A simple centripetal force model for explaining the focusing effect of ion funnels

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Abstract

The ion funnel is one of the key components for transferring ions from higher pressure into vacuum. While known for over twenty years and thoroughly analyzed by mathematical means and simulations, its working principle might be difficult to understand sometimes. In this work, we propose a simple thought experiment based on the centripetal force ions experience inside the ion funnel, which offers a simplistic explanation for the focusing force in an ion funnel. Our centripetal force model can predict the proportionalities of the resulting pseudopotential and should be a good didactical tool.

Keywords: Ion funnel; centripetal force model; focusing effect

Centripetal force model

Since their first description more than 20 years ago [1,2], ion funnels have been widely used in mass spectrometers with ionization sources that operate at higher pressure. The ability to focus ions at higher pressure into a small orifice allows for high gain in signal intensity of one to two orders of magnitude in comparison to standard orifice-skimmer interfaces [3,4]. This is not only true for research instruments; also commercial instruments have widely adopted this technology. Ion funnels are related to stacked ring radio frequency (RF) ion guides [5], which usually consist of a series of cylindrical ring electrodes of fixed inner diameter. A constant (DC) electrical field drives the ions axially through the ion guide towards the exit aperture. In addition, superimposed RF potentials of opposite polarity are applied to adjacent electrodes. The RF field creates a strongly repulsive effective potential near the surface of each electrode, repelling the ions and focusing the ion beam towards the center of the ion guide. The origin of such repulsive effective potentials near the electrodes seems to be the fundamental problem of understanding ion guides and ion funnels. An ion funnel is simply a stacked ring ion guide with continuously decreasing inner diameter, as shown in Figure 1, focusing the ions radially onto a small exit aperture.

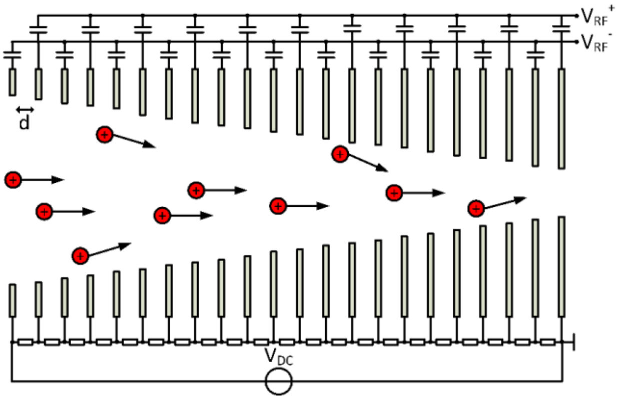

Figure 1: Schematic of an ion funnel. The electric DC field is created by a resistive voltage divider, while the RF field is capacitively coupled.

Starting from the very first publications, thorough analytical and numerical studies of the ion motion inside stacked ring ion guides and ion funnels have been published, leading to precise mathematical descriptions through the corresponding differential equations and resulting pseudopotentials describing the radial focusing of ions inside the ion guide [1,2,5–13]. Most importantly, Gerlich [5] derived the maximum value of the effective potential at the surface of the electrodes in the absence of collisions according to Eq. 1 [11].

$$V_{max} = \frac{q\,{V_{RF}}^2}{\frac{4}{\pi} m\, d^2 \omega^2} \quad (1)$$

Here, V_{RF} is the RF voltages amplitude, ω its angular frequency, m the ion mass, q the ion charge and d the distance between electrodes. Further considerations by Tolmachev et. al [2] include the influence of pressure on this result.

However, understanding the creation of a repulsive potential from a pure RF field and the resulting ion focusing force from the equations given in literature is, even when neglecting collisions with neutrals, most likely not trivial for everybody. Therefore, we propose a more intuitive thought experiment shown in Figure 2. It depicts two electrodes of an ion funnel or ion guide, the electric field lines related to the RF field and a model ion positioned on one of the field lines. Depending on the direction of the electric field, the ion will be accelerated in one of the directions marked by the vector $\vec{a}$, see Figure 2 (left). In the absence of collisions within the free path length at the given pressure, it will not follow the field line but rather its tangent due to mass inertia. As the field lines are convex, the tangent in either direction leads the ion away from the initial field line to another field line further away from the electrodes. Repeating this motion while being accelerated in alternating directions by the RF field leads to a zig-zag motion towards the center axis of the ion funnel, as shown in Figure 2 (right). The ion trajectory simulation shown here was carried out using the particle tracing module of COMSOL Multiphysics 5.1.

