GENERALIZATION OF THE PSEUDOPOTENTIAL CONCEPT FOR RADIO-FREQUENCY QUADRUPOLE FIELDS

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It is shown that the pseudopotential function, which describes the averaged motion of charged particles with accuracy up to quadratic terms for nonuniform radio-frequency fields, can be replaced by an infinite pseudopotential series for quadrupole radio-frequency electric fields. This replacement provides a more accurate description. It allows us to extend the parameter's range of the radio-frequency field; in this range, it makes possible to describe the motion of charged particles quantitatively and not just qualitatively. Unfortunately, even this extended concept of pseudopotential is not suitable enough for describing the motion of charged particles when approaching the region of the parametric resonance, where the motion of charged particles loses stability in the quadrupole radio-frequency fields.

Key words: high-frequency electric field, quadrupole mass filter, secular oscillation, pseudopotential

Citation: A.S. Berdnikov, L.N. Gall, N.R. Gall, K.V. Solovyev, Generalization of the pseudopotential concept for radio-frequency quadrupole fields, St. Petersburg Polytechnical State University Journal. Physics and Mathematics. 11 (3) (2018) 38–48. DOI: 10.18721/JPM.11305

Introduction

The pseudopotential approach is a useful tool for qualitatively describing ion motion in nonuniform radio-frequency (RF) electric fields [1 – 12]. However, the accuracy of the classical pseudopotential approach is too low for RF quadrupole mass filters [11 – 15] and (to a lesser extent) for RF quadrupole traps [16, 17], so the approach can hardly be regarded as useful for investigating the motion of charged particles in these devices. Exceptions from this include pseudopotential functions for calculating the stroboscopic values of coordinates and velocities [18 – 20], or interpretation of Floquet – Lyapunov matrices for solutions of linear differential equations with periodic coefficients in the sense of a pseudopotential model of motion [21, 22]. These pseudopotential functions are based on a fundamentally different mathematical formalism; still, these models of motion are not very convenient for practical calculations.

In this study, we have considered a reasonable compromise between classical models that are practical but not particularly accurate in terms of analyzing the motion of charged particles in RF quadrupole fields [1 – 12], and models that are mathematically accurate but not very practical [18 – 22]. The models we have proposed make it possible to significantly expand the range of parameters of the RF quadrupole electric field within the first stability zone. Using these parameters allows to fit (not only qualitatively but also quantitatively) the approximate motion trajectories to exact solutions of the corresponding differential equations.

The pseudopotential models of motion discussed in the paper follow the general ideology of the classical pseudopotential theory [1 – 12] and produce easily calculable algebraic expressions. However, these models work poorly near the boundary of the stability region of RF quadrupoles which corresponds to parametric resonance between the driving RF field and the secular motion of charged particles violating the basic assumptions that the RF component of charged particle motion is small compared to the "slow" (averaged over RF oscillations) component of motion. Furthermore, the formulae obtained are specific for RF quadrupole electric fields and cannot be generalized to motion of charged particles in nonlinear RF electric fields.

Classical pseudopotential model for motion in a RF quadrupole field

Let us consider the motion of an ion in a RF electric field of a linear quadrupole with hyperbolic rods [11 – 17]. The electric potential $U(x, y, t)$ for such a system has the form

$$U(x,y,t) = = (U_0 + V_0\cos(\Omega t + \varphi_0))\,(x^2 - y^2)/r_0^2\,, \quad (1)$$

where U_0 is the constant component of the voltages applied to the electrodes; V_0 is the amplitude of the cosinusoidal RF component of the voltages applied to the electrodes; Ω is the circular frequency of the RF voltage, φ_0 is the phase of the RF voltage at the start of ion motion; r_0 is the shortest distance from the quadrupole axis to the hyperbolic electrodes (characterizing the interelectrode gap of the RF linear quadrupole); x and y are the Cartesian coordinates; t is the time of motion.

In dimensionless coordinates, the trajectory $x(t)$, $y(t)$ for an ion with the mass m and charge e satisfies the Mathieu-type equations [23 – 30], which are a particular case of linear differential equations with periodic coefficients:

$$\frac{d^2x}{d\xi^2} + (a + 2q\cos(2\xi + \varphi_0))x = 0, \quad (2)$$

$$\frac{d^2y}{d\xi^2} - (a + 2q\cos(2\xi + \varphi_0))y = 0, \quad (3)$$

where $\xi = \Omega t/2$ is the dimensionless time; $a = 8eU_0/m\Omega^2 r_0^2$, $q = 4eV_0/m\Omega^2 r_0^2$ are the dimensionless parameters; $f(\xi) = \cos(2\xi + \varphi_0)$ is the cosinusoidal periodic function with a dimensionless period $T' = \pi$ (the dimensionless circular frequency $\Omega' = 2$) and the initial phase φ_0.

