A Theory of Anharmonic Perturbations in a Penning Trap

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Classical hamiltonian perturbation theory formulated in terms of action-angle variables is applied to develop a general and systematic method for calculating the influence of anharmonic perturbations on the motion of a charged particle in a Penning trap. Action-angle variables are ideally suited to determine the shifts of the characteristic frequencies in a perturbed orbit. The application of the method is demonstrated by several case studies.

1. Introduction

In the fifty years since its invention the Penning trap [1] has developed into a very important tool of experimental physics, useful wherever high precision experiments demand a long time storage of charged particles [2, 3]. The field configuration of an ideal Penning trap consists of a static electric field, derived from a potential $\Phi \propto (2z^2 - x^2 - y^2)$, and a superimposed static homogeneous magnetic field parallel to the z-axis. It is well known that the motion of a charged particle in this field can be described in terms of three independent harmonic oscillators. In real experimental devices the field configuration differs from the ideal one for a variety of reasons: finite size, imperfections of the geometry of the electrodes, holes, slits and other modifications of the electrodes as required by experiment, misalignments and inhomogeneities of the magnetic field, space charge effects when a large number of ions is trapped, and so on. In as far as these perturbations can be described by harmonic terms added to the hamiltonian of the ideal configuration, they can be taken into account by a principal axis transformation [3, 4]. Anharmonic perturbations lead to more complicated phenomena, instead of three uncoupled harmonic oscillators one has to confront, in general, three coupled anharmonic oscillators. The characteristic frequencies then depend on the constants of motion of the individual particle orbit, and a small change of the particle orbit is accompanied by a corresponding change of the characteristic frequencies.

The aim of this paper is to provide a deeper understanding of these anharmonic effects, assuming they are small enough to be treated by perturbation methods. Already in the last century, problems in celestial mechanics stimulated the development of a systematic perturbation theory, based on the formulation of classical hamiltonian mechanics in terms of action-angle variables [5–7]. Subsequently these methods became very important in the early development of quantum theory, in fact Max Born's "Lectures on the Mechanics of Atoms" [8] are nowadays considered as a standard reference for classical perturbation theory. These methods are likewise applicable to the motion of a charged particle in a Penning trap, because the orbits mostly involve large quantum numbers.

In the following sections we first give a brief sketch of the theory of the ideal Penning trap, followed by an outline of classical hamiltonian perturbation theory applied to a Penning trap with anharmonic perturbations, finally the general results are illustrated by several specific case studies.

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2. The Ideal Penning Trap

The ideal Penning trap consists of the following configuration: A particle of mass m and electric charge q is moving in a static electromagnetic field $\boldsymbol{E} = -\nabla\Phi_0$, $\boldsymbol{B} = \nabla \times \boldsymbol{A}_0$ with potentials given by

$$\Phi_0(x, y, z) = \frac{U_0}{3r_0^2}(2z^2 - x^2 - y^2), \tag{2.1}$$

$$\boldsymbol{A}_0(x, y, z) = \tfrac{1}{2} B_0(-y\,\hat{\boldsymbol{e}}_x + x\,\hat{\boldsymbol{e}}_y). \tag{2.2}$$

Equipotential surfaces of Φ_0 are hyperboloids of revolution. To manufacture an ideal Penning trap, two of these hyperboloids have to be realized as conducting surfaces (see Figure 1). In particular, the one-sheeted hyperboloid containing the point $(x, y, z) = (r_0, 0, 0)$ (i.e. the ring electrode) is on potential $-\frac{1}{3}U_0$, while

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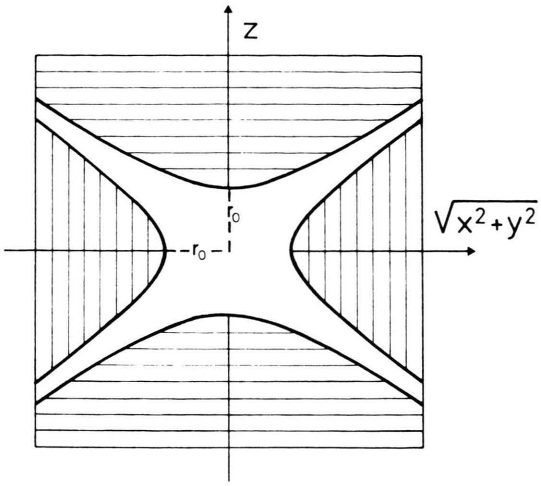

Fig. 1. The figure shows the intersection of an ideal Penning trap with a plane containing the axis of rotational symmetry (z-axis). The heavy lines represent equipotential surfaces realized by the conducting surfaces of the electrodes. In particular, the end cap electrodes (horizontally hatched area) are given by $2z^2 - x^2 - y^2 = 2r_0^2$, the ring electrode (vertically hatched area) by $2z^2 - x^2 - y^2 = -r_0^2$. The case study of Sect. 4.3 assumes the hatched areas to be filled with a material of permeability μ.

the two-sheeted hyperboloid containing the point $(x, y, z) = (0, 0, r_0)$ (i.e. the two cap electrodes) is on potential $+\frac{2}{3}U_0$. The vector potential $\boldsymbol{A}_0$ represents a homogeneous magnetic field parallel to the z-axis, $\boldsymbol{B}_0 = B_0 \hat{\boldsymbol{e}}_z$. The motion of the charged particle is described by the hamiltonian [9]

$$H_0 = \frac{1}{2m}\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}_0\right)^2 + q\Phi_0. \tag{2.3}$$

The equations of motion have the general solution

$$\begin{aligned} x(t) &= +R_+^{(0)} \cos \varphi_+^{(0)}(t) + R_-^{(0)} \cos \varphi_-^{(0)}(t), \\ y(t) &= -R_+^{(0)} \sin \varphi_+^{(0)}(t) - R_-^{(0)} \sin \varphi_-^{(0)}(t), \\ z(t) &= Z^{(0)} \cos \varphi_z^{(0)}(t), \end{aligned} \tag{2.4}$$

where $R_+^{(0)}, R_-^{(0)}, Z^{(0)}$ are constants of motion characterizing the particle orbit, and where the linear functions

$$\begin{aligned} \varphi_+^{(0)}(t) &= \omega_+ t + \alpha_+, \\ \varphi_-^{(0)}(t) &= \omega_- t + \alpha_-, \\ \varphi_z^{(0)}(t) &= \omega_z t + \alpha_z \end{aligned} \tag{2.5}$$

are the "angle variables" that describe the progression of the particle on its orbit. The phases $\alpha_+, \alpha_-, \alpha_z$ are determined e.g. by initial conditions, and the characteristic frequencies are defined by

$$\begin{aligned} \omega_c &= \frac{qB_0}{mc} \quad \text{(cyclotron frequency)}, \\ \omega_z &= \sqrt{\frac{4qU_0}{3mr_0^2}} \quad \text{(axial frequency)}, \\ \omega_1 &= \sqrt{\omega_c^2 - 2\omega_z^2}, \\ \omega_+ &= \tfrac{1}{2}(\omega_c + \omega_1) \quad \text{(modified cyclotron frequency)}, \\ \omega_- &= \tfrac{1}{2}(\omega_c - \omega_1) \quad \text{(magnetron frequency)}. \end{aligned}$$

Confinement of the charged particle to the center of the trap requires $qU_0 > 0$. Under the usual operating conditions [2, 3] one has $\omega_c \gg \omega_z$, and thus

$$\omega_c \approx \omega_+ \gg \omega_z \gg \omega_-. \tag{2.7}$$

The frequencies $\omega_+, \omega_z, \omega_-$ usually differ by one or several orders of magnitude.

The canonical equations of motion also yield the canonical momenta as functions of time

$$\begin{aligned} p_x(t) &= \frac{m\omega_1}{2}\left(-R_+^{(0)} \sin \varphi_+^{(0)}(t) + R_-^{(0)} \sin \varphi_-^{(0)}(t)\right), \\ p_y(t) &= \frac{m\omega_1}{2}\left(-R_+^{(0)} \cos \varphi_+^{(0)}(t) + R_-^{(0)} \cos \varphi_-^{(0)}(t)\right), \\ p_z(t) &= -m\omega_z Z^{(0)} \sin \varphi_z^{(0)}(t). \end{aligned} \tag{2.8}$$

By a canonical transformation [9]

$$\begin{aligned} q_+ &= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_1}{2}}\, x - \sqrt{\frac{2}{m\omega_1}}\, p_y\right), \\ q_- &= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_1}{2}}\, x + \sqrt{\frac{2}{m\omega_1}}\, p_y\right), \\ q_3 &= \sqrt{m\omega_z}\, z, \\ p_+ &= \frac{1}{\sqrt{2}}\left(+\sqrt{\frac{m\omega_1}{2}}\, y + \sqrt{\frac{2}{m\omega_1}}\, p_x\right), \\ p_- &= \frac{1}{\sqrt{2}}\left(-\sqrt{\frac{m\omega_1}{2}}\, y + \sqrt{\frac{2}{m\omega_1}}\, p_x\right), \\ p_3 &= \frac{1}{\sqrt{m\omega_z}}\, p_z \end{aligned} \tag{2.9}$$

the hamiltonian equation (2.3) is brought into the form

$$H_0 = \frac{\omega_+}{2}(q_+^2 + p_+^2) - \frac{\omega_-}{2}(q_-^2 + p_-^2) + \frac{\omega_z}{2}(q_3^2 + p_3^2). \tag{2.10}$$