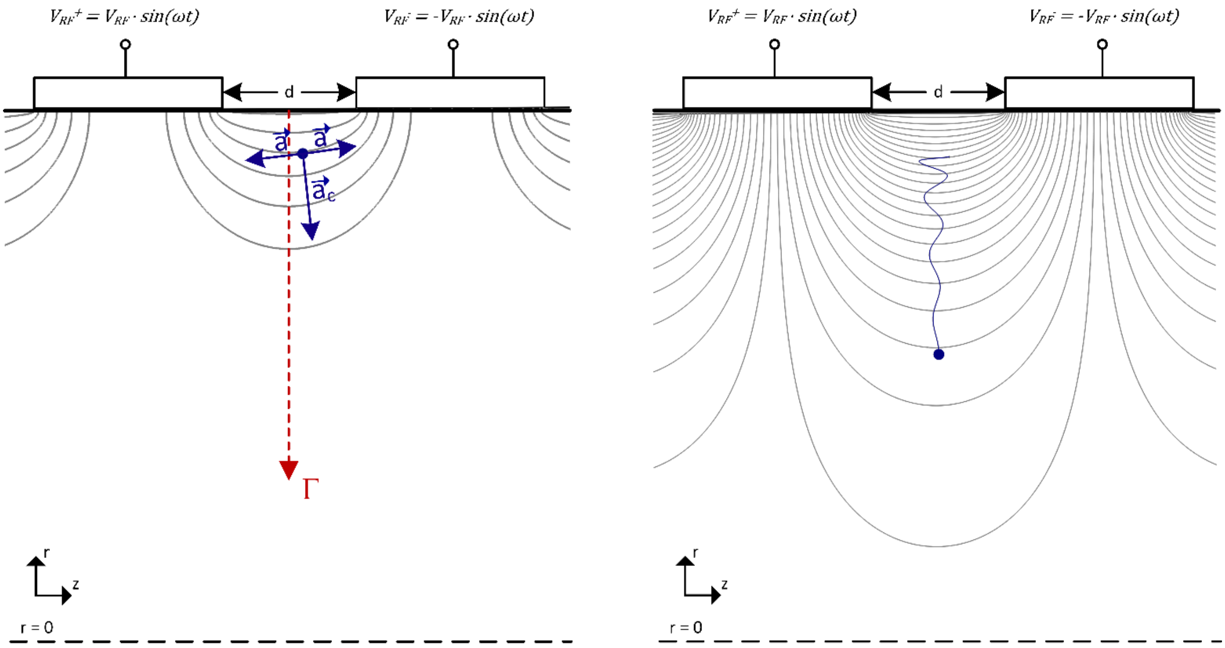

Figure 2: Left: Model ion positioned between two electrodes of an ion funnel. The ion is accelerated in the direction $\vec{a}$ by the electric RF field, leading to an additional effective motion in the direction $\vec{a}_c$ due to centripetal force. The electric field strength depends on the distance from the electrode surface Γ. Right: Simulated ion trajectory for four periods of the RF voltage. Electrode width: 1 mm, distance between two adjacent electrodes d = 0.75 mm, RF voltage amplitude V_{RF} = 50 V, DC voltage V_{DC} = 0V, angular frequency $\boldsymbol{\omega = 2\pi \cdot 2MHz}$, single charged model ion with mass 500 u.