To illustrate the principles of the classical pseudopotential approach, let us consider one-dimensional motion of an ion with mass m and charge e in an RF electric field with an electric potential of the general form

$$U(x,t) = U^0(x,t) + V(x,t)\cos(\Omega t + \varphi_0) + + W(x,t)\sin(\Omega t + \varphi_0), \quad (4)$$

where $U^0(x, t)$, $V(x, t)$, $W(x, t)$ are assumed to be "slow" functions of time, in comparison with "rapidly" oscillating sinusoidal functions $\cos(\Omega t + \varphi_0)$, $\sin(\Omega t + \varphi_0)$.

Newton's equations of motion of an ion in such an electric field take the form

$$(m/e)\ddot{x} = -U_x^0(x,t) - V_x(x,t)\cos(\Omega t + \varphi_0) - - W_x(x,t)\sin(\Omega t + \varphi_0), \quad (5)$$

where the subscripts denote partial derivatives, which helps subsequently avoid unnecessarily cumbersome mathematical expressions.

We assumed for the pseudopotential motion model [1 – 12] that the solution of differential equation (5) can be represented with good accuracy as a sum

$$x(t) = x_0(t) + \delta x(t),$$
$$\delta x(t) \approx \sum_{k=0}^{\infty}\frac{1}{\Omega^k}(x_k^c(t)\cos(\Omega t + \varphi_0) + + x_k^s(t)\sin(\Omega t + \varphi_0) + x_k^{2c}(t)\cos 2(\Omega t + \varphi_0) + + x_k^{2s}(t)\sin 2(\Omega t + \varphi_0) + \cdots), \quad (6)$$

where the "rapid" component of the trajectory $\delta x(t)$, like its time derivative, has a zero mean (calculated over the period of the RF field (4)) and is small, compared with the principal ("slow") component of the trajectory $x_0(t)$.

Let us substitute sum (6) into Eq. (5) and expand both the functions $U^0(x, t)$, $V(x, t)$ and $W(x, t)$ and their partial derivatives to truncated Taylor series with respect to the small $\delta x(t)$ increment. In this case, under certain conditions, namely:

a) assuming that the functions $x_k^c(t)$, $x_k^s(t)$, $x_k^{2c}(t)$, $x_k^{2s}(t)$, ... are "slow",

b) combining together terms that are basic trigonometric functions with the same frequencies and the same powers of Ω,

c) demanding that the corresponding coefficients (except the terms corresponding to the zero harmonic of the RF field) vanish separately, the following approximate relations can be obtained:

$$x(t) \approx x_0(t) + \frac{e}{m\Omega^2} V_x(x_0(t), t)\cos(\Omega t + \varphi_0) + \frac{e}{m\Omega^2} W_x(x_0(t), t)\sin(\Omega t + \varphi_0) + \cdots; \quad (7)$$

$$\dot{x}(t) \approx \dot{x}_0(t) + \frac{e}{m\Omega} W_x(x_0(t), t)\cos(\Omega t + \varphi_0) - \frac{e}{m\Omega} V_x(x_0(t), t)\sin(\Omega t + \varphi_0) - \frac{e}{m\Omega^2}[V_{xt}(x_0(t), t) + \dot{x}_0(t)V_{xx}(x_0(t), t)] \times \cos(\Omega t + \varphi_0) - \frac{e}{m\Omega^2}[W_{xt}(x_0(t), t) + \dot{x}_0(t)W_{xx}(x_0(t), t)]\sin(\Omega t + \varphi_0) + \cdots; \quad (8)$$

$$\ddot{x}_0(t) \approx -\frac{e}{m} U_x(x_0(t), t) - \frac{e}{m} \bar{U}_x^{rf}(x_0(t), t) + \cdots. \quad (9)$$

The powers of Ω up to $1/\Omega^2$ are preserved here, and the higher powers, which are small corrections due to the assumption that the RF electric field has a “high” frequency, are omitted.

It should be noted, however, that in order to obtain the correct expression for the velocity $\dot{x}(t)$ (up to the terms of the form $1/\Omega^2$), the cubic terms $1/\Omega^3$ also have to be preserved in the calculations before differentiating the function $x(t)$ with respect to time; these terms can be eliminated only after the function $\dot{x}(t)$ has been determined correctly.

The function

$$\bar{U}^{rf}(x, t) = \frac{e}{4m\Omega^2}[(V_x(x, t))^2 + (W_x(x, t))^2] \quad (10)$$

is called the pseudopotential (effective potential, RF potential, ponderomotive force potential, etc.), and Eq. (9) can be interpreted as the motion of an ion with mass *m* and charge *e* in a quasi-stationary electric field with the potential $U(x, t) + \bar{U}^{rf}(x, t)$.

