The influence of a nonuniform rf field on the ion trajectories in an omegatron

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MS received 18 May 1971

Abstract The quadrupole field component of a nonuniform rf field causes an effect which improves the resolution and is called rf drift-off. This effect is mathematically analysed. Some experimental results are shown which are in good agreement with the theory.

1 Introduction

In the existing theories describing the performance of the omegatron (Berry 1954, Warnecke 1959-60) the rf field is assumed to be uniform. Indeed, omegatrons with a uniform rf field have been developed, but simple omegatrons as the much-used Alpert-type (Alpert and Buritz 1954) and the long omegatron of van der Waal (1963) have a nonuniform field. This nonuniform rf field causes two effects (Bijma et al. 1968):

(i) Near-resonant ions \( \omega - \Omega \neq 0 \) drift off into a direction perpendicular to the magnet field and the rf electric field. This drift-off, which we call rf drift-off, improves the resolving power.

(ii) At a superimposed frequency \( \omega = 2 \Omega \) ions with a cyclotron frequency \( \Omega \) reach the collector and give rise to a harmonic peak. This peak can easily be suppressed.

In this paper the abovementioned rf drift-off is described. The harmonic effect will be described in a next paper.

2 Equations of motion in a nonuniform field

In order to derive an expression for the equations of motion in an omegatron we have to determine the electric field. Therefore the field shape in a long omegatron has been measured with the aid of a model in an electrolytic plotting tank. As expected, in this omegatron the field nonuniformity occurred mainly in the \( x \) and \( z \) direction, with which the coordinate system has been defined in figure 1.

In this paper we only consider the motion in the \( z = 0 \) plane, giving a model with which the most important phenomena can be explained. In the \( z = 0 \) plane the rf electric field can be approximated by

\[
E_x = (a + bx) \sin (\omega t + \phi)
\]

The nonuniformity of the rf field is taken into account by the quadrupole term \( bx \sin (\Omega t + \phi) \). The magnetic field is assumed to be constant, and passes along the \( x \) axis. \( B = (0, 0, B) \). The equations of motion for the ion are derived with the aid of
the Newton–Lorentz relation:

\[ \frac{d}{dt} (m\mathbf{u}) = e(E + \mathbf{u} \times \mathbf{B}). \]  

(2)
e is the positive unit charge; the ion is assumed to be singly ionized. We define:

\[ \alpha = \frac{ea}{m}, \quad \beta = \frac{eb}{m}, \]  
\[ \Omega = \frac{eB}{m} \quad \text{and} \quad \Delta \omega = \omega - \Omega. \]  

(3)

After some elementary work from (2) with (1) and (3) we obtain the following system of differential equations:

\[ \begin{align*}
\dot{x} + \Omega^2 x &= (\alpha + \beta x) \sin (\omega t + \phi) + \Omega \dot{x}(0) + \Omega^2 x(0) \\
\dot{y} &= -\dot{\Omega}(x - x(0)) + \dot{y}(0) \\
\dot{z} &= 0.
\end{align*} \]  

(4)

The homogeneous part of (4):

\[ x + \Omega^2 x = \beta x \sin (\omega t + \phi) \]  

(7)
is known in literature as the Matthieu equation. When \( t = 0 \) the initial conditions are

\[ x(0) = y(0) = z(0) = 0, \quad \text{and} \quad \dot{x}(0), \dot{y}(0) \text{ have given values}. \]  

(8)

To explain the effects mentioned in §1 approximation solutions from (4) are derived in §3. The influence of a dc field can be expressed by including the terms

\[ \alpha' = \frac{ea'}{m} \quad \text{and} \quad \beta' = \frac{eb'}{m}. \]  

(3a)
in the differential equation

\[ \begin{align*}
\dot{x} + (\Omega^2 - \beta') x &= (\alpha + \beta x) \sin (\omega t + \phi) + \Omega \dot{x}(0) + \alpha' \\
\dot{y} &= -\dot{\Omega} x + \dot{y}(0) \\
\dot{z} &= -\beta' z.
\end{align*} \]  

(4a)

In the calculations made in §3 it is assumed that \( \alpha' = \beta' = 0 \) unless the contrary is indicated.