It is important to note the negative sign in front of the term describing the magnetron motion. It requires the equations of motion

$$\dot{q}_- = -\omega_- p_-, \quad \dot{p}_- = +\omega_- q_- \tag{2.11}$$

as opposed to

$$\dot{q}_+ = +\omega_+ p_+, \quad \dot{p}_+ = -\omega_+ q_+,$$
$$\dot{q}_3 = +\omega_z p_3, \quad \dot{p}_3 = -\omega_z q_3. \tag{2.12}$$

The explicit solution of the equations of motion given by (2.5) and (2.9) shows that we are dealing with a multiple periodic system that is amenable to a description in terms of action and angle variables. The action variables are defined by

$$J_+^{(0)} = \frac{1}{2\pi} \oint p_+ \, \mathrm{d}q_+, \quad J_-^{(0)} = \frac{1}{2\pi} \oint p_- \, \mathrm{d}q_-,$$
$$J_z^{(0)} = \frac{1}{2\pi} \oint p_z \, \mathrm{d}q_z \tag{2.13}$$

with the integral extended over one period of the respective oscillator. The equations (2.11) and (2.12) imply

$$J_+^{(0)} \geqq 0, \quad J_-^{(0)} \leqq 0, \quad J_z^{(0)} \geqq 0. \tag{2.14}$$

By a second canonical transformation [9] we introduce the angle variables $\varphi_+^{(0)}$, $\varphi_-^{(0)}$, $\varphi_z^{(0)}$, which were defined in (2.5), as our new canonical coordinates, with the action variables $J_+^{(0)}, J_-^{(0)}, J_z^{(0)}$, as their corresponding canonical momenta. The hamiltonian then takes the form

$$H_0 = \omega_+ J_+^{(0)} + \omega_- J_-^{(0)} + \omega_z J_z^{(0)}. \tag{2.15}$$

Using (2.9), (2.4) and (2.8) we can evaluate the integrals in (2.13) and obtain the connection between the action variables and the orbital constants $R_+^{(0)}$, $R_-^{(0)}$, $Z^{(0)}$.

$$J_+^{(0)} = \tfrac{1}{2} m\omega_1 (R_+^{(0)})^2, \quad J_-^{(0)} = -\tfrac{1}{2} m\omega_1 (R_-^{(0)})^2,$$
$$J_z^{(0)} = \tfrac{1}{2} m\omega_z (Z^{(0)})^2. \tag{2.16}$$

To obtain the cartesian coordinates and conjugate cartesian momenta in terms of action and angle variables, the expression (2.16) must be inserted into (2.4) and (2.8).

The canonical equations of motion following from (2.15) are

$$\dot{\varphi}_+^{(0)} = \omega_+ = \frac{\partial H_0}{\partial J_+^{(0)}}, \quad \dot{\varphi}_-^{(0)} = \omega_- = \frac{\partial H_0}{\partial J_-^{(0)}},$$
$$\dot{\varphi}_z^{(0)} = \omega_z = \frac{\partial H_0}{\partial J_z^{(0)}}. \tag{2.17}$$

These equations are trivial for the ideal Penning trap, their generalization for the perturbed Penning trap forms the basis of the approach to be described in the next section.

3. The Perturbed Penning Trap

3.1. How to Formulate the Problem

The motion of a particle with mass m and electric charge q in a non-ideal Penning trap can be described by the hamiltonian

$$H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}\right)^2 + q\Phi \tag{3.1}$$

with potentials

$$\Phi = \Phi_0 + \delta\Phi, \quad \boldsymbol{A} = \boldsymbol{A}_0 + \delta\boldsymbol{A}, \tag{3.2}$$

where Φ_0 and $\boldsymbol{A}_0$ are the potentials of the ideal Penning trap, given by (2.1) and (2.2), and where $\delta\Phi$ and $\delta\boldsymbol{A}$ represent the potentials of the static perturbing fields. We can thus write

$$H = H_0 + V \tag{3.3}$$

with

$$V = q\,\delta\Phi - \frac{q}{mc}\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}_0\right)\cdot\delta\boldsymbol{A} + \frac{q^2}{2mc^2}(\delta\boldsymbol{A})^2. \tag{3.4}$$

For physical reasons (no pointlike sources inside the trap) the perturbing potentials $\delta\Phi$ and $\delta\boldsymbol{A}$ may be assumed to be free of singularities and to possess power series expansions in the coordinates x, y, z in a neighbourhood of the origin (center of the trap). Including also the canonical momenta p_x, p_y, p_z in the power counting (they appear in 0th or 1st power only), the perturbing interaction V may likewise be written as a power series expansion in x, y, z, p_x, p_y, p_z:

$$V = V_0 + \lambda V_1 + \lambda^2 V_2 + \lambda^3 V_3 + \lambda^4 V_4 + \ldots, \tag{3.5}$$

where $\lambda^n V_n$ is the sum of all terms of degree n, i.e. all terms of the form $x^{k_1} y^{k_2} z^{k_3} p_x^{k_4} p_y^{k_5} p_z^{k_6}$ with $k_1 + k_2 + k_3 + k_4 + k_5 + k_6 = n$. The parameter λ is the usual counting parameter of perturbation theory, that helps us to organize the calculation and which will be set equal to one in the final results.

3.2. How to Prepare the Hamiltonian

Constant terms in the expansion of the potentials $\delta\Phi$, $\delta\boldsymbol{A}$ are physically irrelevant and can be dropped. Thus $V_0 = 0$, while V_1 receives contributions only from the linear terms in the expansion of $\delta\Phi$. Writing $\lambda V_1 = \frac{1}{2} m \omega_z^2 (2cz - ax - by)$ with suitable coefficients a, b, c, this term can be eliminated by a translation of the origin in phase space: $x' = x + a$, $y' = y + b$, $z' = z + c$, $p'_x = p_x - \frac{1}{2} m \omega_c b$, $p'_y = p_y + \frac{1}{2} m \omega_c a$, $p'_z = p_z$.

The next term $\lambda^2 V_2$ receives its contributions from the quadratic terms in the expansion of $\delta\Phi$ and from the linear terms in the expansion of $\delta\boldsymbol{A}$. The latter ones represent a static homogeneous magnetic field $\delta\boldsymbol{B}_0 = \delta B_0^{\parallel} \hat{\boldsymbol{e}}_z + \delta\boldsymbol{B}_0^{\perp}$, which may have a component $\delta\boldsymbol{B}_0^{\perp}$ perpendicular to the symmetry axis (z-axis) of the Penning trap. Our next goal must be to define as a starting point for the desired perturbation scheme a new 0th order hamiltonian H'_0 that already includes the most important contributions from $\lambda^2 V_2$, but still has the same symmetry properties as H_0. Depending on whether we deem an exact treatment of the magnetic field $\boldsymbol{B}_0 + \delta\boldsymbol{B}_0$ or an exact description of the unperturbed electric potential $\Phi_0(x, y, z)$ to be of greater importance, we have the option to decide for either one of two different strategies.

(I) In the first case we introduce rotated coordinates x', y', z', such that the new z'-axis becomes parallel to $\boldsymbol{B}_0 + \delta\boldsymbol{B}_0$, and we include in H'_0 all contributions from the electric potential that can be written in the form $\frac{1}{4} m \omega_z^2 [(1+\mu)\, 2z'^2 - (1+\varkappa)(x'^2 + y'^2)]$, where μ and $\varkappa$ are suitable constants. Remaining contributions from $H_0 + \lambda^2 V_2$ are treated as a perturbation $\lambda^2 V'_2$.

(II) In the second case we keep the original coordinates x, y, z, thus preserving the relation of the coordinates to the geometry of the electrodes. We include in H'_0 the contribution due to $\delta\boldsymbol{B}_0^{\parallel} = \delta B_0^{\parallel} \hat{\boldsymbol{e}}_z$, as well as all contributions from the electric potential that are symmetric under rotations about the z-axis and under reflections by the xy-plane. The remaining terms together with those describing $\delta\boldsymbol{B}_0^{\perp}$ make up the perturbation $\lambda^2 V'_2$.