Importantly, not only the pseudopotential Eq. (9) for the “slow” component of the ion trajectory, but also Eqs. (7), (8) are an integral part of the pseudopotential model of motion. The latter equations allow to explicitly express the high-frequency corrections for the trajectory and velocity of the ion, and thus find an approximate expression for the true trajectory of the ion in the RF electric field. In particular, it follows from Eqs. (7) and (8) that rapidly oscillating corrections to the “slow” component of ion trajectory are directly proportional to the amplitude of the RF component of electric field strength at the given point of the trajectory. Moreover, nonlinear algebraic Eqs. (7), (8) can be used to express the functions $x_0(t)$, $\dot{x}_0(t)$ in terms of functions $x(t)$, $\dot{x}(t)$ as a series in the powers of $1/\Omega^k$:

$$x_0(t) \approx x(t) - \frac{e}{m\Omega^2} V_x(x(t), t)\cos(\Omega t + \varphi_0) - \frac{e}{m\Omega^2} W_x(x(t), t)\sin(\Omega t + \varphi_0) + \cdots; \quad (11)$$

$$\dot{x}_0(t) \approx \dot{x}(t) - \frac{e}{m\Omega} W_x(x(t), t)\cos(\Omega t + \varphi_0) + \frac{e}{m\Omega} V_x(x(t), t)\sin(\Omega t + \varphi_0) + \frac{e}{m\Omega^2}[V_{xt}(x(t), t) + \dot{x}(t)V_{xx}(x(t), t)] \times \cos(\Omega t + \varphi_0) + \frac{e}{m\Omega^2}[W_{xt}(x(t), t) + \dot{x}(t)W_{xx}(x(t), t)]\sin(\Omega t + \varphi_0) + \cdots, \quad (12)$$

where the terms are preserved up to $1/\Omega^2$ both for $x_0(t)$ and for $\dot{x}_0(t)$.

In particular, Eqs. (11) and (12) allow to explicitly express the initial conditions for “slow” motion (9) in terms of the initial conditions of true motion (5) in the RF field.

Notice that the discrepancy between the initial conditions for the functions $x_0(t)$, $\dot{x}_0(t)$ and $x(t)$, $\dot{x}(t)$, as well as the difference between the averaged $x_0(t)$, $\dot{x}_0(t)$ trajectories and the approximate $x(t)$, $\dot{x}(t)$ trajectories are not always taken into account in studies on assessing the accuracy of the pseudopotential model of motion, which yields estimates worse than the actual accuracy.

The normalized equation of motion (2) is obtained from Eq. (5) by the following substitution:

$$U^0(x, t) = ax^2/2, \quad V(x, t) = qx^2,$$

$$W(x, t) = 0, , \quad \Omega = 2,$$

$$e = 1, \quad m = 1, \quad t = \xi.$$

As a result, the pseudopotential model of ion motion (7) – (12) yields an approximate solution for Eq. (2), written in dimensionless form:

$$x_0''(\xi) \approx -\left(a + \frac{q^2}{2}\right)x_0(\xi) + \cdots; \quad (13)$$

$$x_0(0) \approx x(0)\left(1 - \frac{q}{2}\cos\varphi_0\right) + \cdots;$$
$$x_0'(0) \approx x(0)q\sin\varphi_0 + x'(0)\left(1 + \frac{q}{2}\cos\varphi_0\right) + \cdots; \quad (14)$$

$$x(\xi) \approx x_0(\xi)\left(1 + \frac{q}{2}\cos(2\xi + \varphi_0)\right) + \cdots; \quad (15)$$

$$x'(\xi) \approx -qx_0(\xi)\sin(2\xi + \varphi_0) + $$
$$+ x_0'(\xi)\left(1 - \frac{q}{2}\cos(2\xi + \varphi_0)\right) + \cdots. \quad (15)$$

It is assumed here that

$$a + q^2/2 = \tilde{\beta}^2 > 0,$$

where $\tilde{\beta} = \sqrt{a + q^2/2}$ is the pseudopotential approximation for the exact value of the normalized secular frequency β [23 – 31].

