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Second Order Hamiltonian and F-Matrix for an RFQ: A Step-by-Step Approach

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Abstract: This report details a step-by-step procedure to manually expand the Hamiltonian for a Radiofrequency Quadrupole (RFQ) linear accelerator to second order, largely following that which was done for the axially symmetric linac by Baartman. This technique is applied using the well known 2-term RFQ potential expansion, defined in terms of the vane parameters. The F-matrix, or infinitesimal transfer matrix, describes the point-to-point connection of the beam matrix undergoing a differential step ds along the Frenet-Serret orbit through the structure. This is essential for the computation of the linear optics about the accelerating reference particle.

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Preface

The present procedure closely follows that developed for an axially symmetric linac [1]. Our goal is to produce a Hamiltonian with separated transverse and longitudinal variables, which will allow computation of the F-matrix needed for `TRANSOPTR` implementation of an RFQ. This procedure may be accomplished in three steps. First, we perform two successive canonical transformations to render coordinates 5 and 6 suitable for use with `TRANSOPTR`. Secondly, we perturb time and energy around the reference particle, rendering these variations within an RFQ bunch explicit. Finally, the two-term RFQ potential will be separated into two separate components: a purely longitudinal one along with a mixed transverse-longitudinal term, which will allow for the expansion of the Hamiltonian, to second order.

Introduction

The generalized s-based Hamiltonian, in absence of vector potentials may be written:

$$H(x, P_x, y, P_y, t, E) = \sqrt{\left(\frac{E - q\Phi}{c}\right)^2 - m_0^2c^2 - P_x^2 - P_y^2} \tag{1}$$

the total momentum of a charged reference particle within an electric field with scalar potential Φ may be written:

$$P_0 = \sqrt{\left(\frac{E - q\Phi}{c}\right)^2 - m^2c^2} \tag{2}$$

In the case of an RFQ, we note the two term scalar potential [2]:

$$\Phi(x, y, s, t) = \left[A_{01}\frac{V_0}{2}(x^2 - y^2) + A_{10}\frac{V_0}{2}\cos(kz)I_0(k\sqrt{x^2 + y^2})\right]\sin(\omega t + \theta) \tag{3}$$

the parameters A_{01} and A_{10} define RFQ quadrupole focussing and acceleration, respectively, with given vane voltage V_0, RFQ design wavenumber k, aperture a and modulation factor m:

$$A_{01} = \frac{1}{a^2}\frac{I_0(ka) + I_0(mka)}{m^2I_0(ka) + I_0(mka)} \tag{4}$$

$$A_{10} = \frac{m^2 - 1}{m^2I_0(ka) + I_0(mka)} \tag{5}$$

that is, the two term potential expansion is separated into a transverse focussing term, defined by the $(x^2 - y^2)$ contribution and a longitudinal accelerating term whose radial fall-off is represented with $I_0(r)$, the modified Bessel function of the first kind. The scale of the transverse dimensions in an RFQ make clear that the potential will be dominated by the longitudinal accelerating term. Typically apertures are on the order of 1cm while the length is several meters. We also note that the transverse focussing term has no explicit s dependance.

Canonical Transformations to (z, P_z)

The Hamiltonian (1) is written with canonical coordinates 5,6 expressed as $(t, -E)$, but since it is desired to work with the coordinate pair $(-\beta c\Delta t, \Delta E/(\beta c))$, in line with `TRANSOPTR`, two successive canonical transformations must be performed upon the Hamiltonian, first transforming them to $(-\Delta t, \Delta E)$, where Δt is negative, since an early particle arrives before the reference particle. The generating function that accomplishes this is [3]:

$$G_1 = -\left(t - \int \frac{ds}{\beta c}\right)(\Delta E + E_0) \tag{6}$$

The partial derivative $\partial G_1/\partial s$ is added to the Hamiltonian (1). The generating function G_1 produces the Hamiltonian-added terms:

$$\frac{\partial G_1}{\partial s} = \frac{\Delta E + E_0(s)}{\beta c} - \Delta t \frac{dE_0}{ds}(s) \tag{7}$$

Next, we transform once more from $(-\Delta t, \Delta E)$ to $(-\beta c\Delta t, \Delta E/(\beta c))$, accomplished by using a second Hamiltonian generating function [3]:

$$G_2 = -\beta c\Delta t P_z \tag{8}$$

The full canonical transformation is accomplished by adding the partial derivatives of both generating functions G_1 and G_2 to the Hamiltonian H_s, replacing explicit $(\Delta t, \Delta E)$ dependency by $(-\beta c\Delta t, \Delta E/(\beta c)) = (z, P_z)$, the definitions for coordinates 5 and 6 as implemented in `TRANSOPTR`.

