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Numerical and graphical description on the 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 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 $\omega_{rf} = \omega_c$.

1. Introduction

Penning traps have become very accurate tools for mass determination both on stable and unstable isotopes. There are many Penning traps which are in operation or under construction all over the world, such as ISOLTRAP [1] in CERN, SHIPTRAP [2] in GSI, LEBIT [3] in MSU, CPT [4] in ANL, JYFLTRAP in JYFL [5] and so on. At the Institute of Modern Physics, Chinese Academy of Sciences, the LPT (Lanzhou Penning Trap) is also under construction [6].

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

The ion motion can be driven by oscillating electric fields and this in general results in a change of the amplitudes of the eigenmotions. The effect of the driving field on the 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 this dipolar excitation at $\omega_{rf} = \omega_-$ is generally a significant step to remove the unwanted ions. If ion is excited by a quadrupolar field with a frequency $\omega_{rf} = \omega_c$, where ω_c is the cyclotron frequency of the ion, the magnetron motion and cyclotron motion will be continuously converted into each other, and this is always used to determine the true value of ω_c. If all three eigenfrequencies are measured, the invariance theorem of Brown and Gabrielse [7] can be used.

Cooling of stored ions results in a reduction of the motional amplitudes, and the cooled ions can be trapped in a much smaller volume and thus probe less of the imperfections in the trapping electric and magnetic fields. The technique of buffer gas cooling is commonly applied for radioactive ions stored in a Penning trap, and noble gases are typically used because of their high ionization potential and thus minimum losses due to charge exchange.

So an ion confined in a Penning trap will experience the forces from both the electrostatic field and the magnetic field, and the effects of rf excitation and buffer gas. The equations of ion motion become very complicated and it is very difficult to solve them analytically without any approximation.

Starting from analytical solution, Bollen et al. [8] described ion trajectories under different excitation scenarios qualitatively and identified the important causes of uncertainty in high-precision mass measurements of heavy ions. Savard et al. [9] presented ion trajectories in Penning traps in the presence of buffer gas from Runge–Kutta integration of the relevant equations of motion and

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demonstrated experimentally the effect of buffer gas cooling. König et al. [10] investigated the ion motion in the presence of an azimuthal quadrupolar rf field and buffer gas cooling and excellent agreement was observed between theoretical results and experimental data.

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

2. Dynamical equations of ion motion

Fig. 1 shows the schematic layout of a typical Penning trap. In an ideal Penning trap a charged particle with a mass of m and a charge of q is confined by the combination of a homogeneous magnetic field $\overrightarrow{B}=B\hat{e_z}$ and an axial quadrupolar potential $\Phi(z,\rho)=(U_0/(2d^2)(z^2-\rho^2/2)$, where U_0 is the applied trapping voltage between the ring electrode and the two endcap electrodes, d describes the dimension of the trap and is defined by $d=\sqrt{2z_0^2+\rho_0^2}/2$, where ρ_0 is the inner radius of the ring electrode and $2z_0$ the distance between the endcaps. The forces that the ion in the trap will suffer are

$$\begin{cases} m\ddot{\overrightarrow{z}}=q\overrightarrow{E_z} \\ m\ddot{\overrightarrow{\rho}}=q(\overrightarrow{E_\rho}+\dot{\overrightarrow{\rho}}\times\overrightarrow{B}), \end{cases} \tag{1}$$

where $\overrightarrow{E_z}=-U_0/d^2\cdot z\hat{e_z}$ and $\overrightarrow{E}_\rho=U_0/(2d^2)\cdot\rho\hat{e_\rho}$. Therefore, the axial motion is a harmonic oscillation parallel to the magnetic field with a frequency of

$$\omega_z=\sqrt{\frac{qU_0}{md^2}}, \tag{2}$$

and the radial motion is a superposition of two eigenmotions with frequencies of

$$\omega_\pm=\frac{\omega_c}{2}\pm\sqrt{\frac{\omega_c^2}{4}-\frac{\omega_z^2}{2}}, \tag{3}$$