The condition

$$a + q^2/2 = \tilde{\beta}^2 > 0$$

corresponds to stable ion motion in the RF qua-

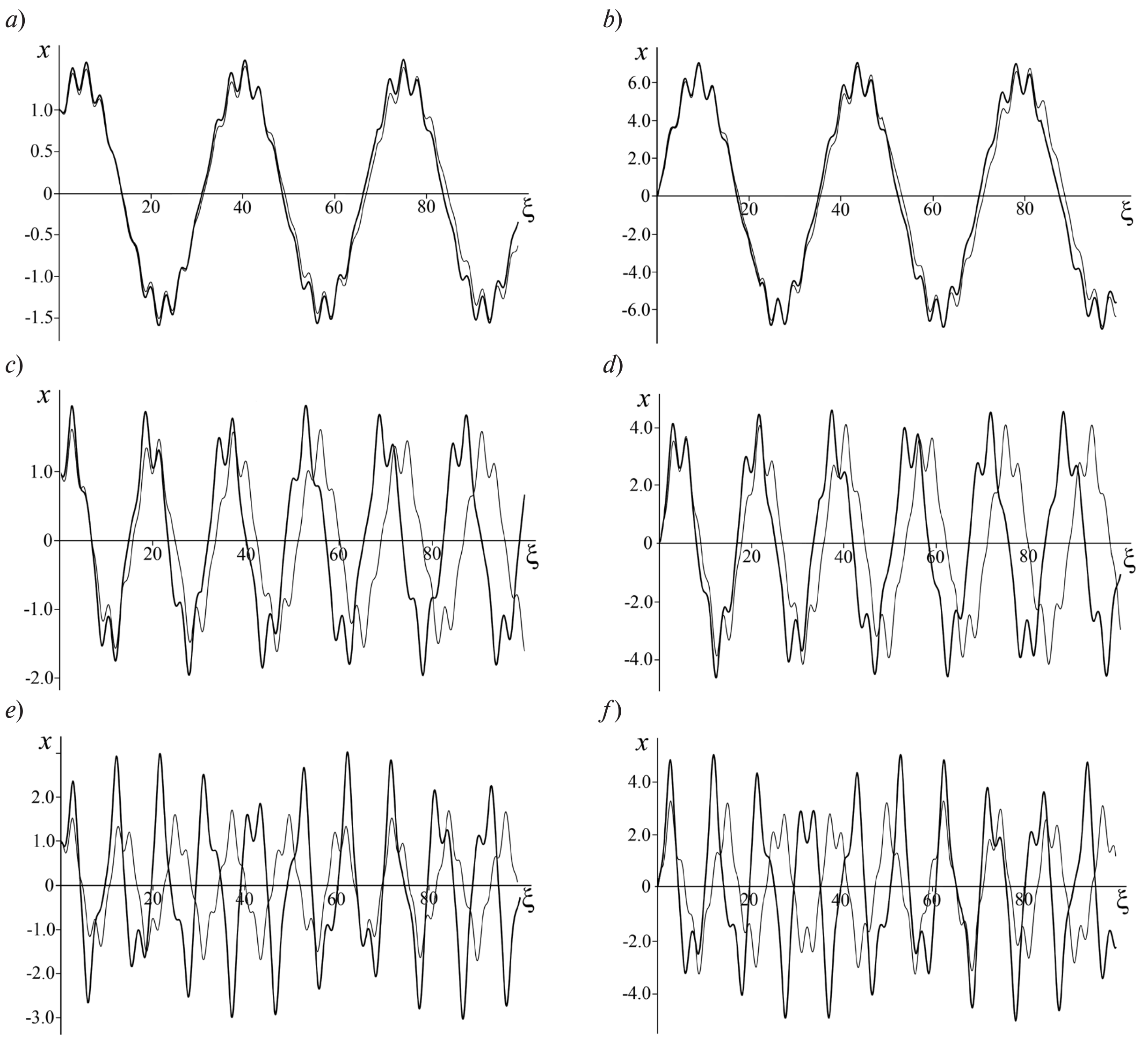

Fig. 1. Comparison of numerically obtained trajectories of Eq. (2) (thin lines) with approximate trajectories calculated by pseudopotential theory (14), (15) (solid lines).
The values of the parameters in Eq. (2) are given in Table

Table

Values of parameters in Eq. (2) for calculating its exact solutions

Fig. 1, 2	q	$x(0)$	$x'(0)$
a	0.25	1	0
b	0.25	0	1
c	0.50	1	0
d	0.50	0	1
e	0.75	1	0
f	0.75	0	1

Note. The parameter $a = 0$ for the entire given set of other parameters

drupole electric field within the pseudopotential model. Fig. 1 shows the difference between the approximate trajectories (13) – (15) and the exact (calculated) solutions of Eq. (2) with $a = 0$ for different values of the parameter q.

Pseudo-potential expansion in an infinite series

If more powers of the form $1/\Omega^k$ are preserved in expansion (6), refined equations can be obtained for "slow" motion, as well as refined coupling equations for true motion $x_0(t)$ and for slow (averaged) motion $x_0(t)$. Unfortunately, in the general case of an arbitrary RF electric field, the expressions obtained by this method turn out to be extremely complex and it is no longer possible to use the elegant and physically transparent classical pseudopotential model to interpret them (conversely, however, see Ref. [32]). Quadrupole electric fields (where the dependence of the electric potential on the coordinates is expressed by a quadratic polynomial) are an exception: high-order corrections for these fields still keep the form of an artificially constructed pseudopotential function.

As an example, let us consider one-dimensional motion in a cosinusoidal RF electric field with a quadratic electric potential:

$$\frac{dx}{dt} = v;$$
$$\frac{dv}{dt} = -\hat{U}x - \hat{V}x\cos(\Omega t + \varphi_0), \tag{16}$$

where, with respect to the linear quadrupole with electric potential (1), the quantity

$$(m/2e)\hat{U}x^2 = U_0\, x^2/r_0^2$$

is the constant component of the electric potential, and the quantity

$$(m/2e)\hat{V}x^2 = V_0\, x^2/r_0^2$$

is the amplitude of the RF component of the electric potential.

