this phenomenon was performed [2] and it was found that a necessary, but not sufficient, condition for this phenomenon to occur was that the dispersion of the trap, i.e. the derivative of the oscillation period (T) by the kinetic energy (E_0), had to be positive: $dT/dE_0 > 0$. Here we present a formal demonstration of this condition, and we show that the phenomenon belongs to a much larger class of behaviour which can be expected whenever classical interacting particles are bound by a soft wall potential.

2. The motion of bound interacting particles

We represent the motion of the particles in the trap using a one-dimensional model potential, as suggested by Pedersen *et al* [2], with sloping walls (see figure 1):

$$V(\mathcal{X}) = \begin{cases} 0, & \text{if } |\mathcal{X}| \leq L/2 \\ F(|\mathcal{X}| - L/2), & \text{if } |\mathcal{X}| > L/2 \end{cases} \quad (1)$$

where L is the length of the field-free region between the mirrors and F is the electric field generated by the potential wall, representing the field produced by the mirror electrodes in the real trap. To represent the motion of N charged particles of identical mass m and charge q we study the dynamics of a single (test) particle with mass m and charge q , relative to a homogeneously charged sphere of radius R_0 and mass Nm , with a charge density ρ so that its total charge is $Q = Nq$, where $N \gg 1$ (see figure 1).

The Hamiltonian for the system is given by

$$H = \frac{p_1^2}{2Nm} + \frac{p_2^2}{2m} + QV(x_1) + qV(x_2) + qU(x_1 - x_2), \quad (2)$$

where x_1 and x_2 are the coordinates of the sphere and test particle, respectively, relative to the centre of the potential well and p_1 and p_2 are their momenta. The interaction between the sphere and the test particle (as long as it is located inside the sphere) is given by

$$U(\Delta x) = \frac{1}{2}\mathcal{K}\Delta x^2 + U_0 \quad (3)$$

where $\Delta x = x_1 - x_2$, U_0 is a constant and $\mathcal{K} = -\rho q/3\epsilon_0$, where ϵ_0 is the vacuum permittivity. Assuming that $\Delta x < L$, we obtain the following simple equations of motion:

$$\Delta \dot{x} = \frac{\Delta p}{\mu} \simeq \frac{\Delta p}{m} \quad (4)$$

$$\Delta \dot{p} = -\frac{N}{N+1}\Delta x q V''(X) - \mathcal{K}\Delta x \simeq -\Delta x q V''(X) - \mathcal{K}\Delta x \quad (5)$$

where $\mu = Nm/(N + 1) \simeq m$ is the reduced mass, Δp is the conjugate momentum of Δx and X is the centre-of-mass coordinate.

We use mapping matrices, which propagate the system in the $(\Delta x, \Delta p)$ phase space, producing a Poincaré map at the centre of the trap to follow the particle motion. If we neglect the interaction between the sphere and test particle, we get the following mapping matrix M_T for a half-oscillation of the system in the trap:

$$\begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix}_n = (M_T)^n \begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix}_0 = (-1)^n \begin{pmatrix} 1 & \frac{T}{m^*} \\ 0 & 1 \end{pmatrix}^n \begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix}_0 \tag{6}$$

where $m^* = -m/\eta$ is the effective mass and

$$\eta = \frac{|P_0|}{T} \frac{dT}{d|P_0|}, \tag{7}$$

where P_0 is the initial centre-of-mass momentum and the half-oscillation time T is given by

$$T = \frac{2|P_0|}{F(Q + q)} + \frac{(M + m)L}{|P_0|}. \tag{8}$$

From equation (6), it is clear that Δx will grow as a function of the half-oscillation number n , unless $dT/d|P_0| = 0$, as in a harmonic potential. It is now possible to include the particle–particle interaction in the solution above, assuming that the force is small and does not change much during T . This yields an additional change in the relative momentum $\Delta p \rightarrow \Delta p - \mathcal{K}T \Delta x$, which can be expressed in matrix form as

$$M_i = \begin{pmatrix} 1 & 0 \\ -\mathcal{K}T & 1 \end{pmatrix} \tag{9}$$

yielding a complete propagation matrix:

$$M = M_T \cdot M_i = - \begin{pmatrix} 1 - \frac{\mathcal{K}T^2}{m^*} & \frac{T}{m^*} \\ -\mathcal{K}T & 1 \end{pmatrix}. \tag{10}$$

Note that the determinant of this matrix $\det(M) = 1$ (area preserving map [6]).