However, while this seems to be a physically sound explanation, does it also lead to the same parameter dependencies of the ion focusing effect described by Eq. 1? Let us assume a sine voltage with amplitude V_{RF} and angular frequency ω is applied between the two electrodes. The field lines near the electrodes are somewhat circular as shown in Figure 2 and thus the length of a field line is proportional to its distance from the electrode surface Γ. Therefore, the electric field E is given by Eq. 2.

$$E \sim \frac{V_{RF}}{\Gamma}\sin(\omega t) \quad (2)$$

This electric field creates a coulomb force periodically accelerating the model ion based on its mass m and charge q as given by Eq. 3.

$$a \sim \frac{q}{m}E = \frac{q}{m}\frac{V_{RF}}{\Gamma}\sin(\omega t) \quad (3)$$

This periodic acceleration a will lead to the oscillating velocity v given by Eq. 4, which is found by integrating Eq. 3 assuming no initial ion velocity.

$$v \sim \frac{q}{m}\frac{V_{RF}}{\Gamma}\frac{1}{\omega}\cos(\omega t) \quad (4)$$

Due to inertia, the ion starts deviating from the circular field line, as it continues to move in a straight line. This deviation depends on the centripetal acceleration a_c that would be needed to keep the ion on its circular field line as shown by Eq. 5.

$$a_c \sim \frac{v^2}{\Gamma} \sim \frac{q^2 {V_{RF}}^2}{m^2\Gamma^3\omega^2}\cos^2(\omega t) \quad (5)$$

To compare this result with the known Eq. 1 for the pseudopotential, it is necessary to derive an average acceleration that can be converted to such a pseudopotential. While the acceleration points in different directions depending on the ion position, its average direction is pointing perpendicular to the electrode surface towards the center of the ion funnel. Just considering the proportionality between the average acceleration and the instantaneous acceleration, the direction of the instantaneous acceleration can be omitted during averaging. Thus, the average acceleration over one period $a_{c,avg}$ is given by Eq. 6.

$$a_{c,avg} = \frac{1}{T}\int_0^T a_c(t)dt = \frac{1}{T}\cdot\frac{q^2 {V_{RF}}^2}{m^2\Gamma^3\omega^2}\cdot\frac{T}{2} \sim \frac{q^2 {V_{RF}}^2}{m^2\Gamma^3\omega^2} \quad (6)$$

The average acceleration $a_{c,avg}$ can be converted to a coulomb force considering the ion mass m, and this force can be converted to an electric field strength E_c considering the ion charge q given by Eq. 7.

$$E_c \sim a_{c,avg}\frac{m}{q} \sim \frac{q\,{V_{RF}}^2}{m\,\Gamma^3\omega^2} \quad (7)$$

Now, it is necessary to integrate Eq. 7 across the distance from the electrode surface Γ to derive the maximum pseudopotential generated by this electric field. As the field can be neglected for large distances Γ, the lower limit of integration is set to infinity. The smallest possible distance from the electrode surface, where the field lines still show a circular shape necessary for focusing, depends on the electrode distance d. Thus, we integrate to some multiple k of d, leading to the pseudopotential V_c^* given by Eq. 8. The value of k is not of importance for the proportionality.

$$V_c^* \sim \int_{\infty}^{k\cdot d} E_c \,\mathrm{d}\Gamma \sim \frac{q\, {V_{RF}}^2}{m\, d^2 \omega^2} \quad (8)$$

This pseudopotential V_c^* has identical dependencies on the amplitude of the RF voltage V_{RF}, the ion charge q, the ion mass m, the distance between electrodes d and the angular frequency ω as the pseudopotential given by Eq. 1, which was derived by solving the differential equations neglecting ion-neutrals collisions.

However, to understand the focusing effect of ion funnels completely, the consideration of ion-neutral collisions is essential. It is well known that the transmission efficiency of ion funnels is a function of neutral background gas density since ion-neutral collisions are required to effectively confine energetic ion motion in multipole RF devices, known as the collisional focusing effect [2,14]. This effect increases with gas pressure up to a point where ion scattering becomes the dominant process. Thus, ion funnels typically work in a pressure range from 1 to 10 Torr [8,15].

From the pictured ions motions in this paper, it is also possible to understand the influence of neutral background gas density. When looking at the ion in Figure 2, it is clear that due to the lower curvature of the field lines, the acceleration will decrease when approaching the center axis of the ion funnel. The ion's momentum however, will be retained. Thus, when reaching the axis of the ion funnel, it will still be moving at considerable speed in radial direction and thus reach a distance from the axis equal to its starting distance. This process will repeat in reverse direction, leading to radial oscillations and thus a wide ion beam, as shown in the left part of Figure 3.