The pseudopotential expansion for the solutions of system of equations (16) can be written in the form of a specific series representing a hybrid of trigonometric Fourier series and Taylor power series:

$$x(t) = x_0(t) +$$
$$+ x_0(t)\sum_{k=1,\infty}\cos k(\Omega t + \varphi_0)\left(\sum_{j=k,\infty}\frac{x_{k,2j}^{(c)}}{\Omega^{2j}}\right) +$$
$$+ v_0(t)\sum_{k=1,\infty}\sin k(\Omega t + \varphi_0)\left(\sum_{j=k,\infty}\frac{x_{k,2j+1}^{(s)}}{\Omega^{2j+1}}\right);$$
$$v(t) = v_0(t) + \tag{17}$$
$$+ x_0(t)\sum_{k=1,\infty}\sin k(\Omega t + \varphi_0)\left(\sum_{j=k,\infty}\frac{v_{k,2j-1}^{(s)}}{\Omega^{2j-1}}\right) +$$
$$+ v_0(t)\sum_{k=1,\infty}\cos k(\Omega t + \varphi_0)\left(\sum_{j=k,\infty}\frac{v_{k,2j}^{(c)}}{\Omega^{2j}}\right);$$

$$\dot{x}_0(t) = v_0(t);$$
$$\dot{v}_0(t) = -\left(X_0 + \sum_{j=1,\infty}\frac{1}{\Omega^{2j}}X_{2j}\right)x_0(t). \tag{18}$$

In these equations, $x_{k,2j}^{(c)}$, $x_{k,2j+1}^{(s)}$, $v_{k,2j-1}^{(s)}$, $v_{k,2j}^{(c)}$, X_{2j} are unknown constants, which should be selected so that solution (17), (18) satisfies system of equations (16). Indeed, after substituting solution (17), (18) into system (16) and combining together the coefficients for trigonometric terms similar to

$$\cos k(\Omega t + \varphi_0),\ \ \sin k(\Omega t + \varphi_0)$$

and power terms $1/\Omega^j$, we can express the constants $x_{k,2j}^{(c)}$, $x_{k,2j+1}^{(s)}$, $v_{k,2j-1}^{(s)}$, $v_{k,2j}^{(c)}$, X_{2j} in a consistent manner using the recurrence relations in terms of the constants $\hat{U}$ and $\hat{V}$ entering Eqs. (16). In this case, the function

$$\hat{U}^{rf}(x_0) = \frac{1}{2}\left(X_0 + \sum_{j=1,\infty}\frac{1}{\Omega^{2j}}X_{2j}\right)x_0^2 = \frac{1}{2}\hat{\beta}^2 x_0^2, \tag{19}$$

used for writing the differential equation (18) in the form

$$\ddot{x}_0 = -d\hat{U}^{rf}(x_0)/dx_0,$$

can be interpreted as the refined quadratic pseudopotential. The latter characterizes "slow" (secular) ion motion in a quadratic RF electric field.

In particular, nonzero coefficients $x_{k,2j}^{(c)}$, $x_{k,2j+1}^{(s)}$, $v_{k,2j-1}^{(s)}$, $v_{k,2j}^{(c)}$, X_{2j}, required for calculating Eqs. (17), (18) up to terms of the form $1/\Omega^6$ are determined as

$$
\begin{gathered}
X_0 = \hat{U},\ X_2 = \frac{1}{2}\hat{V}^2,\ X_4 = 2\hat{U}\hat{V}^2,\\
X_6 = \hat{V}^2\left(8\hat{U}^2 + \frac{25}{32}\hat{V}^2\right);\\
v_{1,1}^{(s)} = -\hat{V},\ v_{1,3}^{(s)} = -2\hat{U}\hat{V},\\
v_{1,5}^{(s)} = -\hat{V}\left(8\hat{U}^2 + \frac{9}{16}\hat{V}^2\right);\\
v_{1,2}^{(c)} = -\hat{V},\ v_{1,4}^{(c)} = -4\hat{U}\hat{V},\\
v_{1,6}^{(c)} = -\hat{V}\left(16\hat{U}^2 + \frac{3}{4}\hat{V}^2\right);\\
x_{1,2}^{(c)} = \hat{V},\ x_{1,4}^{(c)} = 4\hat{U}\hat{V},\\
x_{1,6}^{(c)} = \hat{V}\left(16\hat{U}^2 + \frac{25}{16}\hat{V}^2\right);\\
x_{1,3}^{(s)} = -2\hat{V},\ x_{1,5}^{(s)} = -8\hat{U}\hat{V};\\
v_{2,3}^{(s)} = -\frac{1}{4}\hat{V}^2,\ v_{2,5}^{(s)} = -\frac{11}{8}\hat{U}\hat{V}^2,\\
v_{2,4}^{(c)} = -\frac{5}{8}\hat{V}^2,\ v_{2,6}^{(c)} = -\frac{23}{8}\hat{U}\hat{V}^2;\\
x_{2,4}^{(c)} = \frac{1}{8}\hat{V}^2,\ x_{2,6}^{(c)} = \frac{7}{8}\hat{U}\hat{V}^2,\ x_{2,5}^{(s)} = -\frac{3}{8}\hat{V}^2;\\
v_{3,5}^{(s)} = -\frac{1}{48}\hat{V}^3,\ v_{3,6}^{(c)} = -\frac{5}{72}\hat{V}^3,\ x_{3,6}^{(c)} = \frac{1}{144}\hat{V}^3,\ \dots\ .
\end{gathered}
\tag{20}
$$

Functions $x_0(t), v_0(t)$ can be expressed in terms of functions $x(t), v(t)$ with the help of linear equations (17), allowing, in particular, to correctly calculate the initial conditions for "slow" motion $x_0(t), v_0(t)$ in terms of the initial conditions given for the trajectory $x(t), v(t)$.