The necessary condition for which the relative motion in the phase space $(\Delta x, \Delta p)$ is bound for any value of the oscillation n is obtained by requiring $|\text{Trace}(M)| < 2$ [6]. Applying this to equation (10) yields the following general stability condition:

$$0 < \frac{\mathcal{K}T^2}{m^*} < 4. \tag{11}$$

An additional requirement is that the maximum distance between the centre of the sphere and the test particle is smaller than the radius of the sphere R_0 . The condition for this can be obtained from the largest deviation in the Δx coordinate in the Poincaré section produced by the mapping given in equation (10):

$$\Delta x_{\max}^2 = \frac{\Delta x_0^2 + \frac{\eta}{m} (\Delta x_0 \Delta p_0 T - \frac{p_0^2}{\mathcal{K}})}{1 + \frac{\eta \mathcal{K} T^2}{4m}} < R_0^2. \tag{12}$$

Assuming that \mathcal{K} is small (relative to $4m/(\eta T^2)$), which is the case relevant for both the experiment performed by Pedersen *et al* [1, 2] and the approximation used above, and letting $\Delta x_0 \approx R_0/2$, equation (12) can be written as

$$\rho > \frac{4\eta\epsilon_0 \Delta p_0^2}{mq R_0^2}, \tag{13}$$

where we have also used the fact that $R_0 \gg 2\eta p_0 T/3m$.

The results obtained in equations (11) and (13) demonstrate that the relative motion between the test particle and the sphere can, under certain conditions, be bound (self-bunching), and that such an effect is due to the combination of the ion–ion interaction and the special kinematics which are the result of the shape of the external potential $V(\mathcal{X})$. It can be shown that the exact dependence of the force on the particle–sphere distance is not critical, and that other dependencies would yield similar propagation matrices which, under the condition that the trace modulus is less than 2, yield an analogous condition to the one in equation (11).

For the inequality of equation (11) to be true when $\mathcal{K} < 0$ (repulsive interaction), the effective mass m^* must be negative. Such a requirement is equivalent to (see equation (7))

$$\eta > 0, \quad \text{or} \quad \frac{dT}{d|P_0|} > 0. \quad (14)$$

This result is similar to the condition stated by Pedersen *et al* (see equation (26) in [2]), which was shown to be in excellent agreement with both the experimental data and numerical simulations.

Equation (13) demonstrates that there is a minimum density required for stabilizing a bunch of particles of size $\sim 2R_0$. The dependence of the minimum charge density on Δp_0 is as expected, i.e. if the momentum spread of the particles is large, a higher charge density is required, in agreement with the simulation performed in [2]. A numerical evaluation of equation (13) for 4.2 keV Ar⁺ ions, with an energy spread of 1 eV, in a potential with $\eta = 0.5$ gives a minimal density of 100 cm⁻³, which is consistent with the ion densities 10³–10⁵ cm⁻³ used in the experiments [1, 2].

The approximation used above is valid only when the particle–sphere force is repulsive ($\mathcal{K} < 0$), as for an attractive force, an oscillatory motion is obtained and the assumption that the force is approximately constant during half an oscillation is incorrect. However, it is possible to solve the equations of motion exactly for both a particle–sphere attractive or repulsive interaction. In such a case, the mapping matrices are rather complicated (more details will be given in a future publication), but an analytical form for the stability condition can be obtained:

$$\left| \cos(\omega T) - \frac{\sin(\omega T)}{(1 + \eta)\omega T} + 4 \frac{\cos(\omega T) - \cos(\eta\omega T)}{(1 + \eta)^2(\omega T)^2} \right| < 1, \quad (15)$$

where $\omega = \sqrt{\mathcal{K}/m}$.

Figure 2 shows the stability condition graphically for various values of \mathcal{K}/m as a function of ηT^2 . This parametrization allows one to separate the quantities depending on the particle properties (\mathcal{K} and m) from the properties of the external potential (η and T). The shaded area represents the region of stability obtained under the impulse approximation, as given in equation (11) (for $\mathcal{K} < 0$ only), while the dots represent the region of stability as given by equation (15). Figure 2 shows clearly that, for $\mathcal{K} < 0$, the stability condition $\eta > 0$ holds as no stable configurations can be found in the lower left quarter of the plot. It is also interesting to point out that, for $\mathcal{K} > 0$, the system can be unbound, even though the force between the particle and the sphere is attractive.

3. Conclusions

The self-bunching effect described above (for $\mathcal{K} < 0$) is related to the so-called negative mass instability which was first introduced by Nielsen *et al* [7] for relativistic circular accelerators or storage rings, and extensively considered in a number of both experimental and theoretical works [8]. In these machines, the negative mass instability occurs when, for example, the angular velocity decreases with increasing energy, a situation occurring above the so-called