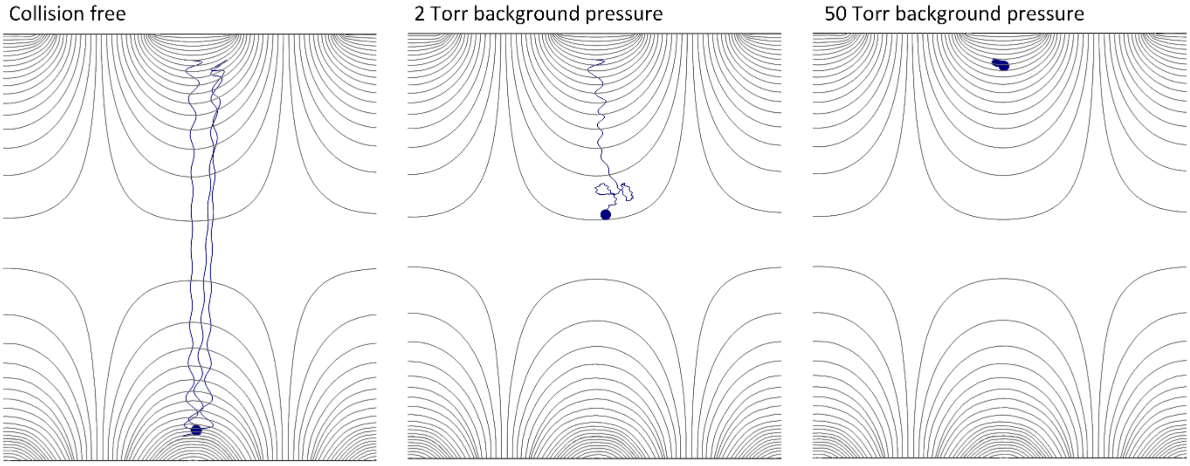

Figure 3: Simulated ion trajectory for 35 periods of the RF voltage at various background pressures. Other conditions are identical to Figure 2: Electrode width: 1 mm, distance between two adjacent electrodes d = 0.75 mm, RF voltage amplitude V_{RF} = 50 V, DC voltage V_{DC} = 0V, angular frequency $\boldsymbol{\omega = 2\pi \cdot 2MHz}$, single charged model ion with mass 500 u.

With increasing density of neutral gas molecules, these will collide with the ion, leading to a loss of its velocity. This dampens the oscillation in radial direction and thus sharpens the ion beam, as illustrated in the center part of Figure 3. However, when the neutral gas density increases even further, it will also dampen the oscillation along the field lines, leading to a loss of focusing as shown in the right part of Figure 3. The determining factor here is the ratio between the average time τ between collisions and the period of the RF voltage, as the shorter one limits the acceleration period. When τ becomes comparable with the period of the RF voltage, the angular frequency ω in Eq. 8 can be replaced by the geometric mean of the two frequencies ω and τ^{-1} leading to an effective angular frequency ω_{eff}.

$$\omega_{eff} = \sqrt{\omega^2 + \frac{1}{\tau^2}} \quad (9)$$

Substituting ω in Eq. 8 by ω_{eff} results in the pressure dependent coefficient originally introduced by Tolmachev et. al. [2].

$$V_{c,eff}{}^{*} \sim \frac{1}{\omega^2 + \frac{1}{\tau^2}} \cdot \frac{q\, V_{RF}{}^{2}}{m\, d^2} = \frac{\omega^2\tau^2}{1+\omega^2\tau^2} \cdot \frac{1}{\omega^2} \cdot \frac{q\, V_{RF}{}^{2}}{m\, d^2} = \frac{\omega^2\tau^2}{1+\omega^2\tau^2} \cdot V_c^{*} \quad (10)$$

Eq. 10 shows that the influence of ion-neutral collisions on the pseudopotential V_c^{*} becomes significant for $\omega\tau \leq 1$.

Conclusion

In this paper, we presented a simple model for explaining the origin of the focusing force of an ion funnel based on a centripetal force approximation. Despite being rather simplistic, it predicts the same proportionalities as derived from solving the full differential equations. However, being more vivid, we hope our centripetal force model may help understanding the focusing characteristics of ion funnels.

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