Making use of our freedom to choose a suitable gauge, we write

$$\delta\boldsymbol{A}_0 = \tfrac{1}{2}(\delta\boldsymbol{B}_0 \times \boldsymbol{x}) = \frac{\delta B_0^{\parallel}}{B_0} \boldsymbol{A}_0 + \tfrac{1}{2}(\delta\boldsymbol{B}_0^{\perp} \times \boldsymbol{x})$$

and define for the above two cases

case (I):

$$\boldsymbol{A}' = \boldsymbol{A}_0 + \delta\boldsymbol{A}_0, \qquad \boldsymbol{B}' = \boldsymbol{B}_0 + \delta\boldsymbol{B}_0, \qquad \delta\boldsymbol{B}' = 0;$$

case (II):

$$\boldsymbol{A}' = \left(1 + \frac{\delta B_0^{\parallel}}{B_0}\right) \boldsymbol{A}_0, \quad \boldsymbol{B}' = (B_0 + \delta B_0^{\parallel})\, \hat{\boldsymbol{e}}_z, \quad \delta\boldsymbol{B}' = \delta\boldsymbol{B}_0^{\perp}.$$

The new 0th order hamiltonian can then be written as

$$H'_0 = \frac{1}{2m}\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}'\right)^2 + \frac{m\omega_z^2}{4}[(1+\mu)\, 2z^2 - (1+\varkappa)(x^2+y^2)]. \qquad (3.6)$$

In case (I) we have for reasons of simplicity suppressed the primes on the coordinates and have denoted the rotated coordinates by x, y, z. The constants μ, $\varkappa$ must be computed from Φ_0 and the power series expansion of $\delta\Phi$. In case (II) x, y, z are the original coordinates and the constants μ, $\varkappa$ are obtained from $\delta\Phi$ alone. The constants μ, $\varkappa$ can assume positive or negative values. The effect of the perturbing terms to be included in the new 0th order hamiltonian H'_0 is merely a redefinition of the frequencies. With $B' = |\boldsymbol{B}'|$ we have

$$\omega'_z = \omega_z \sqrt{1+\mu}, \qquad \omega'_c = \frac{q}{mc} B',$$
$$\omega'_1 = \sqrt{\omega_c'^2 - 2\omega_z^2 (1+\varkappa)}, \quad \omega'_{\pm} = \tfrac{1}{2}(\omega'_c \pm \omega'_1). \qquad (3.7)$$

The remaining perturbation terms of order λ^2 are collected in $\lambda^2 V'_2$. Among these, either the one proportional to xy or the one proportional to $x^2 - y^2$ can be eliminated by a rotation of the coordinate axes in the xy-plane with the z-axis fixed. Thus, without loss of generality the remaining 2nd order perturbation may be assumed to be given in the form

$$\lambda^2 V'_2 = q[a(x^2 - y^2) + bxz + cyz] - \frac{q}{2mc}\, \delta\boldsymbol{B}' \cdot \left[\boldsymbol{x} \times \left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}'\right)\right]. \qquad (3.8)$$

The ideal Penning trap is symmetric with respect to rotations around the z-axis and to reflections by the xy-plane. The first term in the expression (3.8) breaks these symmetries, the second one describes a misalignment of the homogeneous magnetic field. Without anharmonic terms, the 2nd order problem can be solved numerically by a transformation to principal axes [4]. For treating anharmonic perturbations, however, it is more convenient to take advantage of the simplicity and the symmetry properties of the hamiltonian H'_0 of (3.6).

A general parametrisation of the anharmonic terms $\lambda^3 V_3$, $\lambda^4 V_4$, ... in (3.5) involves a large number of arbitrary parameters. This number can be reduced considerably by using the Coulomb gauge for the vector potential and by observing that we must have

$$\Delta(\delta\Phi) = -4\pi\varrho, \quad \Delta(\delta A) = -\frac{4\pi}{c}\boldsymbol{j}, \tag{3.9}$$

where ϱ represents the space charge density inside the trap and $\boldsymbol{j}$ the associated current density [10].

3.3. How to Perform the Perturbation Calculation

We have now set the stage for the perturbation treatment of the hamiltonian

$$H = H_0' + \lambda^2 V_2' + \lambda^3 V_3 + \lambda^4 V_4 + \dots. \tag{3.10}$$

The first step is to express this hamiltonian in terms of the action and angle variables J_k' and φ_k' of the hamiltonian H_0', with $k = +, -, z$. By a slight generalization of the results of Section 2 we find

$$x(t) = \sqrt{\frac{2}{m\omega_1'}}\left(+\sqrt{J_+'}\cos\varphi_+'(t) + \sqrt{|J_-'|}\cos\varphi_-'(t)\right),$$

$$y(t) = \sqrt{\frac{2}{m\omega_1'}}\left(-\sqrt{J_+'}\sin\varphi_+'(t) - \sqrt{|J_-'|}\sin\varphi_-'(t)\right),$$

$$z(t) = \sqrt{\frac{2}{m\omega_z'}}\cdot\sqrt{J_z'}\cos\varphi_z'(t), \tag{3.11}$$

$$p_x(t) = \sqrt{\frac{m\omega_1'}{2}}\left(-\sqrt{J_+'}\sin\varphi_+'(t) + \sqrt{|J_-'|}\sin\varphi_-'(t)\right),$$

$$p_y(t) = \sqrt{\frac{m\omega_1'}{2}}\left(-\sqrt{J_+'}\cos\varphi_+'(t) + \sqrt{|J_-'|}\cos\varphi_-'(t)\right),$$

$$p_z(t) = -\sqrt{2m\omega_z'}\cdot\sqrt{J_z'}\sin\varphi_z'(t) \tag{3.12}$$

with ω_1', ω_z', $\omega_\pm'$ given by (3.7) and $\varphi_k'(t) = \omega_k' t + \alpha_k'$.

The 0th order hamiltonian is, of course,

$$H_0' = \omega_+' J_+' + \omega_-' J_-' + \omega_z' J_z'. \tag{3.13}$$

By inserting (3.11) and (3.12) into the perturbing terms $\lambda^n V_n$, these are immediately obtained as Fourier series

$$\lambda^n V_n = \sum_{j_+, j_-, j_z} A^{(n)}_{j_+, j_-, j_z}(J_+', J_-', J_z') \cdot \exp(i[j_+\varphi_+'(t) + j_-\varphi_-'(t) + j_z\varphi_z'(t)]). \tag{3.14}$$

The j_+, j_-, j_z are integer numbers, positive, negative, or zero, and by construction the range of the summation underlies the restriction $|j_+| + |j_-| + |j_z| \leqq n$. For later purposes it is important to note that for odd (even) n the sum $j_+ + j_- + j_z$ is always an odd (even) integer. Therefore, a time-independent term can occur in the expansion (3.14) only for even n. For more compact notation we shall in the following denote the Fourier coefficients also by $A_j^{(n)}(J')$.

The perturbation method aims at finding new action and angle variables $J_+, J_-, J_z, \varphi_+, \varphi_-, \varphi_z$ such that the full hamiltonian H is a function of the new action variables only. The desired hamiltonian is

$$H = H(J_+, J_-, J_z), \tag{3.15}$$

from which one derives the canonical equations of motion ($k = +, -, z$)

$$\frac{\mathrm{d}}{\mathrm{d}t}\varphi_k(t) = +\frac{\partial H}{\partial J_k} = \Omega_k(J_+, J_-, J_z), \tag{3.16}$$

$$\frac{\mathrm{d}J_k}{\mathrm{d}t} = -\frac{\partial H}{\partial \varphi_k} = 0, \tag{3.17}$$

implying that the new action variables are indeed constants of the motion and that the characteristic frequencies Ω_k, i.e. the time derivatives of the angle variables, depend on the constants of motion J_+, J_-, J_z and thus may differ for different particle orbits. Only when H is a linear function of the action variables (as is the case for H_0') the characteristic frequencies are the same for all particle orbits.

The desired new action and angle variables are constructed by means of a canonical transformation with generating function

$$S(\varphi_+', \varphi_-', \varphi_z', J_+, J_-, J_z) = \sum_{n=0}^{\infty} \lambda^n S_n(\varphi_+', \varphi_-', \varphi_z', J_+, J_-, J_z), \tag{3.18}$$

where

$$S_0(\varphi', J) = \varphi_+' J_+ + \varphi_-' + \varphi_z' J_z \tag{3.19}$$

is the generating function of the identity. In terms of the generating function S we have with $k = +, -, z$

$$\varphi_k = \frac{\partial S}{\partial J_k} = \varphi_k' + \sum_{n=1}^{\infty} \lambda^n \frac{\partial}{\partial J_k} S_n(\varphi', J), \tag{3.20}$$

$$J_k' = \frac{\partial S}{\partial \varphi_k'} = J_k + \sum_{n=1}^{\infty} \lambda^n \frac{\partial}{\partial \varphi_k'} S_n(\varphi', J). \tag{3.21}$$

By the developments leading up to (3.14) we had brought the hamiltonian H into the form

$$H = H_0'(J') + \sum_{n=2}^{\infty} \lambda^n V_n(\varphi', J'). \tag{3.22}$$

By insertion of (3.21) into this result we obtain

$$H(J) = H_0'(J) + \sum_{n=1}^{\infty} \lambda^n \sum_k \omega_k' \frac{\partial S_n}{\partial \varphi_k'} + \sum_{n=2}^{\infty} \lambda^n V_n\left(\varphi', J + \sum_{m=1}^{\infty} \lambda^m \frac{\partial S_m}{\partial \varphi'}\right), \tag{3.23}$$

and by a subsequent Taylor expansion

$$H(J) = H'_0(J) + \sum_{n=2}^{\infty} \lambda^n H_n(J)\,. \qquad (3.24)$$

At this point it is crucial to note that the right hand side must be independent of $\varphi_+, \varphi_-, \varphi_z$ term by term, and that there can be no time dependence via the $\varphi_k(t)$. In the course of our construction of H'_0 the terms linear in x, y, z, p_x, p_y, p_z had been eliminated, and thus the term linear in λ is missing in (3.22). On comparison with (3.23) we conclude that we must have

$$\frac{\partial S_1}{\partial \varphi'_+} = \frac{\partial S_1}{\partial \varphi'_-} = \frac{\partial S_1}{\partial \varphi'_z} = 0\,, \qquad (3.25)$$

so that all summations actually start with $n=2$ and $m=2$, respectively.