3 RF drift-off

3.1 Introduction

Calculations with the aid of a computer show a drift-off effect of near-resonant ions in a nonuniform rf field. This drift-off direction is perpendicular to the electric and magnetic field, i.e. in the chosen coordinate system in the y direction. Figure 2 shows a near-resonant ion trajectory in both a uniform and a nonuniform rf field. In a uniform rf field the path radius is approximated by

\[ r = \frac{a}{B \Delta \omega} \sin \frac{1}{2} \Delta \omega t, \quad \Delta \omega = \omega - \Omega \neq 0 \]  

(9)

On this motion a drift-off effect is superimposed, if we have to deal with a nonuniform field.

3.2 Mathematical treatment

The drift-off effect can be calculated by considering \( \beta x \sin (\omega t + \phi) \) in the differential equation (4) as a perturbation term with respect to the term \( \Omega^2x \). This allows for

\[ | \beta \sin (\omega t + \phi) | \ll \Omega^2 \]  

(10)

which condition has been satisfied for the fields considered by us (see Appendix 4). We shall prove that taking \( \beta = 0 \) in (4) the general solution of this equation can be written in closed form under the initial conditions of (8). We consider the differential equation

\[ x + \Omega^2 x = f(t, x) \]  

(11)

which may be transformed, with the boundary conditions \( x(0) = 0 \) and \( \dot{x}(0) \) and with the aid of Laplace-transformation or variation of constants, to the integral equation

\[ x = \frac{x(0)}{\Omega} \sin \Omega t + \frac{1}{\Omega} \int_0^t f(t, x) \sin \Omega(t - \tau) \, d\tau. \]  

(12)

For \( \beta = 0 \) the right-hand side of equation (4) becomes

\[ f(t, x) = \alpha \sin (\omega t + \phi) + \Omega \dot{x}(0). \]  

(13)

Provided that \( \omega \neq \Omega \), substituting (13) in (12) we obtain the unperturbed solution:

\[ x_a = \frac{x(0)}{\Omega} \sin \Omega t + \frac{y(0)}{\Omega} (1 - \cos \Omega t) + \frac{\alpha}{(\Omega^2 - \omega^2)} \times \left\{ \sin (\omega t + \phi) - \cos \Omega t \sin \phi - \frac{\omega}{\Omega} \sin \Omega t \cos \phi \right\}. \]  

(14)

If \( \beta \neq 0 \) (4), (12) and (14) yield

\[ x = x_a + \frac{\beta}{\Omega} \int_0^t \sin \Omega(t - \tau) \sin (\omega \tau + \phi) \, d\tau. \]  

(15)
An approximated resolution of this equation can be found by the iteration method of Liouville-Neumann, which method can be applied in our case, since \(\sin Q(t-\tau)\) is a continuous kernel function (Gröbner and Lesky 1964). We use the first order approximation which consists of replacing \(x(\tau)\) by \(x_a\) in the integral form (15):

\[
x_p - x_a = \frac{\beta}{\Omega^2} \int_0^\tau \sin \Omega(t-\tau) x_a \sin (\omega t + \phi) d(\Omega \tau)
\]

where \(x_p\) is the approximated resolution.

Since \(\frac{\beta}{\Omega^2} \ll 1\) (see Appendix 4) the first order approximation (16) differs only a little from the exact resolution (15). A second-order approximation gives terms being a factor of \(\frac{\beta}{\Omega^2}\) smaller than the calculated first order terms. For this reason we only apply the first order approximation. Working out (16) gives:

\[
x_p - x_a = \frac{x(0)}{\Omega^2} \frac{\beta}{\Omega^2} (\cos (\Delta \omega t + \phi) - \frac{\beta}{\Omega^2} \sin (\Delta \omega t + \phi))
\]

in which the residual term \(R_1\) consists of oscillating terms with frequency of approximately \(\Omega\) and amplitude less than or equal to \(\alpha \beta / 2 \Omega^2 (\Omega^2 - \omega^2)\). For the considered frequencies \((\Delta \omega / \Omega)^2 \ll 1\) is assumed, in which case the term \((\Delta \omega / \Omega)^2\) is negligible. From (5) and (17) we obtain the perturbation term \(y_p - y_a\), being the rf drift-off:

\[
y_p - y_a = -\frac{x(0)}{\Omega^2} \frac{\beta}{\Delta \omega} \sin \frac{1}{2} \Delta \omega t \cos \left(\frac{3}{4} \Delta \omega t + \phi\right)
\]

