Numerical and Graphical Description of Ion Motions in a Penning Trap for Mass Measurements (Postprint)

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Abstract

The ion motions in a Penning trap have been studied in detail in the presence of azimuthal dipolar and quadrupolar radio-frequency excitations and buffer gas cooling. The numerical solutions by using the Runge-Kutta method and thus the pictures of the ion trajectories in the trap have been obtained for different cases and summarized in graphical form. For the recentering of the ion of interest and to perform the purification of the ion species, one has to set a reasonable buffer gas pressure in the trap and apply azimuthal quadrupolar excitation at frequency ωrf = ωc.

Full Text

Preamble

Numerical and graphical description of ion motions in a Penning trap for mass measurements

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Abstract

The ion motions in a Penning trap have been studied in detail under the influence of azimuthal dipolar and quadrupolar radio-frequency excitations combined with buffer gas cooling. Numerical solutions obtained using the Runge-Kutta method have yielded ion trajectory images in the trap for various cases, which are summarized in graphical form. For recentering the ion of interest and performing purification of ion species, one must set an appropriate buffer gas pressure in the trap and apply azimuthal quadrupolar excitation at frequency ωrf = ωc.

Keywords: Ion trap, ion motion, ion trajectory, numerical description, mass measurement

1. Introduction

Penning traps have become highly accurate tools for mass determination of both stable and unstable isotopes. Numerous Penning traps are currently in operation or under construction worldwide, including ISOLTRAP [?] at CERN, SHIPTRAP [?] at GSI, LEBIT [?] at MSU, CPT [?] at ANL, JYFLTRAP at JYFL [?], and others. At the Institute of Modern Physics, Chinese Academy of Sciences, the LPT (Lanzhou Penning Trap) is also under construction [?].

In an ideal Penning trap, an ion is confined by the combination of an electrostatic quadrupolar field and a homogeneous magnetic field, and its motion is a superposition of three eigenmotions: an axial oscillation (z) with frequency ωz and two radial motions commonly referred to as reduced cyclotron (+) and magnetron motions (−) with frequencies ω+ and ω−, respectively. To measure the ion's mass with high precision, one common method involves performing buffer gas cooling and radio-frequency (rf) excitations to remove unwanted ions from nuclear reactions and other sources. This method has been employed in many Penning traps.

The ion motion can be driven by oscillating electric fields, which generally results in changes to the amplitudes of the eigenmotions. The effect of the driving field on ion motion depends on the multipolarity of the field and its frequency. A dipole field at one of the eigenfrequencies can be used to increase the amplitude of the corresponding eigenmotion, and dipolar excitation at ωrf = ω− is generally a crucial step for removing unwanted ions. When an ion is excited by a quadrupolar field with frequency ωrf = ωc, where ωc is the cyclotron frequency of the ion, the magnetron and cyclotron motions are continuously converted into each other, a technique always used to determine the true value of ωc. If all three eigenfrequencies are measured, the invariance theorem of Brown and Gabrielse [?] can be applied.

Cooling of stored ions results in reduction of motional amplitudes, allowing cooled ions to be trapped in a much smaller volume and thus probe fewer imperfections in the trapping electric and magnetic fields. The technique of buffer gas cooling is commonly applied to radioactive ions stored in Penning traps, with noble gases typically used due to their high ionization potential and thus minimal losses from charge exchange.

An ion confined in a Penning trap experiences forces from both the electrostatic and magnetic fields, as well as the effects of rf excitation and buffer gas. The equations of ion motion become very complicated and are extremely difficult to solve analytically without approximation. Starting from analytical solutions, Bollen et al. [?] described ion trajectories under different excitation scenarios qualitatively and identified important sources of uncertainty in high-precision mass measurements of heavy ions. Savard et al. [?] presented ion trajectories in Penning traps with buffer gas, obtained from Runge-Kutta integration of the relevant equations of motion, and demonstrated the effect of buffer gas cooling experimentally. König et al. [?] investigated ion motion in the presence of an azimuthal quadrupolar rf field and buffer gas cooling, observing excellent agreement between theoretical results and experimental data.

In this paper, we solve the equations of ion motion numerically using the Runge-Kutta method, obtain ion trajectories in the trap for many different cases, and summarize these trajectories in graphical form to help understand the physical picture in a Penning trap.