On comparing (3.23) and (3.24) term by term for $\lambda = 2, \ldots, 6$ one obtains the following relations ($k, l = +, -, z$):

$$H_2(J) = \sum_k \omega'_k \frac{\partial S_2}{\partial \varphi'_k} + V'_2(\varphi', J)\,, \qquad (3.26)$$

$$H_3(J) = \sum_k \omega'_k \frac{\partial S_3}{\partial \varphi'_k} + V_3(\varphi', J)\,, \qquad (3.27)$$

$$H_4(J) = \sum_k \omega'_k \frac{\partial S_4}{\partial \varphi'_k} + V_4(\varphi', J) + \sum_k \frac{\partial V'_2}{\partial J_k} \cdot \frac{\partial S_2}{\partial \varphi'_k}\,, \qquad (3.28)$$

$$H_5(J) = \sum_k \omega'_k \frac{\partial S_5}{\partial \varphi'_k} + V_5(\varphi', J) + \sum_k \left(\frac{\partial V_3}{\partial J_k} \cdot \frac{\partial S_2}{\partial \varphi'_k} + \frac{\partial V'_2}{\partial J_k} \cdot \frac{\partial S_3}{\partial \varphi'_k} \right), \qquad (3.29)$$

$$H_6(J) = \sum_k \omega'_k \frac{\partial S_6}{\partial \varphi'_k} + V_6(\varphi', J) + \sum_k \left(\frac{\partial V_4}{\partial J_k} \cdot \frac{\partial S_2}{\partial \varphi'_k} + \frac{\partial V_3}{\partial J_k} \cdot \frac{\partial S_3}{\partial \varphi'_k} + \frac{\partial V'_2}{\partial J_k} \cdot \frac{\partial S_4}{\partial \varphi'_k} \right) + \frac{1}{2} \sum_k \sum_l \frac{\partial^2 V'_2}{\partial J_k \, \partial J_l} \cdot \frac{\partial S_2}{\partial \varphi'_k} \cdot \frac{\partial S_2}{\partial \varphi'_l}\,. \qquad (3.30)$$

As emphasized before, the right hand sides must actually be independent of $\varphi_+, \varphi_-, \varphi_z$.

Similar to the perturbation V the generating function S may be assumed to be given in the form of a Fourier series

$$\lambda^n S_n = \sum_{j_+, j_-, j_z} B^{(n)}_{j_+, j_-, j_z}(J_+, J_-, J_z) \cdot \exp(i[j_+ \varphi'_+(t) + j_- \varphi'_-(t) + j_z \varphi'_z(t)]) \qquad (3.31)$$

with the derivative

$$\lambda^n \frac{\partial}{\partial \varphi'_k} S_n = \sum_{j_+, j_-, j_z} i j_k \, B^{(n)}_{j_+, j_-, j_z}(J_+, J_-, J_z) \cdot \exp(i[j_+ \varphi'_+(t) + j_- \varphi'_-(t) + j_z \varphi'_z(t)])\,. \qquad (3.32)$$

Note that (3.32) contains no term constant in time, i.e. with $j_+ = j_- = j_z = 0$. The time average of (3.32) must therefore vanish. Equation (3.26) implies, because the left hand side is constant in time,

$$\lambda^2 H_2(J) = A'^{(2)}_{000}(J) \qquad (3.33)$$

and

$$B^{(2)}_{j_+ j_- j_z}(J) = i \frac{A'^{(2)}_{j_+ j_- j_z}(J)}{j_+ \omega'_+ + j_- \omega'_- + j_z \omega'_z}\,, \qquad (j_+, j_-, j_z) \neq (0, 0, 0)\,. \qquad (3.34)$$

Recalling our remarks following (3.14) we know that the time average of V_3 must vanish, and thus we can conclude $H_3(J) = 0$ and

$$B^{(3)}_{j_+ j_- j_z}(J) = i \frac{A'^{(3)}_{j_+ j_- j_z}(J)}{j_+ \omega'_+ + j_- \omega'_- + j_z \omega'_z}\,, \qquad (j_+, j_-, j_z) \neq (0, 0, 0)\,. \qquad (3.35)$$

Quite generally we observe that the structure of our perturbation expansion is such that the Fourier series for $\lambda^n S_n$ contains for odd (even) n only terms, for which $j_+ + j_- + j_z$ is an odd (even) integer. This follows from the corresponding observation after (3.14) on the Fourier series of $\lambda^n V_n$ and the structure of (3.26)–(3.30). The immediate consequence is

$$H_n(J) = 0 \quad \text{for all odd } n. \qquad (3.36)$$

The expression for $H_4(J)$ is obtained as the time average, denoted by $\langle \cdots \rangle$, of the right hand side of (3.28).

$$\lambda^4 H_4(J) = A^{(4)}_{000}(J) + \lambda^4 \left\langle \sum_k \frac{\partial V'_2}{\partial J_k} \cdot \frac{\partial S_2}{\partial \varphi'_k} \right\rangle. \qquad (3.37)$$

Using $A'^{(2)}_{-j}(J) = (A'^{(2)}_j(J))^*$ and (3.32), (3.34), this can be evaluated in the form

$$\lambda^4 H_4(J) = A^{(4)}_{000}(J) - \frac{1}{2} \sum_{j_+, j_-, j_z} \sum_k \frac{j_k}{j_+ \omega'_+ + j_- \omega'_- + j_z \omega'_z} \cdot \frac{\partial}{\partial J_k} (|A^{(2)}_{j_+ j_- j_z}(J)|^2)\,. \qquad (3.38)$$

The sextic contribution to $H(J)$ is obtained as the time average of the right hand side of (3.30):

$$\lambda^6 H_6(J) = A_{000}^{(6)}(J) + \lambda^6 \left\langle \sum_k \left(\frac{\partial V_4}{\partial J_k} \cdot \frac{\partial S_2}{\partial \varphi_k'} + \frac{\partial V_3}{\partial J_k} \cdot \frac{\partial S_3}{\partial \varphi_k'} + \frac{\partial V_2'}{\partial J_k} \cdot \frac{\partial S_4}{\partial \varphi_k'} \right) \right\rangle + \frac{1}{2} \lambda^6 \left\langle \sum_k \sum_l \frac{\partial^2 V_2'}{\partial J_k \partial J_l} \cdot \frac{\partial S_2}{\partial \varphi_k'} \cdot \frac{\partial S_2}{\partial \varphi_l'} \right\rangle, \tag{3.39}$$

which can be further evaluated using (3.32), (3.34) and (3.35), the expression for $B_j^4(J)$ being determined by (3.28).

The main goal of these developments has now been reached: The characteristic frequencies of a perturbed Penning trap can be calculated as a perturbation series up to any desired order, using (3.16), (3.24), (3.33), (3.38), and so on. Thus, including all terms up to 4th order we have (for $k = +, -, z$)

$$\Omega_k(J_+, J_-, J_z) = \omega_k' + \frac{\partial}{\partial J_k} A_{000}'^{(2)}(J) + \frac{\partial}{\partial J_k} A_{000}^{(4)}(J) - \frac{1}{2} \sum_{j_+, j_-, j_z} \sum_l \frac{j_l}{j_+ \omega_+' + j_- \omega_-' + j_z \omega_z'} \cdot \frac{\partial^2}{\partial J_k \partial J_l} (|A_{j_+ j_- j_z}'^{(2)}(J)|^2). \tag{3.40}$$

In the next section the application of this formula will be demonstrated by several typical case studies.

4. Applications

In this section we demonstrate the application of the general theory to several specific problems, which we hope are instructive and useful examples for the type of questions that are encountered in practice.

4.1. Perturbations of the Electric Potential

Perturbations of the electric potential can be caused by deviations of the geometric shape of the electrodes from ideal hyperboloids of revolution, by misalignments, by the finite size of the apparatus, by holes and slits in the electrodes as are necessary for experimental purposes, by additional surface charges on the electrodes, as may be the case when these are covered with a nonconducting oxyde layer, and by other similar causes. We expressly assume that there are no space charges (due to a particle cloud) at the center of the trap. Under this assumption the perturbations $\delta\Phi$ considered here must satisfy Laplace's differential equation in the interior of the trap

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \delta\Phi(x) = 0 . \tag{4.1}$$

This fact implies that $\delta\Phi$ must possess an expansion in spherical harmonics

$$\delta\Phi(x) = \sum_{l=1}^{\infty} \sum_{m=-l}^{m=+l} \sqrt{\frac{4\pi}{2l+1}} Q_{lm} \cdot (x^2+y^2+z^2)^{l/2} Y_{lm}\left(\frac{x}{|x|}\right). \tag{4.2}$$

The coefficients Q_{lm} (analogous to multipole moments) completely characterize the perturbation $\delta\Phi$, and because $\delta\Phi$ is real, they must satisfy

$$Q_{l,-m} = (-1)^m Q_{lm}^* . \tag{4.3}$$

In the expansion (4.2) the $l=0$ term has been omitted as physically irrelevant. The $l=1$ terms can be eliminated, as discussed in Sect. 3, by a translation of the origin of our coordinates in phase space. It is conceivable, however, that in certain situations this translation would render the computation of higher order terms more difficult, e.g. when surface integrals over the hyperboloids of the electrodes have to be evaluated or other geometric considerations come into play. We may then choose the alternative procedure of treating the $l=1$ terms by perturbation theory too. In that case, in the language of Sect. 3, we have $\lambda V_1 \neq 0$, and we must in the formal developments of Sect. 3 keep all terms involving V_1 or S_1. In the following, the $l=1$ terms will not further be considered, and the summation in (4.2) will be assumed to start with $l=2$.