When the resulting expressions are expanded in a power series with respect to $1/\Omega^k$, we obtain expressions of the form

$$
\begin{aligned}
x_0(t) &= x(t)\left(1 + \sum_{k=2,\infty}\frac{\tilde{x}_{2k}^{(0)}}{\Omega^{2k}}\right) + \\
&+ x(t)\sum_{k=1,\infty}\cos k(\Omega t + \varphi_0)\left(\sum_{j=k,\infty}\frac{\tilde{x}_{k,2j}^{(c)}}{\Omega^{2j}}\right) + \\
&+ v(t)\sum_{k=1,\infty}\sin k(\Omega t + \varphi_0)\left(\sum_{j=k,\infty}\frac{\tilde{x}_{k,2j+1}^{(s)}}{\Omega^{2j+1}}\right);\\
v_0(t) &= v(t)\left(1 + \sum_{k=2,\infty}\frac{\tilde{v}_{2k}^{(0)}}{\Omega^{2k}}\right) + \\
&+ x(t)\sum_{k=1,\infty}\sin k(\Omega t + \varphi_0)\left(\sum_{j=k,\infty}\frac{\tilde{v}_{k,2j-1}^{(s)}}{\Omega^{2j-1}}\right) + \\
&+ v_0(t)\sum_{k=1,\infty}\cos k(\Omega t + \varphi_0)\left(\sum_{j=k,\infty}\frac{\tilde{v}_{k,2j}^{(c)}}{\Omega^{2j}}\right).
\end{aligned}
\tag{21}
$$

In particular, substituting expressions (21) into relations (17) and combining such terms, we can express the unknown coefficients $x_{k,2j}^{(c)}$, $x_{k,2j+1}^{(s)}$, $\tilde{x}_{2k}^{(0)}$, $v_{k,2j-1}^{(s)}$, $v_{k,2j}^{(c)}$, $\tilde{v}_{2k}^{(0)}$ directly through a system of recurrent algebraic relations:

$$
\begin{gathered}
\tilde{v}_4^{(0)} = \frac{3}{2}\hat{V}^2,\ \tilde{v}_6^{(0)} = 10\hat{U}\hat{V}^2;\\
\tilde{x}_4^{(0)} = \frac{3}{2}\hat{V}^2,\ \tilde{x}_6^{(0)} = 10\hat{U}\hat{V}^2;\\
\tilde{v}_{1,1}^{(s)} = \hat{V},\ \tilde{v}_{1,3}^{(s)} = 2\hat{U}\hat{V},\ \tilde{v}_{1,5}^{(s)} = \hat{V}\left(8\hat{U}^2 + \frac{33}{16}\hat{V}^2\right);\\
\tilde{v}_{1,2}^{(c)} = \hat{V},\ \tilde{v}_{1,4}^{(c)} = 4\hat{U}\hat{V},\\
\tilde{v}_{1,6}^{(c)} = -\hat{V}\left(16\hat{U}^2 + \frac{49}{16}\hat{V}^2\right);\\
\tilde{x}_{1,3}^{(s)} = 2\hat{V},\ \tilde{x}_{1,5}^{(s)} = 8\hat{U}\hat{V};\\
\tilde{x}_{1,2}^{(c)} = -\hat{V},\ \tilde{x}_{1,4}^{(c)} = -4\hat{U}\hat{V},\\
\tilde{x}_{1,6}^{(c)} = -\hat{V}\left(16\hat{U}^2 + \frac{9}{4}\hat{V}^2\right);\\
\tilde{v}_{2,3}^{(s)} = \frac{1}{4}\hat{V}^2,\ \tilde{v}_{2,5}^{(s)} = \frac{11}{8}\hat{U}\hat{V}^2,\ \tilde{v}_{2,4}^{(c)} = \frac{1}{8}\hat{V}^2,\\
\tilde{v}_{2,6}^{(c)} = \frac{7}{8}\hat{U}\hat{V}^2;\\
\tilde{x}_{2,5}^{(s)} = \frac{3}{8}\hat{V}^2,\ \tilde{x}_{2,4}^{(c)} = -\frac{5}{8}\hat{V}^2,\ \tilde{x}_{2,6}^{(c)} = -\frac{23}{8}\hat{U}\hat{V}^2;\\
\tilde{v}_{3,5}^{(s)} = \frac{1}{48}\hat{V}^3,\ \tilde{v}_{3,6}^{(c)} = \frac{1}{144}\hat{V}^3,\ \tilde{x}_{3,6}^{(c)} = -\frac{5}{72}\hat{V}^3,\ \dots\ .
\end{gathered}
\tag{22}
$$

For transition from system of equations (16) to the dimensionless equation, we use the substitution

$$\hat{U} = a,\ \hat{V} = 2q,\ \Omega = 2.$$

Fig. 2 compares approximate solutions, constructed with the help of relations (17),