The residual term \(R_2\), consisting of oscillating terms with a frequency approximately \(\Omega\) and an amplitude less than or equal to \(\alpha \beta / 2 \Omega^2 (\Omega^2 - \omega^2)\), can be neglected. With substitution of (3), (18) is reducible to:

\[
y_p - y_a = -\frac{x(0)}{\Omega^2} \frac{\beta}{\Delta \omega} \sin \frac{1}{2} \Delta \omega t \cos \left(\frac{3}{4} \Delta \omega t + \phi\right)
\]

with

\[
R_3 = -\frac{\Delta \omega}{2 \Omega} \left[\frac{\sin \Delta \omega t}{\Delta \omega t} - 1 + \frac{1}{4} \Delta \omega t\right]
\]

In Appendix 5 the residual term \(R_3\) is shown to be small with respect to the leading term, on conditions fulfilled in practice. The rf drift-off \(y_p - y_a\) is approximated by:

\[
y_p - y_a \approx -\frac{ab}{4 B^2 \Delta \omega r} \left(1 - \frac{\sin \Delta \omega t}{\Delta \omega t}\right).
\]

Besides the rf drift-off in an omegatron an additional dc drift-off occurs as a result of the dc field we applied in the \(x\) direction. This dc drift-off is approximated by:

\[
y_{dc} = -\frac{a'}{B} t.
\]

The total drift-off \(y_{tr}\) is the sum of the dc drift-off and the rf drift-off \(y_p - y_a\), so

\[
y_{tr} = (y_p - y_a) + y_{dc} = -\frac{ab}{4 B^2 \Delta \omega r} \left(\frac{\sin \Delta \omega t}{\Delta \omega t} - 1\right) - \frac{a'}{B} t.
\]

We now choose a new origin \(O'\) moving with the drifting-off ion. This is

\[
O' \left(0, -\frac{ab}{4 B^2 \Delta \omega r} \left(\frac{\sin \Delta \omega t}{\Delta \omega t} - 1\right) - \frac{a'}{B} t\right).
\]

With respect to \(O'\) the drifting-off ions have the same radius as the nondrifting-off ions had with respect to \(O\), given by (9):

\[
r' = \frac{a}{B \Delta \omega r} \sin \frac{1}{4} \Delta \omega t.
\]

3.3 The influence of rf and dc drift-off on the resolving power

The influence of rf and dc drift-off on the resolving power can easily be explained in case of an omegatron with, for instance, three collectors \(C_1\), \(C_2\) and \(C_3\) with a mutual distance \(2l\). The distance between the \(y\) axis and the collectors is \(d\).

If the drift-off distance of \(O'\) is smaller than \(3l\), ions for which \(r' > d\) hit one of these three collectors. In the omegatron drawn in figure 3 ions reach

\[
\begin{align*}
\text{collector } C_1 & \text{ if } -3l < y_{tr} < -l \\
\text{collector } C_2 & \text{ if } -l < y_{tr} < +l \\
\text{collector } C_3 & \text{ if } +l < y_{tr} < +3l.
\end{align*}
\]

We now determine the frequency range for which \(r' > d\). With the maximum value of \(r'\)

\[
r'_{max} = \frac{a}{B} \frac{1}{\Delta \omega}
\]

we define

\[
\Delta \omega_1 = \frac{\Delta \omega}{|\Delta \omega|} \text{ if } r'_{max} = d
\]

hence

\[
\Delta \omega_1 = \frac{a}{B \Delta \omega}.
\]