Symmetries of the perturbation $\delta\Phi$ can be used to reduce the number of relevant coefficients Q_{lm}. Rotational symmetry around the z-axis requires the vanishing of all coefficients Q_{lm} with $m \neq 0$, i.e. $Q_{lm} = \delta_{0m} Q_{l0}$. Symmetry under space reflections with respect to the origin requires $Q_{lm} = 0$ for all odd l. Symmetry with respect to reflections by the xz-plane implies that all Q_{lm} must be real.

Thus a perturbation invariant under rotations around the z-axis and under space reflections can be expanded in the form

$$\delta\Phi(x) = \sum_{k=1}^{\infty} Q_{2k,0} \cdot (x^2+y^2+z^2)^k P_{2k}\left(\frac{z}{\sqrt{x^2+y^2+z^2}}\right). \tag{4.4}$$

Inserting the expressions for the spherical harmonics and using $r^2 = x^2 + y^2$ we obtain

$$\delta\Phi(x) = Q_{20} \cdot \tfrac{1}{2}(2z^2 - r^2) + Q_{40} \cdot \tfrac{1}{8}(8z^4 - 24z^2r^2 + 3r^4) + Q_{60} \cdot \tfrac{1}{16}(16z^6 - 120z^4r^2 + 90z^2r^4 - 5r^6) + \ldots \tag{4.5}$$

The quadratic term can be absorbed into H_0 by redefinition of the frequencies ω_z and ω_1, as discussed in Section 3. The quartic and sextic anharmonic terms are uniquely determined in their functional form, only their strength parameters Q_{40} and Q_{60} are variable.

Let us now apply the perturbation theory of Section 3 to evaluate the effect of the perturbing potential given by (4.5). We first define a new 0th order hamiltonian

$$H'_0 = H_0 + \lambda^2 V_2 = H_0 + q Q_{20} \cdot \tfrac{1}{2}(2z^2 - r^2) \tag{4.6}$$

and the modified frequencies:

$$\begin{aligned} \omega'_z &= \sqrt{\frac{2q}{m}\left(\frac{2U_0}{3r_0^2} + Q_{20}\right)}, \\ \omega'_1 &= \sqrt{\omega_c^2 - 2\omega_z'^2}, \\ \omega'_\pm &= \tfrac{1}{2}(\omega_c \pm \omega'_1). \end{aligned} \tag{4.7}$$

The remaining perturbation is

$$V' = \lambda^4 V_4 + \lambda^6 V_6 \tag{4.8}$$

with

$$\lambda^4 V_4 = q Q_{40} \cdot \tfrac{1}{8}(8z^4 - 24 z^2 r^2 + 3r^4), \tag{4.9}$$

$$\lambda^6 V_6 = q Q_{60} \cdot \tfrac{1}{16}(16 z^6 - 120\, z^4 r^2 + 90 z^2 r^4 - 5 r^6). \tag{4.10}$$

With $V'_2 = V_3 = V_5 = 0$ our general equations (3.26) to (3.30) imply $S_2 = S_3 = S_5 = 0$, and thus

$$\begin{aligned} H(J) &= H'_0(J) + \lambda^4 H_4(J) + \lambda^6 H_6(J) \\ &= H'_0(J) + A^{(4)}_{000}(J) + A^{(6)}_{000}(J). \end{aligned} \tag{4.11}$$

All that is still required is the calculation of the Fourier coefficients $A^{(4)}_{000} = \langle \lambda^4 V_4 \rangle$ and $A^{(6)}_{000} = \langle \lambda^6 V_6 \rangle$. From (3.11) we have

$$r^2(t) = \frac{2}{m\omega'_1}\left(J'_+ - J'_- + 2\sqrt{J'_+ |J'_-|}\cos(\varphi'_+(t) - \varphi'_-(t))\right), \tag{4.12}$$

$$z^2(t) = \frac{J'_z}{m\omega'_z}(1 + \cos 2\varphi'_z(t)). \tag{4.13}$$

By straightforward algebra, using identities for the trigonometric functions, we find

$$A^{(4)}_{000}(J) = \frac{3}{2} \cdot \frac{qQ_{40}}{m^2}\left[\frac{J_z^2}{\omega_z'^2} - \frac{4J_z(J_+ - J_-)}{\omega'_1 \omega'_z} + \frac{J_+^2 + J_-^2 - 4J_+ J_-}{\omega_1'^2}\right], \tag{4.14}$$

$$\begin{aligned} A^{(6)}_{000}(J) = \frac{5}{2} \cdot \frac{qQ_{60}}{m^3}\Bigg[&\frac{1}{\omega_z'^3} J_z^3 - \frac{5}{\omega_z'^2 \omega'_1} J_z^2 (J_+ - J_-) \\ &+ \frac{5}{\omega'_z \omega_1'^2} J_z (J_+^2 + J_-^2 - 4J_+ J_-) - \frac{1}{\omega_1'^3}(J_+^3 - 9J_+^2 J_- + 9J_+ J_-^2 - J_-^3)\Bigg]. \end{aligned} \tag{4.15}$$

From (3.40) we now obtain immediately the characteristic frequencies of the orbit of the trapped particle:

$$\begin{aligned} \Omega_+(J_+, J_-, J_z) &= \omega'_+ + \frac{3qQ_{40}}{m^2}\left[-\frac{2}{\omega'_1\omega'_z} J_z + \frac{1}{\omega_1'^2}(J_+ - 2J_-)\right] \\ &\quad + \frac{5}{2} \cdot \frac{q\,Q_{60}}{m^3}\left[-\frac{5}{\omega_z'^2 \omega'_1} J_z^2 + \frac{10}{\omega'_z \omega_1'^2} J_z(J_+ - 2J_-) - \frac{3}{\omega_1'^3}(J_+^2 - 6J_+ J_- + 3J_-^2)\right], \\ \Omega_-(J_+, J_-, J_z) &= \omega'_- + \frac{3qQ_{40}}{m^2}\left[+\frac{2}{\omega'_1\omega'_z} J_z + \frac{1}{\omega_1'^2}(J_- - 2J_+)\right] \\ &\quad + \frac{5}{2} \cdot \frac{q\,Q_{60}}{m^3}\left[+\frac{5}{\omega_z'^2 \omega'_1} J_z^2 + \frac{10}{\omega'_z \omega_1'^2} J_z(J_- - 2J_+) + \frac{3}{\omega_1'^3}(J_-^2 - 6J_+ J_- + 3J_+^2)\right], \\ \Omega_z(J_+, J_-, J_z) &= \omega'_z + \frac{3qQ_{40}}{m^2}\left[+\frac{1}{\omega_z'^2} J_z - \frac{2}{\omega'_1\omega'_z}(J_+ - J_-)\right] \\ &\quad + \frac{5}{2} \cdot \frac{q\,Q_{60}}{m^3}\left[\frac{3}{\omega_z'^3} J_z^2 - \frac{10}{\omega_z'^2 \omega'_1} J_z(J_+ - J_-) + \frac{5}{\omega'_z \omega_1'^2}(J_+^2 - 4J_+ J_- + J_-^2)\right]. \end{aligned} \tag{4.16}$$

This result has a rather abstract appearance. To cast it into a more practical form we write on the basis of (3.21), (3.11), and (2.16)

$$J_k = J'_k - \lambda^4 \frac{\partial}{\partial \varphi'_k} S_4(\varphi', J) + \ldots \approx J'_k, \qquad (4.17)$$

$$J_+ \approx +\tfrac{1}{2} m\omega'_1 R'^2_+, \quad J_- \approx -\tfrac{1}{2} m\omega'_1 R'^2_-,$$

$$J_z \approx +\tfrac{1}{2} m\omega'_z Z'^2, \qquad (4.18)$$

where R'_+, R'_-, Z' denote the amplitudes of the three harmonic oscillators contained in H'_0. Dropping for further simplification the contributions from sextic perturbations, (4.16) assumes the form

$$\Omega_+(R'_+, R'_-, Z') = \omega'_+ + \frac{3}{2} \cdot \frac{qQ_{40}}{m\omega'_1} (R'^2_+ + 2R'^2_- - 2Z'^2), \qquad (4.19)$$

$$\Omega_-(R'_+, R'_-, Z') = \omega'_- + \frac{3}{2} \cdot \frac{qQ_{40}}{m\omega'_1} (-2R'^2_+ - R'^2_- + 2Z'^2),$$

$$\Omega_z(R'_+, R'_-, Z') = \omega'_z + \frac{3}{2} \cdot \frac{qQ_{40}}{m\omega'_z} (-2R'^2_+ - 2R'^2_- + Z'^2),$$

When these equations are applied to an ensemble of trapped particles, with orbit parameters R'_+, R'_-, Z' distributed over a finite interval, then a finite linewidth is expected for the three characteristic frequencies.