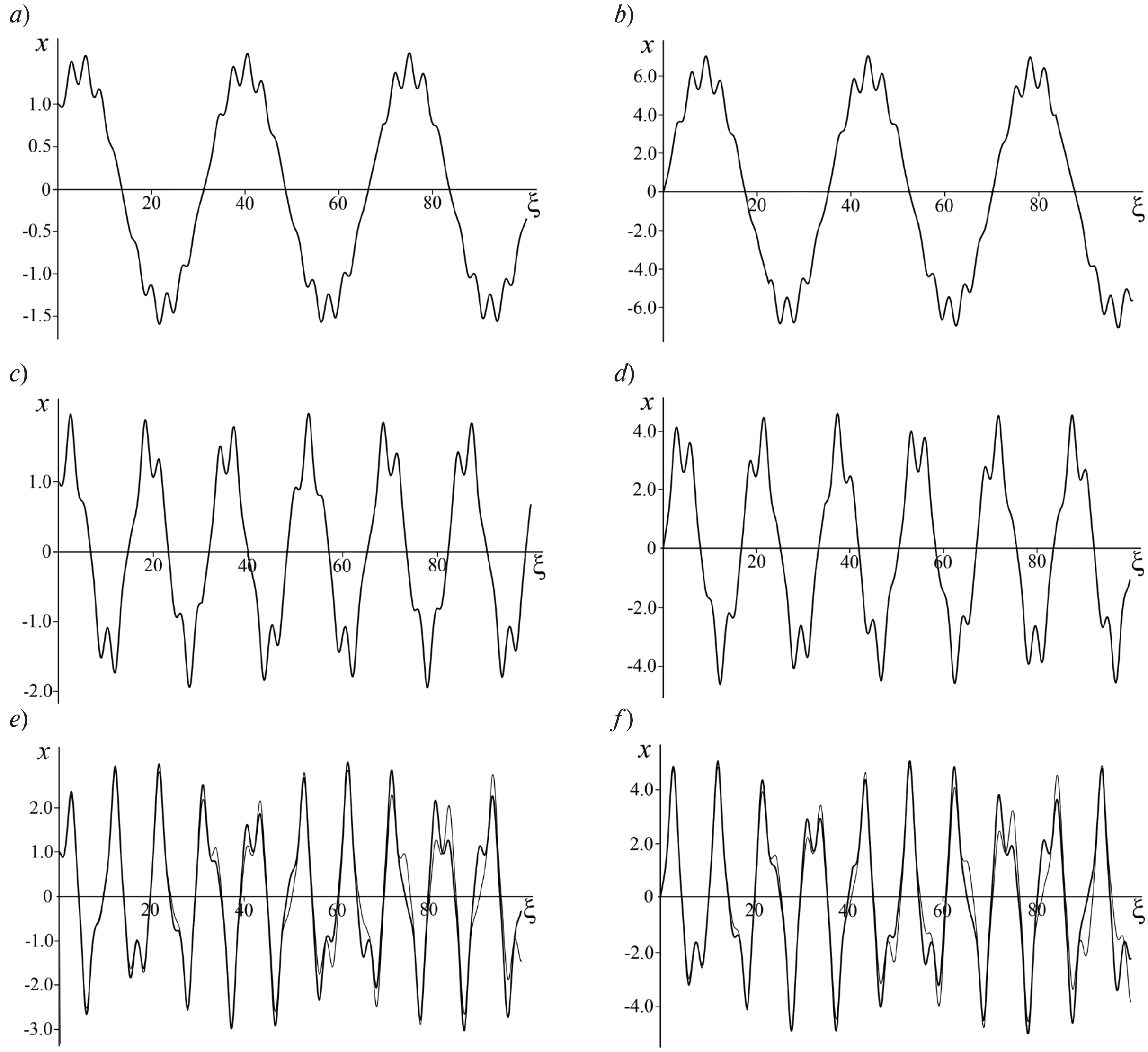

Fig. 2. Comparison of numerically obtained trajectories of Eq. (2) (thin lines) with approximate trajectories calculated by pseudopotential decomposition (17) – (22) up to terms of the form $1/\Omega^{14}$ (solid lines).
The parameter values used are given in Table. Thin and solid lines in Figs. *a* – *d* overlap, so they are visually indistinguishable (in contrast to the curves in Fig. 1)

(18), (20) and including expansion terms up to $1/\Omega^{14}$, with exact (numerical) solutions of system of equations (16). As expected, the accuracy deteriorates rapidly as the parameter q increases (i.e., when approaching the far end of the stability region), so the expressions obtained above are suitable only for moderately high q values (more precisely, only for moderately high secular frequencies $\beta \le 0,62$). Divergence is quite natural when approaching the far end of the stability region corresponding to the secular frequency $\beta = 1$, since the basic assumptions that using the representation of solutions in the form (17) is based on and derivation of the final expressions are not satisfied under parametric resonance between the proper secular oscillations of ions and the forced RF oscillations. The latter are due to external effect of the radio frequency electric field. However, ion trajectories can be calculated with sufficient accuracy using the approximate formulae obtained for the range of secular frequencies $0 \le \beta \le 0,62$.