2. Dynamical equations of ion motion

Figure 1 [Figure 1: see original paper] shows the schematic layout of a typical Penning trap. In an ideal Penning trap, a charged particle with mass m and charge q is confined by the combination of a homogeneous magnetic field $\vec{B} = B\hat{e}_z$ and an axial quadrupolar potential $\Phi(z,\rho) = \frac{U_0}{2d^2}(z^2 - \frac{\rho^2}{2})$, where U_0 is the applied trapping voltage between the ring electrode and the two endcap electrodes, and d describes the trap dimension defined by $d = \sqrt{\frac{\rho_0^2}{4} + \frac{z_0^2}{2}}$, with ρ_0 being the inner radius of the ring electrode and $2z_0$ the distance between the endcaps.

The forces acting on the ion in the trap are:

$$m\ddot{\vec{z}} = q\vec{E}_z \cdot \hat{e}_z$$

$$m\ddot{\vec{\rho}} = q(\vec{E}_\rho + \dot{\vec{\rho}} \times \vec{B})$$

where $\vec{E}_z = -\frac{U_0}{d^2} z\hat{e}_z$ and $\vec{E}_\rho = \frac{U_0}{2d^2}\rho\hat{e}_\rho$.

Therefore, the axial motion is a harmonic oscillation parallel to the magnetic field with frequency $\omega_z = \sqrt{\frac{qU_0}{md^2}}$, and the radial motion is a superposition of two eigenmotions with frequencies:

$$\omega_\pm = \frac{1}{2}\left(\omega_c \pm \sqrt{\omega_c^2 - 2\omega_z^2}\right)$$

where $\omega_c = \frac{qB}{m}$.

To remove unwanted ions and measure the ion's mass, one method is to perform buffer gas cooling and rf excitations on the ion. This makes the equations of ion motion more complicated than in the ideal case mentioned above.

A dipole field is created by applying an rf voltage with amplitude V_d and frequency ω_{rf} with a 180° phase difference between two opposite segments of the ring electrode, producing an additional electric field [?, ?]. For example, for the radial x-component:

$$\vec{E}_x = \frac{V_d}{a}\cos(\omega_{rf}t - \phi_{rf}) \cdot \hat{e}_x$$

where a is the inner radius of the trap.

An azimuthal quadrupolar rf field with amplitude V_q and frequency ω_{rf} is applied with 180° phase shifts on sets of ring-electrode segments perpendicular to each other, giving an additional electric field [?]:

$$\vec{E}_x = \frac{2V_q}{a^2}\cos(\omega_{rf}t - \phi_{rf}) \cdot y\hat{e}_x$$

$$\vec{E}_y = \frac{2V_q}{a^2}\cos(\omega_{rf}t - \phi_{rf}) \cdot x\hat{e}_y$$

where $\hat{e}_x$ and $\hat{e}_y$ are the unit vectors along the x and y axes, respectively.

Zhu et al. [?] studied the energy limitations for models simulating buffer gas cooling and suggested that the viscous drag force model should be used when the ion's energy is less than ~5 eV/u. Thus, the effect of buffer gas on ion motion in a Penning trap can be described as:

$$\vec{F} = -\delta m\vec{v}$$

where δ is the damping parameter describing the effect of the buffer gas. With the ion mobility K_0, δ can be expressed as:

$$\delta = \frac{q}{m}\frac{1}{K_0}\frac{P}{T}\frac{T_N}{P_N}$$

Here, q/m is the ion's charge-to-mass ratio, and P and T are the gas pressure and temperature in units of normal pressure P_N and temperature T_N [?], respectively.

The dynamical equations including all effects from dipolar rf excitation and buffer gas cooling can be written as:

$$\begin{cases} \ddot{x} - \frac{qU_0}{2md^2}x - \frac{qB}{m}\dot{y} + \delta\dot{x} = \frac{qV_d}{ma}\cos(\omega_{rf}t - \phi_{rf}) \\ \ddot{y} - \frac{qU_0}{2md^2}y + \frac{qB}{m}\dot{x} + \delta\dot{y} = 0 \\ \ddot{z} + \frac{qU_0}{md^2}z + \delta\dot{z} = 0 \end{cases}$$

And those for quadrupolar excitation and buffer gas cooling:

$$\begin{cases} \ddot{x} - \frac{qU_0}{2md^2}x - \frac{qB}{m}\dot{y} + \delta\dot{x} = \frac{2qV_q}{ma^2}\cos(\omega_{rf}t - \phi_{rf}) \cdot y \\ \ddot{y} - \frac{qU_0}{2md^2}y + \frac{qB}{m}\dot{x} + \delta\dot{y} = \frac{2qV_q}{ma^2}\cos(\omega_{rf}t - \phi_{rf}) \cdot x \\ \ddot{z} + \frac{qU_0}{md^2}z + \delta\dot{z} = 0 \end{cases}$$

Here, the first part describes ion motion in an ideal Penning trap, the second part arises from the dipolar/quadrupolar rf electric field, and the third part originates from buffer gas cooling.