The considerations above have assumed rotational invariance around the z-axis. There are, however, interesting applications for which this assumption is too stringent. For example, experimental techniques often require that the ring electrode be divided into two equal pieces by a slit of finite width coincident with the xz-plane. In this situation we still have invariance with respect to reflections by the xy-plane, by the xz-plane, and by the yz-plane, implying symmetries also under space reflections with respect to the origin and under rotations by 180° around the z-axis. As consequence, in (4.2) the coefficients Q_{lm} must vanish when l is odd or when l is even and m is odd. The nonvanishing coefficients must be real. Thus, inluding contributions up to $l=4$, (4.2) reads

$$\delta\Phi(x) = \sqrt{\frac{4\pi}{5}} (x^2+y^2+z^2) [Q_{20} Y_{20} + Q_{22}(Y_{22} + Y_{2-2})]$$
$$+ \sqrt{\frac{4\pi}{9}} (x^2+y^2+z^2)^2 [Q_{40} Y_{40} + Q_{42}(Y_{42} + Y_{4-2}) + Q_{44}(Y_{44} + Y_{4-4})] + \ldots \qquad (4.20)$$

By insertion of the expressions for the spherical harmonics we obtain

$$\delta\Phi(x) = Q_{20} \cdot \tfrac{1}{2}(2z^2 - x^2 - y^2) + Q_{22} \cdot \sqrt{\tfrac{3}{2}}(x^2 - y^2)$$
$$+ Q_{40} \cdot \tfrac{1}{8}(8z^4 - 24z^2(x^2+y^2) + 3(x^2+y^2)^2)$$
$$+ Q_{42} \cdot \sqrt{\tfrac{5}{8}}(6z^2 - x^2 - y^2)(x^2 - y^2)$$
$$+ Q_{44} \cdot \sqrt{\tfrac{35}{32}}(x^4 - 6x^2y^2 + y^4) + \ldots \qquad (4.21)$$

The coefficients Q_{lm} must be computed by analyzing the geometry of the modified Penning trap. Brown and Gabrielse [3] argue that this can be done to a good approximation by representing the slit by a layer of electric dipoles. We will not further pursue this question but assume the coefficients to be known.

For the perturbation treatment we proceed in a similar fashion as before. A new 0th order hamiltonian and new 0th order frequencies are defined by (4.6) and (4.7). The remaining perturbation of order λ^2

$$\lambda^2 V'_2 = qQ_{22} \cdot \sqrt{\tfrac{3}{2}}(x^2 - y^2) \qquad (4.22)$$

is Fourier analyzed using

$$x^2 - y^2 = \frac{2}{m\omega'_1} (J'_+ \cos 2\varphi'_+(t) - J'_- \cos 2\varphi'_-(t) + 2\sqrt{J'_+ |J'_-|} \cos[\varphi'_+(t) + \varphi'_-(t)]). \qquad (4.23)$$

This expression contains no constant term, and thus we obtain no contribution of order λ^2 to (3.24). The contribution to $H(J)$ of order λ^4 can be read off from (3.37) or (3.38). We find that the terms in $\delta\Phi$ coming from $l=4$, $m=\pm 2$ and from $l=4$, $m=\pm 4$ have no constant term in their Fourier expansion, and thus $A^{(4)}_{000}(J)$ is again given by (4.14). Including all contributions up to order λ^4, the hamiltonian in terms of action-angle variables is given, according to (3.38), by

$$H(J) = H'_0(J) + \frac{3(qQ_{22})^2}{m^2 \omega'_1 \omega_c} \left(\frac{J_+}{\omega'_+} - \frac{J_-}{\omega'_-} \right) + A^{(4)}_{000}(J) + \ldots \qquad (4.24)$$

The second term on the right hand side implies a well defined constant shift of the modified cyclotron frequency and of the magnetron frequency.

4.2. Misalignment of the Magnetic Field and the Electrodes

In the ideal Penning trap as described in Sect. 2 the magnetic field $\boldsymbol{B}_0 = B_0 \hat{\boldsymbol{e}}_z$ is strictly parallel to the axis of rotational symmetry of the electrodes. In actual experimental devices the magnetic field $\boldsymbol{B}$ is sometimes slightly tilted against this symmetry axis, causing a shift of the characteristic frequencies:

$$\boldsymbol{B}=B_0(\hat{\boldsymbol{e}}_x \sin\alpha\cos\beta+\hat{\boldsymbol{e}}_y \sin\alpha\sin\beta+\hat{\boldsymbol{e}}_z\cos\alpha). \quad (4.25)$$

Setting $\boldsymbol{B}=\boldsymbol{B}_0+\delta\boldsymbol{B}_0$, we can study the perturbation due to $\delta\boldsymbol{B}_0$ by either one of the two strategies outlined in Section 3. Beyond its experimental significance, this problem is very interesting because it permits an assessment of the accuracy of our perturbation method by comparing its results numerically against the exact values of characteristic frequencies for a misaligned magnetic field, which can be found as solutions of an eigenvalue problem according to work by Brown and Gabrielse [4]. It will be shown below that our computational Method (I), which uses rotated coordinates with the direction of $\boldsymbol{B}$ as new z-direction and considers the electrodes rather than the magnetic field as misaligned, leads to much more accurate results than the Method (II), which considers $\boldsymbol{B}$ as misaligned and treats $\delta\boldsymbol{B}_0$ as a perturbation.

Our calculations below will be based on the hamiltonian

$$H=\frac{1}{2m}\left(\boldsymbol{p}-\frac{q}{c}\boldsymbol{A}\right)^2+\tfrac{1}{4}m\omega_z^2[2z^2-x^2-y^2-\varepsilon(x^2-y^2)], \quad (4.26)$$

where $\boldsymbol{A}=\frac{1}{2}(\boldsymbol{B}\times\boldsymbol{x})$, with $\boldsymbol{B}$ given by (4.25). For more complete comparison with the work by Brown and Gabrielse [4] we have included in H also an axial asymmetry of the electrodes described by the parameter ε.

Method I: Introducing a rotated cartesian coordinate frame with coordinates x', y', z' and unit vectors

$$\begin{aligned}\hat{\boldsymbol{e}}'_x &= \hat{\boldsymbol{e}}_x\cos\alpha\cos\beta+\hat{\boldsymbol{e}}_y\cos\alpha\sin\beta-\hat{\boldsymbol{e}}_z\sin\alpha,\\ \hat{\boldsymbol{e}}'_y &= -\hat{\boldsymbol{e}}_x\sin\beta+\hat{\boldsymbol{e}}_y\cos\beta, \qquad (4.27)\\ \hat{\boldsymbol{e}}'_z &= \hat{\boldsymbol{e}}_x\sin\alpha\cos\beta+\hat{\boldsymbol{e}}_y\sin\alpha\sin\beta+\hat{\boldsymbol{e}}_z\cos\alpha\end{aligned}$$

we have

$$\boldsymbol{B}=B_0\hat{\boldsymbol{e}}'_z \quad\text{and}\quad \boldsymbol{A}=\tfrac{1}{2}(\boldsymbol{B}\times\boldsymbol{x})=\tfrac{1}{2}B_0(-y'\hat{\boldsymbol{e}}'_x+x'\hat{\boldsymbol{e}}'_y).$$

The hamiltonian (4.26) can then be rewritten as

$$H=H'_0+V' \quad (4.28)$$

with

$$H'_0=\frac{1}{2m}\left(\boldsymbol{p}-\frac{q}{c}\boldsymbol{A}\right)^2+\tfrac{1}{4}m\omega_z^2[1-\tfrac{1}{2}\sin^2\alpha\cdot(3+\varepsilon\cos2\beta)]\cdot[2z'^2-x'^2-y'^2], \quad (4.29)$$

$$V'=a(x'^2-y'^2)+b\cdot2x'y'+c\cdot2x'z'+d\cdot2y'z' \quad (4.30)$$

and

$$\begin{aligned}a&=+\tfrac{1}{4}m\omega_z^2\cdot[\tfrac{1}{2}\sin^2\alpha\cdot(3+\varepsilon\cos2\beta)-\varepsilon\cos2\beta],\\ b&=+\tfrac{1}{4}m\omega_z^2\cdot\cos\alpha\cdot\varepsilon\sin2\beta,\\ c&=-\tfrac{1}{4}m\omega_z^2\cdot\sin\alpha\cdot\cos\alpha\cdot(3+\varepsilon\cos2\beta),\\ d&=+\tfrac{1}{4}m\omega_z^2\cdot\sin\alpha\cdot\varepsilon\sin2\beta. \qquad (4.31)\end{aligned}$$

The hamiltonian H'_0 describes an ideal Penning trap with the characteristic frequencies

$$\begin{aligned}\omega_c&=\frac{qB_0}{mc},\\ \omega'_z&=\omega_z\cdot\sqrt{1-\tfrac{1}{2}\sin^2\alpha\cdot(3+\varepsilon\cos2\beta)},\\ \omega'_1&=\sqrt{\omega_c^2-2\omega_z'^2}=\sqrt{\omega_1^2+\omega_z^2\sin^2\alpha\cdot(3+\varepsilon\cos2\beta)},\\ \omega'_+&=\tfrac{1}{2}(\omega_c+\omega'_1),\\ \omega'_-&=\tfrac{1}{2}(\omega_c-\omega'_1). \qquad (4.32)\end{aligned}$$

The problem has thus been reduced to that of an ideal Penning trap with a purely electrostatic perturbing potential quadratic in the coordinates. This type of problem was treated in full detail in the first part of this section. In particular, arguments such as those leading to (4.23) show that the time-independent term in the Fourier expansion of V' vanishes, and with it the term λ^2H_2 of the perturbation series (cf. (3.33)). The lowest nonvanishing term of the perturbation series is λ^4H_4, which can be computed using (3.38). In the approximation $H\approx H'_0+\lambda^4H_4$ the characteristic frequencies are obtained from (3.40) as

$$\begin{aligned}\Omega_+&=\omega'_++\frac{2(a^2+b^2)}{m^2\omega'_1\,\omega_c}\cdot\frac{1}{\omega'_+}+\frac{2(c^2+d^2)}{m^2\omega'_1}\cdot\frac{1}{\omega_+'^2-\omega_z'^2},\\ \Omega_-&=\omega'_--\frac{2(a^2+b^2)}{m^2\omega'_1\,\omega_c}\cdot\frac{1}{\omega'_-}-\frac{2(c^2+d^2)}{m^2\omega'_1}\cdot\frac{1}{\omega_-'^2-\omega_z'^2},\\ \Omega_z&=\omega'_z+\frac{3(c^2+d^2)}{m^2}\cdot\frac{\omega'_z}{(\omega_+'^2-\omega_z'^2)(\omega_-'^2-\omega_z'^2)}. \qquad (4.33)\end{aligned}$$