The frequency range for which \(r' > d\) is equal to \(2 \Delta \omega_1\). Hence it follows that the total peak width is \(2 \Delta \omega_1\). The resolving power in connection with this total peak width is

\[
S = \frac{M}{2 \Delta M} \approx \frac{e B d}{2 a m}
\]
As a result of this drift-off ions from a frequency range $2\Delta \omega$ can hit different collectors, in this case three collectors, dividing the total peak in subpeaks, each of them of course, smaller than $2\Delta \omega$. The resolving power, measured on each single collector, can be determined as follows. With the radius $r'=d$ the drift-off position $O'$ depends on the shift of $\Delta \omega$ and can be expressed as a function of a shifting parameter $k$, defined by

$$k = \frac{\Delta \omega}{\Delta \omega_1}, \quad |k| \ll 1. \quad (28)$$

From (23) we derive

$$r' = \frac{a}{B\Delta \omega_1} \frac{\Delta \omega_1}{\Delta \omega} \sin \frac{1}{2} \Delta \omega t = \frac{d}{k} \sin \frac{1}{2} \Delta \omega t. \quad (29)$$

For $r'=d$ with $t=t_1$ it is necessary that

$$\frac{1}{k} \sin \frac{1}{2} \Delta \omega t_1 = 1, \quad \sin \frac{1}{2} \Delta \omega t_1 = k. \quad (30)$$

The drift-off distance $y_{dr}$ of $O'$ at $t=t_1$ is equal to

$$y_{dr} = \frac{-ab}{4b^2 \Delta \omega} t_1 \left( \frac{\sin \Delta \omega t_1}{\Delta \omega t_1} - 1 \right) - \frac{a'}{B} t_1. \quad (31)$$

$$= \frac{-ab}{4b^2 \Delta \omega} \left( \frac{\Delta \omega}{\Delta \omega_1} \right)^2 \left( \sin \Delta \omega t_1 - \Delta \omega t_1 \right) - \frac{a'}{B} t_1. \quad (32)$$

With (26), (28) and (30) this can be turned into:

$$y_{dr} = \frac{bd^2}{a} K(k, C) \quad (33)$$

where

$$K(k, C) = \frac{1}{2k^2} \left( k(1-k^2)^{1/2} - \sin^{-1} k \right) \frac{C}{k} \sin^{-1} k \quad (34)$$

and

$$C = \frac{2a'}{db} = \frac{2a'}{ab} \frac{a}{bd}. \quad (35)$$

The factor $bd^2/a$ in formula (33) is a constant for a given omegatron configuration, so that the drift-off $y_{dr}$ is proportional to the function $K(k, C)$. In figure 4 the function $K(k, C)$ has been drawn.

Connected with this function $K=K(k, C)$ (34) is the function $C=C(k, K)$ (35) for which we can write

$$C(k, K) = \frac{-2KK + (1-k^2)^{1/2}}{2 \sin^{-1} k} - \frac{1}{2k^2} \quad (36)$$

In figure 5 this function has been drawn for discrete values of K. The relation (24), which gives the collection ranges for the different collectors, can be transferred into

$$K_{-31} = -3 \frac{a}{bd^2} < K(k, C) < K_{-1} = -\frac{a}{bd^2} \quad \text{for collector C}_1$$

$$K_{-1} = -\frac{a}{bd^2} < K(k, C) < K_{+1} = +\frac{a}{bd^2} \quad \text{for collector C}_2$$

$$K_{+1} = +\frac{a}{bd^2} < K(k, C) < K_{+31} = +3 \frac{a}{bd^2} \quad \text{for collector C}_3 \quad (37)$$

$K_{-31}, K_{-1}, \ldots, K_{-1}$ are discrete values for $K$ in a given omegatron. At a given rf and dc field the function $C(k, K)$ = $(2a'/a)(a/bd)$ has a constant value. The intersection of $C(k, K) = \text{constant}$ with $(K_{-31}, K_{-1}), (K_{-1}, K_{+1})$ and $(K_{+1}, K_{+31})$ gives the peak distribution over the collectors $C_1, C_2$ and $C_3$. It can be seen from figure 5 that the peak frequency is shifted by variation of $C$. $C=(2a'/a)(a/bd)$ depends on the rf field $a$ and the drift-off field $a'$; the factor $a/bd$ is a constant for a given omegatron configuration. Furthermore, the frequency is shifted by the dc trapping field. It follows from (4a) that

$$\Omega^* = (\Omega^2 - \beta')^{1/2} \approx \Omega - \beta'/2\Omega. \quad (38)$$