Eq. (19) yields an improved version of the approximate formula

$$\tilde{\beta}^2 \approx a + q^2/2$$

for the secular oscillation frequency, which is obtained from classical pseudopotential theory:

$$\hat{\beta}^2(a,q) \approx a + \frac{1}{2}q^2 + \frac{1}{2}aq^2 + \left(\frac{1}{2}a^2q^2 + \frac{25}{128}q^4\right) + \left(\frac{1}{2}a^3q^2 + \frac{273}{512}aq^4\right) + \left(\frac{1}{2}a^4q^2 + \frac{2049}{2048}a^2q^4 + \frac{1169}{9216}q^6\right) + \ldots \quad (23)$$

The inequality $0 \le \hat{\beta}^2 \le 1$, or, more precisely, a pair of inequalities

$$\beta_x^2 = \beta^2(a,q) \le 1, \ \ \beta_y^2 = \beta^2(-a,-q) \ge 0,$$

with $a \ge 0$, $q \ge 0$, can be used to approximately calculate the boundaries of the first stability region. Notably, while the inequality $\beta_y^2 = \beta^2(-a,-q) \ge 0$ is sufficiently accurate for describing the near end of the first stability region, then the inequality $\beta_x^2 = \beta^2(a,q) \le 1$ at best provides a qualitative description of the far end of the first stability region.

It follows from the data in Fig. 3 that series (23) diverges near the far end of the first stability region, and, therefore, when approaching the far end of the first stability region, reasonable accuracy can only be achieved by using an incredibly large number of terms in the series.

Conclusion

As a result of the study we have carried out, we have found that the concept of a pseudopotential function can be generalized in a completely constructive way for RF quadrupole fields. The purpose of such generalization is in reducing the discrepancy between the exact and analytical solutions obtained in analysis of simplified models of the object under consideration. In this case, exact solutions cannot be obtained analytically. The resulting algebraic expression in the form of a truncated pseudopotential series allows to significantly expand the range of parameters of the RF field. Motion of charged particles within the framework of the traditional pseudopotential approach, which is characterized by conceptual simplicity and physical clarity, can be described not only qualitatively but also quantitatively in this range. Notably, the approaches offered in [21, 22] lack these advantages.

Unfortunately, the concept of the pseudopotential expanded in this way is not particularly suitable for describing the motion of charged particles when approaching the region of parametric

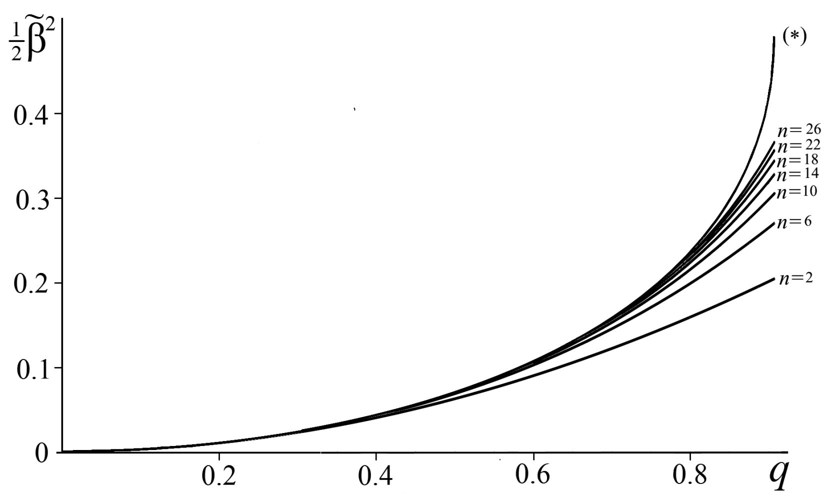

Fig. 3. Quadratic coefficient of pseudopotential (PP) function (23), calculated via PP expansions (17) – (22) with different accuracy orders $1/\Omega^n$ for n = 2 – 26 in the range $0 \le q \le 0,9080$ (a = 0), as a function of q.

The curve (*) corresponds to the function for an analytically accurate value of secular oscillation frequency (calculated in accordance with [21, 22, 31]) resonance $(\beta \approx 1)$, where the motion of charged particles in RF quadrupole fields loses stability. In this case, pseudopotential models [21, 22] that are accurate yet rather cumbersome turn out to be a preferable alternative. The results prove to be acceptable for moderately high secular frequencies lying in the range $0 \le \beta \le 0,62$, while the range of permissible values of the parameter providing acceptable accuracy of calculations is far more narrow $(0 \le \beta \le 0,2)$ for the classical pseudopotential theory.

It is recommended to use the exact theory of quadratic pseudopotential for RF quadrupole fields [21, 22], rather than approximate pseudopotential expansions, for large values of secular frequencies.

Acknowledgment

The authors are grateful to the developers, employees and sponsors of the Numdam digital library [37] for providing open access to a rare publication [23].

This study was carried out within the framework of state task no. 007-00229-18-00 for the Institute of Analytical Instrumentation for the Russian Academy of Sciences.

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Received 18.07.2018, accepted 26.07.2018.

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