One can try to improve this result by computing also the perturbation term of order λ^6 using (3.39). The result is

$$\lambda^6H_6=+\frac{C}{m^3\omega_1'^2}\left[\frac{\omega'_+}{\omega_c}\cdot\frac{\omega_1'^2-\omega_z'^2-\omega'_1\,\omega_c}{(\omega_+'^2-\omega_z'^2)(\omega_-'^2-\omega_z'^2)}-\frac{2\omega'_-}{\omega_c}\cdot\frac{1}{\omega_+'^2-\omega_z'^2}\right]\frac{J_+}{\omega'_+}$$

$$+\frac{C}{m^3\omega_1'^2}\left[\frac{\omega_-'}{\omega_c}\cdot\frac{\omega_1'^2-\omega_z'^2+\omega_1'\omega_c}{(\omega_+'^2-\omega_z'^2)(\omega_-'^2-\omega_z'^2)}\right.$$
$$\left.-\frac{2\omega_+'}{\omega_c}\cdot\frac{1}{\omega_-'^2-\omega_z'^2}\right]\frac{J_-}{\omega_-'}$$
$$+\frac{C}{m^3\omega_1'^2}\left[\frac{2\omega_1'^2}{(\omega_+'^2-\omega_z'^2)(\omega_-'^2-\omega_z'^2)}\right]\frac{J_z}{\omega_z'} \quad (4.34)$$

with

$$C=(a+ib)(c-id)^2+(a-ib)(c+id)^2$$
$$=2a(c^2-d^2)+4bcd.$$

Method II: This approach treats the magnetic field as misaligned, causing a perturbing vector potential $\delta\boldsymbol{A}_0=\frac{1}{2}(\delta\boldsymbol{B}_0\times\boldsymbol{x})$. As a new 0th order hamiltonian we introduce

$$H_0'=\frac{1}{2m}\left(\boldsymbol{p}-\frac{q}{c}\boldsymbol{A}_0\cos\alpha\right)^2+\tfrac{1}{4}m\omega_z^2(2z^2-x^2-y^2)$$
$$+\frac{m}{16}\left(\frac{qB_0}{mc}\right)^2\sin^2\alpha\cdot(2z^2+x^2+y^2). \quad (4.35)$$

Defining

$$\mu=-\varkappa=\frac{\omega_c^2}{4\omega_z^2}\sin^2\alpha, \quad (4.36)$$

this can be rewritten as

$$H_0'=\frac{1}{2m}\left(\boldsymbol{p}-\frac{q}{c}\boldsymbol{A}\cos\alpha\right)^2$$
$$+\tfrac{1}{4}m\omega_z^2[2z^2(1+\mu)-(x^2+y^2)(1-\mu)]. \quad (4.37)$$

From this expression the characteristic frequencies of H_0' can be read off to be (cf. (3.7))

$$\omega_c'=\omega_c\cos\alpha,$$
$$\omega_z'=\omega_z\sqrt{1+\mu},$$
$$\omega_1'=\sqrt{\omega_c'^2-2\omega_z^2(1-\mu)}=\sqrt{\omega_c^2-2\omega_z'^2}, \quad (4.38)$$
$$\omega_+'=\tfrac{1}{2}(\omega_c'+\omega_1'),$$
$$\omega_+'=\tfrac{1}{2}(\omega_c'-\omega_1').$$

The complete hamiltonian H can then be written as

$$H=H_0'+V' \quad (4.39)$$

with the new perturbation term

$$V'=-\tfrac{1}{4}m\omega_z^2[(\varepsilon+\mu\cos 2\beta)(x^2-y^2)+\mu\sin 2\beta\cdot 2xy]$$
$$-\tfrac{1}{2}\omega_c\sin\alpha[\cos\beta(L_x+\tfrac{1}{2}m\omega_c\cos\alpha\cdot xz)$$
$$+\sin\beta(L_y+\tfrac{1}{2}m\omega_c\cos\alpha\cdot yz)], \quad (4.40)$$

where L_x, L_y are components of the canonical angular momentum $\boldsymbol{L}=\boldsymbol{x}\times\boldsymbol{p}$. The new perturbation term V' is of order λ^2 and the time-independent term in its Fourier expansion vanishes, $A_{000}'^{(2)}=0$. According to Sect. 3, the lowest nonvanishing term in the perturbation series is of order λ^4 and can be computed from (3.38), $H(J)=H_0'(J)+\lambda^4H_4(J)+\ldots$, using (3.11)–(3.14), (3.32), (3.34). The characteristic frequencies to order λ^4 are given by (3.40). Omitting all further details we quote the final results:

$$\Omega_+=\omega_+'+\frac{\omega_c^2\sin^2\alpha}{8\omega_1'}\cdot\frac{3\omega_+'^2+\omega_z'^2}{\omega_+'^2-\omega_z'^2}+\frac{\omega_z^4\cdot|\varepsilon+\mu e^{2i\beta}|^2}{8\omega_1'\omega_c'\omega_+'},$$

$$\Omega_-=\omega_-'-\frac{\omega_c^2\sin^2\alpha}{8\omega_1'}\cdot\frac{3\omega_-'^2+\omega_z'^2}{\omega_-'^2-\omega_z'^2}-\frac{\omega_z^4\cdot|\varepsilon+\mu e^{2i\beta}|^2}{8\omega_1'\omega_c'\omega_-'},$$

$$\Omega_z=\omega_z'-\frac{\omega_c^2\sin^2\alpha}{8\omega_1'\omega_z'}$$
$$\cdot\left[\omega_+'\frac{\omega_+'^2+3\omega_z'^2}{\omega_+'^2-\omega_z'^2}-\omega_-'\frac{\omega_-'^2+3\omega_z'^2}{\omega_-'^2-\omega_z'^2}\right]. \quad (4.41)$$

Note that the second term in these equations contains ω_c, not ω_c', and that the third term in the first two equations contains ω_z, not ω_z'.

The results of both calculational methods can now be compared numerically against the exact values of the characteristic frequencies as obtained by the method of Brown and Gabrielse [4]. Our calculations were done with trapping parameters appropriate for a proton ($\nu_+=76.34$ MHz, $\nu_-=662.85$ kHz, $\nu_z=10.06$ MHz) [3]. In Table 1 we have collected the relative errors $(\Omega_{\text{approx}}-\Omega_{\text{exact}})/\Omega_{\text{exact}}$ of the characteristic frequencies for both methods and two sets of perturbation parameters.

One notes at once that Method I yields results that are in comparison to those of Method II more accurate by several orders of magnitude, in particular for the modified cyclotron frequency and the axial frequency. Going from H_0 to H_0' means an improvement of the frequencies in Method I but a deterioration in Method II. This can be understood from the fact that the perturbation parameter μ of Method II contains the large factor $(\omega_c/\omega_z)^2$ (cf. (4.36)). Physically, the superiority of Method I tells us that the direction and strength of the magnetic field is a much more important feature than the details of the geometry of the electrodes. This fact should be kept in mind also in setting up perturbation schemes for more general situations.

Table 1. Accuracy of the perturbation approach in case of misaligned geometry.

Approximation	Method I			Method II		
	$\delta\Omega_+/\Omega_+$	$\delta\Omega_-/\Omega_-$	$\delta\Omega_z/\Omega_z$	$\delta\Omega_+/\Omega_+$	$\delta\Omega_-/\Omega_-$	$\delta\Omega_z/\Omega_z$
Perturbation parameters: $\alpha=1°$, $\beta=0°$, $\varepsilon=0$						
H_0	-4.11×10^{-6}	$+2.38\times10^{-4}$	-2.33×10^{-4}	-4.11×10^{-6}	$+2.38\times10^{-4}$	-2.33×10^{-4}
H_0'	-1.06×10^{-7}	$+9.13\times10^{-6}$	-6.94×10^{-4}	-1.20×10^{-4}	$+2.47\times10^{-3}$	-4.58×10^{-3}
$H_0'+\lambda^4H_4$	-4.17×10^{-13}	$+9.82\times10^{-9}$	-8.60×10^{-8}	-1.61×10^{-8}	$+2.62\times10^{-6}$	-1.12×10^{-5}
$H_0'+\lambda^4H_4+\lambda^6H_6$	$<10^{-13}$	$+8.43\times10^{-9}$	$+2.29\times10^{-7}$	–	–	–
Perturbation parameters: $\alpha=3°$, $\beta=45°$, $\varepsilon=0.3$						
H_0	-4.03×10^{-5}	$+2.14\times10^{-3}$	$+4.61\times10^{-2}$	-4.03×10^{-5}	$+2.14\times10^{-3}$	$+4.61\times10^{-2}$
H_0'	-4.34×10^{-6}	$+8.14\times10^{-5}$	$+4.18\times10^{-2}$	-1.08×10^{-3}	$+2.20\times10^{-2}$	$+5.17\times10^{-3}$
$H_0'+\lambda^4H_4$	$+5.05\times10^{-10}$	-8.83×10^{-7}	$+1.21\times10^{-3}$	$+1.31\times10^{-6}$	$+2.04\times10^{-4}$	-1.79×10^{-3}
$H_0'+\lambda^4H_4+\lambda^6H_6$	$+4.69\times10^{-11}$	$+6.55\times10^{-7}$	$+8.43\times10^{-4}$	–	–	–

The table lists the relative errors $\delta\Omega/\Omega=(\Omega_{\text{approx}}-\Omega_{\text{exact}})/\Omega_{\text{exact}}$, assuming for the ideal configuration ($\alpha=\beta=\varepsilon=0$) the frequency $\nu_+=76.34$ MHz, $\nu_-=662.85$ MHz, $\nu_z=10.06$ MHz (appropriate for a trapped proton).