Though the theory of rf drift-off is new, all simple omegatrons with a nonuniform rf field show this effect. The extent of advantage of this effect depends on the place of the collector and the dimensions of the collection range. The theory described by Petley and Morris (1968) can be applied only
Figure 6  This three-dimensional display of measurements shows a number of mass peaks recorded at distinct values of the drift-off field $a'$. $a$ being constant, $a'$ is proportional to $C(k, K)$. The frequency shift $k = \Delta \omega / \Delta \omega_1$ is indicated. The peak height is proportional to the measured ion current on the collector. The peak shift is in good agreement with the shift theoretically indicated in figure 5. The resolving power is up to a factor 6 better than the classical value given by 27. More details of this measurement are to be published.

on omegatrons with a uniform rf field. The elongated shape with hyperbolic electrodes may be the most favourable shape for an omegatron. For, then the coefficients $b$ and $b'$ determined in §2, which were only valid for the plane $z=0$, can be applied in the entire omegatron. Consequently, we obtain a frequency shift of $\Omega'=\Omega=-\beta'/2\Omega$ no longer being dependent on the place in the omegatron. This is one of the conditions to obtain a great resolving power with small rf signals. The coefficient $b$ which causes the rf drift-off is also independent of the place in a quadrupole omegatron. Some typical results of such a quadrupole omegatron are given in figure 6.

Appendix 1  Review of the theory of the ion trajectories in a uniform field

Ion trajectories in a uniform field are determined by the differential equations (4) and (5) with boundary conditions (8) and $\beta=0$. This system can be resolved elementarily by (see §3)

$$x_0 = \frac{x(0)}{\Omega} \sin \Omega t + \frac{j(0)}{\Omega} (1-\cos \Omega t) + \frac{\alpha}{\omega} \sin \Omega t \sin \phi \cos \Omega t$$

$$y_0 = \frac{x(0)}{\Omega} \cos (\Omega t - 1) + \frac{j(0)}{\Omega} \sin \Omega t - \frac{\alpha}{\omega} \sin \Omega t \cos \phi $$

The influence of the initial velocities and of the terms with forefactor $\alpha/\Omega^2$ can be neglected. $\alpha/\Omega^2$ is assumed to be small with respect to $\alpha/\Omega \Delta \omega$, which is consistent with the assumption that $\Delta \omega/\Omega < 1$:

$$x_0 = \frac{x(0)}{\Omega} \sin \Delta \omega t \cos (\frac{1}{2}(\Omega + \omega) t + \phi)$$

$$y_0 = \frac{x(0)}{\Omega} \sin \Delta \omega t \sin (\frac{1}{2}(\Omega + \omega) t + \phi)$$

From this it follows that

$$r = \frac{\alpha}{\Omega \Delta \omega} \sin \frac{1}{2} \Delta \omega t = \frac{\alpha}{B \Delta \omega} \sin \frac{1}{2} \Delta \omega t.$$  (A4)

Appendix 2  The influence of a uniform dc field on the ion trajectories

In equation (4a) the influence of a dc field in the $x$ direction is given by the term $a'$. We consider $\beta = \beta'=0$:

$$x= -\Omega \Delta x = \alpha \sin (\omega t + \phi) + \Omega j(0) + a'$$

$$y = -\Delta (x-x(0)) + y(0).$$

The resolutions of this system are given by

$$x = x_0 + x_{dc}$$

$$y = y_0 + y_{dc}.$$ (A5)

(A6)

The resolutions $x_0$ and $y_0$ have been given by (14) and (A1), whilst

$$x_{dc} = \frac{a'}{B} (1-\cos \Omega t) = \frac{a'}{B} (1-\cos \Omega t)$$

$$y_{dc} = \frac{a'}{B} + \frac{a'}{B} \sin \Omega t = -\frac{a'}{B} + \frac{a'}{B} \sin \Omega t.$$ (A7)

The influence of the term $x_{dc}$ on the given derivation from the rf drift-off ($\beta \neq 0$) is negligible, which appears from the relative perturbation term:

$$-\Omega \int_{0}^{t} dt_1 \frac{1}{\Omega^2} \sin \Omega (t_1 - \tau) \frac{a'}{B} (1-\cos \Omega \tau) \sin (\omega t + \phi) \, d\tau.$$ (A8)

In §3 only the asymptotic behaviour of $y_{dc}$ given by

$$y_{dc} = -\frac{a'}{B} t$$

is important.