As these are nonlinear differential equations, obtaining an analytic solution is difficult. The known method involves using variable substitution twice ($\vec{V}^{\pm}(t) = \dot{\vec{\rho}}(t) - \omega_{\mp}\vec{\rho}(t) \times \hat{e}_z,\ \vec{A}^{\pm}(t) = \vec{V}^{\pm}(t)e^{\mp i(\omega_{\pm}t+\phi_{\pm})}$) and neglecting high-frequency terms [**?**, **?**]. Here, we obtain the numerical solution of the above equations using the Runge-Kutta method.

3. Numerical solution by the Runge-Kutta method

The common fourth-order Runge-Kutta method is used to obtain numerical solutions of ion motions in a Penning trap. Specifying the first-order differential equation in the form $y'(t) = f(t, y)$ and defining its initial value as $y(t_0) = y_0$, the following equations are introduced:

$$y_{k+1} = y_k + \frac{h}{6}(f_1 + 2f_2 + 2f_3 + f_4)$$

$$t_{k+1} = t_k + h$$

where h is the time interval, y_{k+1} is the approximation of $y(t_{k+1})$, and:

$$\begin{cases} f_1 = f(t_k, y_k) \\ f_2 = f(t_k + \frac{h}{2}, y_k + \frac{h}{2}f_1) \\ f_3 = f(t_k + \frac{h}{2}, y_k + \frac{h}{2}f_2) \\ f_4 = f(t_k + h, y_k + hf_3) \end{cases}$$

Studies show that the error per step is on the order of h^5, while the total accumulated error has order h^4 [**?**, **?**]. Four slopes corresponding to each dependent variable need to be calculated using the same method mentioned above. Equations (7) and (8) can be rewritten as first-order differential equations by defining new variables $x_1 = \dot{x}$ and $y_1 = \dot{y}$.

Table 1 shows parameters used in the calculations. A proper interval value h was chosen to reduce accumulated error and computation time. The parameters B, U_0, d, and a for the LPT [**?**, **?**] are used. To clearly demonstrate excitation effects, larger values were chosen for V_d (driving rf amplitude for dipolar excitation), V_q (for quadrupolar excitation), and P (helium buffer gas pressure for cooling). Trajectories for ions with mass 200 u have been obtained for many different cases.

3.1. Axial motion

Figure 2 [Figure 2: see original paper] shows ion trajectories in the axial direction along the magnetic field as a function of elapsed time. Without buffer gas

(Figure 2(a)), the motion is a harmonic oscillation with frequency ω_z that can be obtained from the analytic solution of equation (1). However, with buffer gas present, obtaining an analytic solution without approximation becomes difficult. The numerical solution (Figure 2(b)) shows that the ion experiences damped vibration, with its distance from the trap center decreasing continuously until the ions are concentrated very close to the trap center.

3.2. Radial motion without excitation

In an ideal trap without excitation fields and without buffer gas, radial motion is a superposition of reduced cyclotron motion with frequency ω_+ and magnetron motion with frequency ω_-. The ion trajectory is shown in Figure 3 Figure 3: see original paper. The cyclotron radius depends on the ion's initial velocity—the greater the initial velocity, the larger the cyclotron radius. The magnetron radius depends on the initial distance from the trap center, with greater distances producing larger magnetron radii. Without buffer gas, the cyclotron and magnetron motions maintain their initial status. With buffer gas present, the cyclotron motion is damped while the magnetron motion increases steadily but slowly, as shown in Figure 3(b).

3.3. Radial motion with azimuthal dipolar excitation

The phase of the exciting dipolar rf field relative to the initial magnetron motion has a very strong effect on the magnetron radius [**?**, **?**]. Depending on this phase difference, one may actually decrease the magnetron radius. In all calculations shown in this section, we choose the phase difference as the most favorable value to enhance the magnetron radius.