4.3. Perturbation by Inhomogeneities of the Magnetic Field

Our last case study deals with the perturbation of the characteristic frequencies by inhomogeneities of the magnetic field, which may for instance be caused by the magnetization of the electrodes. As in our previous examples two clearly separated problems have to be solved: (i) the geometry of the specific experimental arrangement must be analyzed to determine the perturbing vector potential δA, (ii) the perturbation theory of Sect. 3 must be applied to find the shifts of the characteristic frequencies due to δA.

For the purpose of demonstration it is sufficient to discuss the simplest possible geometry. The electrodes are assumed to be manufactured of a paramagnetic ($\mu>1$) or diamagnetic ($\mu<1$) metal and to possess uniform magnetization

$$\boldsymbol{M}=\frac{3}{4\pi}\left(\frac{\mu-1}{\mu+2}\right)\boldsymbol{B}_0\,. \tag{4.42}$$

For uniform magnetization, the perturbation $\delta\boldsymbol{A}$ of the vector potential stems solely from the sudden change of $\boldsymbol{M}$ at the surface of the electrodes. According to Jackson [11] we have

$$\delta\boldsymbol{A}(\boldsymbol{x})=\oint_S \mathrm{d}a'\,\frac{\boldsymbol{M}\times\boldsymbol{n}'(\boldsymbol{x}')}{|\boldsymbol{x}-\boldsymbol{x}'|}\,, \tag{4.43}$$

where the integration extends over the surface area of the electrodes and where $\boldsymbol{n}'(\boldsymbol{x}')$ is a unit vector normal to the surface at the surface point $\boldsymbol{x}'$ and pointing into the region of the electrodes. Our perturbation approach of Sect. 3 requires knowledge of $\delta\boldsymbol{A}$ near the center of the trap. It is therefore sufficient to introduce into (4.43) an expansion in terms of spherical harmonics and to compute the first few coefficients. Denoting spherical coordinates for $\boldsymbol{x}$ by $r=|\boldsymbol{x}|$, θ, ϕ (similarly $r'=|\boldsymbol{x}'|$, θ', ϕ' for $\boldsymbol{x}'$) we have

$$\delta\boldsymbol{A}(\boldsymbol{x})=\sum_{l=0}^{\infty}\sum_{m=-l}^{m=+l}\frac{4\pi}{2l+1}\,r^l\,Y_{lm}(\theta,\phi)\cdot\oint_S \mathrm{d}a'\,\boldsymbol{M}\times\boldsymbol{n}'(\boldsymbol{x}')\,\frac{Y_{lm}^*(\theta',\phi')}{r'^{\,l+1}}\,. \tag{4.44}$$

For a further evaluation of the integral we must choose some definite geometry. The simplest situation is obtained when the outer surfaces of the electrodes are removed to infinity and only the inner surfaces facing the interior of the trap are kept. In other words, except for the interior of the trap the whole space (hatched region in Fig. 1) is assumed to be filled with material of permeability μ and uniform magnetization $\boldsymbol{M}$. An approximately similar situation is encountered in practice when the trap is constructed with massive metal electrodes. Assuming the electrodes to be realized as hyperboloids of revolution,

$$\begin{aligned}&\text{ring electrode:} && x^2+y^2-2z^2=r_0^2\,,\\ &\text{cap electrodes:} && 2z^2-x^2-y^2=2r_0^2\,,\end{aligned} \tag{4.45}$$

the integrals in (4.44) can easily be evaluated. The only nonvanishing terms are those with odd l and $m=\pm1$.

One obtains

$$\delta A(x) = \frac{3(\mu-1)}{\mu+2}\left[-\left(\frac{1}{\sqrt{3}}+\frac{2}{3}\ln(1+\sqrt{3})\right) + \frac{1}{4\sqrt{3}}(4z^2-x^2-y^2)+\ldots\right]A_0(x). \quad (4.46)$$

To find the shift of the characteristic frequencies we define, according to Sect. 3,

$$\begin{aligned}
\omega_c' &= \omega_c\left[1-\frac{3(\mu-1)}{\mu+2}\left(\frac{1}{\sqrt{3}}+\frac{2}{3}\ln(1+\sqrt{3})\right)\right],\\
\omega_1' &= \sqrt{\omega_c'^2-2\omega_z^2}, \qquad (4.47)\\
\omega_+' &= \tfrac{1}{2}(\omega_c'+\omega_1'), \quad \omega_-' = \tfrac{1}{2}(\omega_c'-\omega_1'),
\end{aligned}$$

thus taking into account the constant term in the square bracket of (4.46). The remaining term gives rise to a perturbation of order λ^4, which according to (3.38) requires the computation of the time average

$$\langle (4z^2-x^2-y^2)(x p_y - y p_x - \tfrac{1}{2} m\omega_c'(x^2+y^2))\rangle.$$

The result is

$$\begin{aligned}
&\lambda^4 H_4(J_+, J_-, J_z)\\
&= \frac{3(\mu-1)}{\mu+2}\cdot\frac{\omega_c}{\sqrt{3}mr_0^2}\left[\frac{1}{\omega_1'\omega_z}(\omega_+' J_+ J_z - \omega_-' J_- J_z) - \frac{1}{2\omega_1'^2}(\omega_+' J_+^2 + \omega_-' J_-^2 - 2\omega_c' J_+ J_-)\right]. \quad (4.48)
\end{aligned}$$

Finally the perturbed characteristic frequencies up to order λ^4 are obtained from (3.40) as

$$\begin{aligned}
\Omega_+ &= \omega_+'\left[1+\frac{3(\mu-1)}{\mu+2}\cdot\frac{\omega_c}{\sqrt{3}\omega_1' m r_0^2}\left(+\frac{J_z}{\omega_z}-\frac{J_+}{\omega_1'}+\frac{\omega_c'}{\omega_+'}\cdot\frac{J_-}{\omega_1'}\right)\right],\\
\Omega_- &= \omega_-'\left[1+\frac{3(\mu-1)}{\mu+2}\cdot\frac{\omega_c}{\sqrt{3}\omega_1' m r_0^2}\left(-\frac{J_z}{\omega_z}-\frac{J_-}{\omega_1'}+\frac{\omega_c'}{\omega_-'}\cdot\frac{J_+}{\omega_1'}\right)\right], \qquad (4.49)\\
\Omega_z &= \omega_z\left[1+\frac{3(\mu-1)}{\mu+2}\cdot\frac{\omega_c}{\sqrt{3}\omega_1' m r_0^2}\cdot\frac{1}{\omega_z^2}(\omega_+' J_+ - \omega_-' J_-)\right].
\end{aligned}$$

We note a dependence of the Ω_j on the constants of motion J_k of the individual particle orbit. By means of (2.16) the J_k can be expressed approximately by the amplitudes R_+, R_-, Z. Thus the order of magnitude of the λ^4 contribution is dominated by the factor $(\mu-1)(R/r_0)^2$. For an ensemble of trapped particles a frequency distribution with a small, but finite width will be observed.

5. Concluding Remarks

We have studied in this paper the shifts of the characteristic frequencies of an ion trapped in a Penning cage, with an imperfect geometry causing deviations of the electromagnetic field configuration from the ideal one. The understanding and interpretation of such frequency shifts is a problem of considerable practical importance. Our method is based on classical hamiltonian perturbation theory in terms of action-angle variables, as it was originally developed by Poincaré for the needs of celestial mechanics. The required input are the deviations (near the center of the trap) of the actual electromagnetic potentials Φ, A from the potentials Φ_0, A_0 of the ideal configuration. In practice these deviations $\delta\Phi$, δA can be computed or estimated from the geometry of the actual apparatus, or they follow as consequences of hypotheses that one wants to test as explanations of observed frequency shifts. Once the deviations $\delta\Phi$, δA are given, be it by actual computation or by hypothesis, the general perturbation theory yields a computational prescription suitable for practical calculations. This has been demonstrated by means of several case studies. In one case, where the exact solution is known, the perturbation series was found to give results of high precision in the parameter range that is important in practice. It was found that the direction of the magnetic field is a physical parameter whose importance dominates over details of the geometry of the electrodes. For high precision results, the calculation should therefore be arranged in such a way that the homogeneous magnetic field is in its entirety included in the 0th order hamiltonian.

This paper only has dealt with static perturbations. However, classical hamiltonian perturbation theory can also be applied to perturbations that are periodic in time or otherwise timedependent. Our studies of such problems will be described elsewhere.

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