Appendix 3  Initial velocity of the ions

The velocity distribution of the gas particles at equilibrium at a certain temperature is given by the Maxwell distribution. The ionization of the gas occurs with an electron beam of about 90 eV. If the gas is ionized but not dissociated the energy distribution is only slightly changed. So, for a good approximation we can use the Maxwell distribution. A simple
notation for the Maxwell distribution can be obtained by transformation from Cartesian to cylindrical coordinates in the velocity space:

\[ \dot{x} = \dot{r} \cos \zeta, \]
\[ \dot{y} = \dot{r} \sin \zeta, \]
\[ \dot{z} = \dot{t}. \]  

The velocity distribution in the plane \((x, y) = (r, \zeta)\) is

\[ f(\dot{r}) \, d\zeta = \frac{m}{2\pi kT} \exp \left( -\frac{m \dot{r}^2}{2kT} \right) \dot{r} \, d\zeta. \]  

The average velocity in this plane is

\[ \dot{\zeta} = \frac{\int_0^\infty \dot{r} f(\dot{r}) \, d\zeta}{\int_0^\infty f(\dot{r}) \, d\zeta}. \]  

Appendix 4 Numerical data

In this appendix some physical constants are given. Furthermore some values of the magnitude of the field, as they were found to occur in the omegatron considered by us, are given. With the aid of these data some neglected quantities are finally verified.

\[ \Omega = \frac{eB}{m} \text{ rad s}^{-1}, \]
\[ e = 1.6 \times 10^{-19} \text{ C}, \]
\[ m = M \text{ mo kg}, \]
\[ m_0 = 1.66 \times 10^{-27} \text{ kg} \approx 1 \text{ a.m.u.}, \]
\[ M = \text{ mass in a.m.u.}. \]

For the performance of an omegatron a magnet with a strength of about 0.4 T is often used:

\[ B \approx 0.4 \text{ T}. \]

In a long omegatron which measures 2 cm \(\times\) 2 cm \(\times\) 5 cm an rf voltage with an amplitude of \(V_{rf} V\) gives for the magnitudes defined in formula (1) the following values:

\[ a \approx 50 \, V_{rf} \, \text{V m}^{-1}, \]
\[ b \approx 5 \times 10^9 \, V_{rf} \, \text{V m}^{-2}. \]

Usually \(V_{rf}=1\) or 2 V is applied. \(d \approx 10^{-8} \text{ m}\) is the usual collector distance.

\(B/\Omega^2\): with the above-mentioned numerical magnitudes \(B/\Omega^2 \ll 1\) can now be verified by

\[ \frac{B}{\Omega^2} = \frac{b m_0 M}{B^4 e} \approx 3 \times 10^{-4} \, MV_{rf}. \]

For \(M < 100 \text{ a.m.u.} \) and \(V_{rf}=1 \) or 2 V, \(B/\Omega^2 \ll 1\) is valid.

\(\Delta \omega/\Omega\): in the derivation of formula (20) terms are neglected on account of the assumption that \(|\Delta \omega/\Omega| \ll 1\). This assumption is satisfied by those ions which can be detected, i.e. for which

\[ r = \frac{a}{B \Delta \omega} \sin \frac{1}{2} \Delta \omega t \gg d. \]

Then with the above-mentioned numerical magnitudes

\[ \frac{\Delta \omega}{\Omega} = k \frac{\Delta \omega}{\Omega} = k \frac{am}{B^4 e} \approx 3 \times 10^{-4} k MV_{rf}. \]

For \(M < 100 \text{ a.m.u.} \) and \(V_{rf}=1 \) or 2 V, \(\Delta \omega/\Omega \ll 1\) is valid.