Figures 4 Figure 4: see original paper and (b) show ion trajectories in the radial direction when azimuthal dipolar excitation is applied at $\omega_{rf} = \omega_-$, for cases without and with buffer gas cooling, respectively. The buffer gas has no obvious effect on the magnetron motion, and its amplitude increases continuously. Moreover, all ions can be driven to a larger radius by this azimuthal dipolar excitation because the first-order approximation of ω_- is independent of the ion's mass. For the cyclotron motion, its amplitude becomes progressively smaller when buffer gas is present.

Figures 4(c) and (d) show similar results to Figures 4(a) and (b), but with dipolar excitation applied at $\omega_{rf} = \omega_+$. Clearly, the dipolar field drives the cyclotron motion while the magnetron motion remains constant without buffer gas. With buffer gas present, the cyclotron motion amplitude is damped while the magnetron motion amplitude increases slowly and continuously.

When dipolar excitation is applied at frequencies other than ω_- and ω_+, the picture becomes more complex because other sidebands, such as $2\omega_-$ and $2\omega_+$, may occur. However, if excitation is performed at frequencies other than these particular values, the field does not drive the cyclotron or magnetron motion and has almost no effect on ion trajectories. The ion trajectories shown in Figures

4(e) and (f) are very similar to those obtained without any excitation (Figure 3).

3.4. Radial motion with azimuthal quadrupolar excitation

Figure 5 [Figure 5: see original paper] shows ion trajectories in the radial direction when azimuthal quadrupolar excitation is applied at the resonant mode, $\omega_{rf} = \omega_c = \omega_+ + \omega_-$, and at the non-resonant mode, $\omega_{rf} \neq \omega_c$, for cases without and with buffer gas cooling. Initially, there is only magnetron motion. Without buffer gas, the two eigenmotions are coupled and full periodic conversion between the two motions occurs after a certain time (depending on the excitation amplitude V_q). For non-resonant excitation, the conversion is incomplete. By scanning the frequency of this quadrupolar excitation, the coupled cyclotron frequency can be obtained using the time-of-flight ion cyclotron resonance (TOF-ICR) detection technique [**?**], and the ion mass can then be calculated using equation (4). This is the typical method used for mass measurement in most Penning traps worldwide.

When buffer gas is present in the trap, the ion behavior becomes quite different. When in resonance, if a reasonable buffer gas pressure is applied, both cyclotron and magnetron motions decrease as a function of time, and eventually the ion returns to the trap center. Conversely, when out of resonance, the ion continues moving in a larger orbit and never returns to the center. Thus, this mass-selective centering can be used to purify ion species, with contaminants being lost through a very small pore during ion transportation.

In fact, when in resonance, the decrease of motional amplitudes as a function of time depends heavily on the damping constant. This has not been studied in detail and has been overlooked in previous research papers. Figure 6 [Figure 6: see original paper] shows ion trajectories in the radial direction when azimuthal quadrupolar excitation is applied at the resonant mode with different buffer gas pressures. When the buffer gas pressure in the trap is too low (Figure 6(a)), some periodic conversion can still occur because the gas cannot cool the ion fast enough. As the pressure increases, the ion can be cooled more rapidly, and both cyclotron and magnetron motions decrease as a function of time until the ion returns to the trap center (Figure 6(c)). However, if the buffer gas pressure is too high, the increase in magnetron radius becomes significant, and the ion never returns to the center (Figure 6(e)). Therefore, to use this method for recentering the ion of interest and purifying ion species, one must set a reasonable buffer gas pressure.

Figure 7 [Figure 7: see original paper] shows the centering time as a function of helium buffer gas pressure P and driving rf amplitude V_q for azimuthal quadrupolar excitation. All excitations are performed at $\omega_{rf} = \omega_c$, and all ions start at the point (1.0 mm, 0.0 mm). The centering time is defined as the time when the distance between the ion's position and the trap center has decreased to less than 0.1 mm for 0.1 ms, which we consider as recentering. Obviously, to obtain a shorter centering time, one must find a reasonable combination of P and V_q. In our calculations, when different buffer gases such as helium, neon, and argon are used, the corresponding shortest centering times are found to be 0.36 ms at ~10 Pa and ~28 V, 0.53 ms at ~5 Pa and ~28 V, and 0.90 ms at ~0.5 Pa and ~16 V, respectively. As heavier buffer gas is used, the optimal gas pressure becomes lower, possibly due to increased stopping power. For lower buffer gas pressure, the centering time becomes longer, but too much buffer gas causes the ion to move to a larger radius. The amplitude of the driving rf field also affects the centering time, but we cannot apply a very high amplitude in practice because it distorts the electric field in the trap too much. Therefore, to achieve a reasonable centering time in a real experiment, we recommend that the helium gas pressure should be set in the range of 0.01–5 Pa and the driving rf amplitude for quadrupolar excitation should be set in the range of 2–15 V.