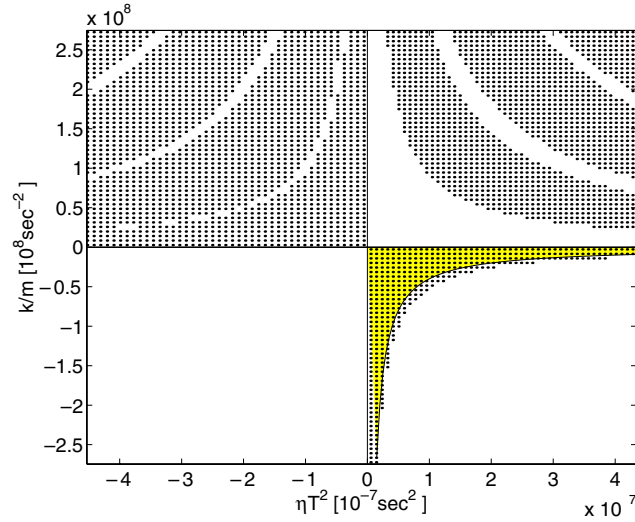


Figure 2. Stability diagram for the system described in figure 1. The shaded area represents the stability condition as expressed in equation (11) and the dots represent the stability condition obtained from the exact solution, equation (15).

transition energy. This effect has been, to our knowledge, observed only in accelerators working at relativistic energies, and the theoretical treatment has been implemented using the Vlasov equation [8].

However, unlike the large accelerators where the negative mass instability is a nuisance, it leads to an interesting application in the electrostatic trap. The self-bunching effect, discovered by Pedersen *et al* [1, 2] and theoretically explained here, shows that it is possible to trap a bunch without its size changing with time. Since the oscillation frequency of the ions in the trap is proportional to $\sqrt{q/m}$, and the shape of the signal induced by the bunch on the capacitive pickup near the centre of the trap is independent of trapping time, a measurement of the oscillation frequency directly yields a mass spectrum of the stored ions.

The application of our trap as a folded, time-of-flight (TOF) mass spectrometer, albeit without self-bunching, has been previously described [9]. A mass resolution of $\Delta m/m = 3.5 \times 10^{-4}$ for $m = 40$ was obtained. Figure 3 shows a frequency spectrum of data taken in the same instrument, in the self-bunching configuration. Two isotopes of xenon, $^{131}\text{Xe}^+$ and $^{132}\text{Xe}^+$, were injected into the trap with a kinetic energy of 4.2 keV. The signal from the pickup was recorded for 300 ms and the Fourier transform in figure 3 shows the seventh harmonics. The width of the peaks (about 1.5 channels wide) is <4 Hz, which corresponds to $\Delta m/m = 2\Delta f/f \sim 7 \times 10^{-6}$, while the distance between the peaks is consistent with the mass difference between the two isotopes. As the detection efficiency of the capacitive pickup is mass-independent, and trapping of very heavy species is possible in this electrostatic trap, such a system is well suited for heavy masses, where the detectors in standard TOF spectrometers are less efficient. In principle, the mass resolution is proportional to the measurement time, so that even higher resolution is feasible. In practice, however, there are several limiting factors. The most important one is the finite lifetime of the bunch in the trap (about 300 ms with the configuration described in [2]), which limits the overall measuring time to about 1 s at a background pressure of 5×10^{-10} Torr. In any case, the resolution obtained here is superior to the one obtained in standard TOF mass spectrometry [10] and

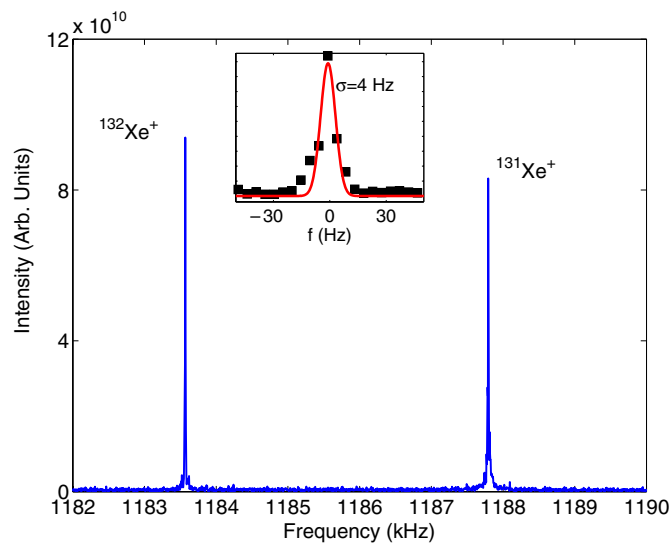


Figure 3. Frequency spectrum obtained by fast Fourier transform of the pickup signal when a bunch comprising two isotopes of singly charged xenon ions is injected into the trap. Only the seventh harmonics are shown. The inset shows an enhanced view of the left peak.

approaches the values measured using the Fourier transform ion cyclotron resonance (FTICR) technique [11], which is considered to be the most precise technique in general use available today, but requires superconductor magnets to achieve high resolution. Additional studies are needed to understand the limit of the mass separation: preliminary data show that, when the mass difference between two species is very small, they tend to produce a single bunch under the self-bunching conditions, a phenomenon known in FTICR as well, called peak coalescence [11].

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