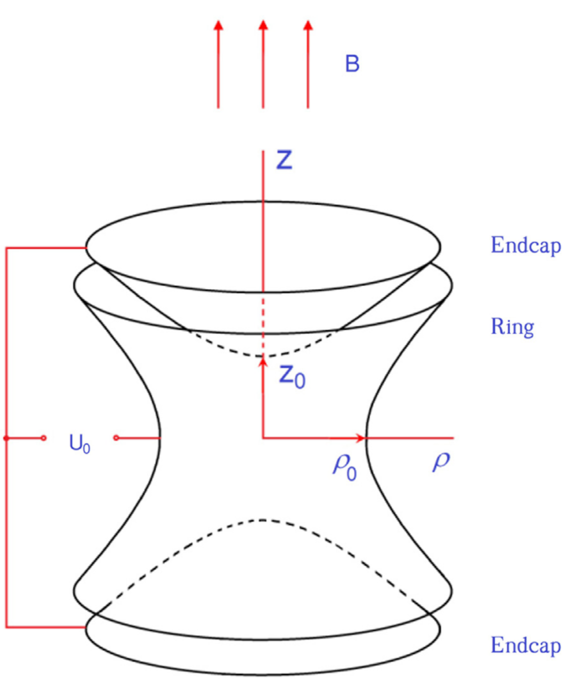

Fig. 1. Schematic layout of a typical Penning trap.

where

$$\omega_c=\frac{q}{m}B. \tag{4}$$

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

A dipole field is created by an rf voltage with amplitude V_d and frequency ω_{rf} applied with a phase difference of 180° between two opposite segments of the ring electrode, and it gives an additional electric field [11,12], for example, for the radial x-component

$$\overrightarrow{E_x}=\frac{V_d}{a}\cos\,(\omega_{rf}t-\phi_{rf})\cdot\hat{e_x}, \tag{5}$$

where a is the inner radius of the trap.

An azimuthal quadrupolar rf field with amplitude V_q and frequency ω_{rf} applied with 180° phase shifts on sets of ring-electrode segments perpendicular to each other gives an additional electric field [10]

$$\begin{cases} \overrightarrow{E_x}=\frac{2V_q}{a^2}\cos\,(\omega_{rf}t-\phi_{rf})\cdot y\hat{e_x} \\ \overrightarrow{E_y}=\frac{2V_q}{a^2}\cos\,(\omega_{rf}t-\phi_{rf})\cdot x\hat{e_y}, \end{cases} \tag{6}$$

where $\hat{e_x}$ and $\hat{e_y}$ are the unit vectors on the x- and y-axes, respectively.

Zhu et al. [13] studied the energy limitation for models to simulate the 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 the buffer gas on the ion motion in a Penning trap can be described as $\overrightarrow{F}=-\delta m\overrightarrow{v}$, where δ is the damping parameter describing the effect of the buffer gas. With the ion mobility K_0, δ can be written as $\delta=(q/m)(1/K_0)(P/P_N)/(T/T_N)$. 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 and temperature P_N and T_N [14], respectively.

Thus the dynamical equations including all effects from the dipolar rf excitation and buffer gas cooling can be described as

$$\begin{cases} \left(\ddot{x}-\frac{qU_0}{2md^2}x-\frac{qB}{m}\dot{y}\right)-\frac{qV_d}{ma}\cos\,(\omega_{rf}t-\phi_{rf})+\delta_x\dot{x}=0 \\ \left(\ddot{y}-\frac{qU_0}{2md^2}y+\frac{qB}{m}\dot{x}\right)+\delta_y\dot{y}=0 \\ \left(\ddot{z}+\frac{qU_0}{md^2}z\right)+\delta_z\dot{z}=0, \end{cases} \tag{7}$$

and those for the quadrupolar excitation and buffer gas cooling

$$\begin{cases} \left(\ddot{x}-\frac{qU_0}{2md^2}x-\frac{qB}{m}\dot{y}\right)-\frac{2qV_q}{ma^2}\cos\,(\omega_{rf}t-\phi_{rf})\cdot y+\delta_x\dot{x}=0 \\ \left(\ddot{y}-\frac{qU_0}{2md^2}y+\frac{qB}{m}\dot{x}\right)-\frac{2qV_q}{ma^2}\cos\,(\omega_{rf}t-\phi_{rf})\cdot x+\delta_y\dot{y}=0 \\ \left(\ddot{z}+\frac{qU_0}{md^2}z\right)+\delta_z\dot{z}=0. \end{cases} \tag{8}$$

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

As these are nonlinear differential equations, an analytic solution is difficult to obtain, and the method which has been known is using variable substitution twice $(\overrightarrow{V^\pm}(t)=\dot{\overrightarrow{\rho}}(t)-\omega_\mp\overrightarrow{\rho}(t)\times\hat{e_z}$, $\overrightarrow{A_\pm}(t)=V^\pm(t)e^{\mp i(\omega_\pm t+\phi_\pm)})$ and neglecting the high frequency terms [8,10]. Here we obtain the numerical solution of the above equation by using Runge–Kutta method.

3. Numerical solution by the Runge–Kutta method

Common fourth-order Runge–Kutta method is used to obtain the numerical solution of ion motions in a Penning trap. Specifying the form of first order differential equation as $y'(t)=f(t,y)$ and