4. Summary

Penning traps have become highly accurate tools for mass determination of both stable and unstable isotopes. To manipulate ions in the trap, azimuthal dipolar and quadrupolar rf excitations and buffer gas cooling must be applied, making ion motions very complicated and analytic solutions impossible to obtain without approximation. We have studied in detail the numerical solutions of ion motions using the Runge-Kutta method for different cases applicable to high-precision mass measurement experiments. The ion trajectories in the trap for these various cases have been obtained and summarized in graphical form.

Ion motion in the trap depends heavily on the multipolarity of the rf field, its frequency, and the buffer gas pressure. Azimuthal dipolar excitation at frequency $\omega_{rf} = \omega_-$ can be used to drive all ions to a larger radius. Azimuthal quadrupolar excitation at frequency $\omega_{rf} = \omega_c$ without buffer gas is generally used to measure ion mass. For recentering the ion of interest and performing purification of ion species, one must set a reasonable buffer gas pressure in the trap and apply quadrupolar excitation at frequency $\omega_{rf} = \omega_c$.

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Figure Captions

Figure 1 [Figure 1: see original paper]: Schematic layout of a typical Penning trap.

Figure 2 [Figure 2: see original paper]: Axial ion trajectories in a plane along the magnetic field as a function of elapsed time. (a) without buffer gas; (b) with helium buffer gas at a pressure of 5 Pa.

Figure 3 [Figure 3: see original paper]: Radial ion trajectories in a plane perpendicular to the magnetic field without excitation. The trap center is at the point (0, 0) marked as a cross, and the ion starts at the point (1.0 mm, 0.0 mm). (a) without buffer gas; (b) with helium buffer gas at a pressure of 5 Pa. Note that the ion moves in a clockwise direction.

Figure 4 [Figure 4: see original paper]: Same as figure 3, but with azimuthal dipolar excitation. The left panels are obtained without buffer gas, and the right panels are with helium buffer gas at a pressure of 5 Pa. (a) and (b): $\omega_{rf} = \omega_-$; (c) and (d): $\omega_{rf} = \omega_+$; (e) and (f): $\omega_{rf} \neq \omega_-, \omega_+$ or other sidebands. Note that the ion moves in a clockwise direction.

Figure 5 [Figure 5: see original paper]: Same as figure 3, but with azimuthal quadrupolar excitation. Initially there is only magnetron motion. The left and middle panels are obtained without buffer gas, and the right panels are with helium buffer gas at a pressure of 5 Pa. (a) and (b): $\omega_{rf} = \omega_c$; (c) and (d): $\omega_{rf} \neq \omega_c$. (a1) and (a2) show the first and second half of the conversion. Note that the ion moves in a clockwise direction.

Figure 6 [Figure 6: see original paper]: Same as figure 3, but with azimuthal quadrupolar excitation at $\omega_{rf} = \omega_c$ and with helium buffer gas at pressures of (a) 0.05 Pa, (b) 0.5 Pa, (c) 5 Pa, (d) 30 Pa and (e) 50 Pa. Initially there is only magnetron motion. (a1)–(a3) and (b1)–(b3) show successively the ion trajectories with helium buffer gas at pressures of 0.05 Pa and 0.5 Pa, respectively. Note that the ion moves in a clockwise direction.

Figure 7 [Figure 7: see original paper]: (color online) The centering time T as functions of helium buffer gas pressure P and driving rf amplitude V_q for azimuthal quadrupolar excitation. All excitations are performed at $\omega_{rf} = \omega_c$.

Table Caption

Table 1 : Parameters used in the calculation. a (mm), m (u), d (mm), U_0 (V), P (Pa).

Note: Figure translations are in progress. See original paper for figures.

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