Perturbation About the Reference Particle

The desired perturbation in time and energy is obtained by allowing:

$$t \longrightarrow t_0 + \Delta t \tag{9}$$

$$E \longrightarrow E_0 + \Delta E \tag{10}$$

where the subscript 0 will denote the reference particle from here on. The first consequence may be found in the sinusoidal time-dependence, which after manipulation becomes:

$$\sin(\omega(t_0 + \Delta t) + \theta) = \left(1 - \frac{(\omega \Delta t)^2}{2}\right) S_0 + (\omega \Delta t) C_0 \tag{11}$$

where $\omega \Delta t \ll 1$. For conciseness, we introduce the notation $S = S(t) = \sin(\omega t + \theta)$ and $C = C(t) = \cos(\omega t + \theta)$. The quantities $S_0 = S(t_0)$ and $C_0 = C(t_0)$ correspond to the reference particle's time coordinate.

Longitudinal Isolation and Hamiltonian Expansion

We now look back at the general two-term RFQ potential:

$$\Phi(x, y, s, t) = \frac{V_0}{2} \left[A_{10} \cos(\psi) I_0(kr) + A_{01} \left(x^2 - y^2\right)\right] \sin\left(\omega t + \theta\right) \tag{12}$$

$$r = \sqrt{x^2 + y^2} \tag{13}$$

As written above, the potential $\Phi(x, y, s, t)$ lacks a purely longitudinal component. The set of second partial derivatives that compose the F-matrix in either of (x, y, s, t) will render the computation more difficult, particularly in presence of the square root expression in Eq. (13), which is the sole explicit, transverse-longitudinal dependence in the potential Φ. Should the Bessel function be approximated to first order, we will obtain a pure longitudinal component. The expansion of $I_0(kr)$ about $r = 0$ is:

$$I_0(kr) = 1 + \frac{k^2}{4}(r^2) + \mathcal{O}(r^4), \tag{14}$$

then we write the potential function $\Phi(x, y, s, t)$ as:

$$\Phi(x, y, s, t) = \left(\phi(s) + T(x, y, s)\right) S(t) \tag{15}$$

where

$$\phi(s) = \frac{A_{10} V_0}{2} \cos(\psi), \tag{16}$$

and

$$T(x,y,s) = \left(\frac{A_{01}V_0}{2}(x^2-y^2) + \frac{A_{10}V_0k^2\cos(\psi)}{8}(x^2+y^2) \right) \tag{17}$$

Expanding the Bessel function has allowed us to separate the potential into a purely longitudinal component $\phi(s)$, in addition to a transverse-dependant term $T(x,y,s)$. For clarity and conciseness, $\phi(s)$ and $T(x,y,s)$ shall be denoted ϕ and T from here on. We observe that ϕ depends only on the accelerating efficiency A_{10} and the accumulation of longitudinal spatial phase ψ. Meanwhile, the first term in Eq. (17) represents the quadrupole contribution with (x^2-y^2), featuring the transverse focusing parameter A_{01}. The second term in T contributes to acceleration thanks to its A_{10} and $\psi(s)$ dependence, with radially increasing amplitude. The former encodes a well-known feature of RFQ accelerators, in which the accelerating electric field is stronger off-axis. Due to the second-order truncation, the validity of this analysis is bounded for coordinates where $(x,y) \ll s$. Substituting the potential Φ from Eq. (15) in the expression for the modified canonical energy:

$$\left(\frac{E - q\Phi(x,y,s,t)}{c} \right) = \left(\frac{E - q\phi S(t) - qTS(t)}{c} \right) \tag{18}$$

The above is then squared as it appears in the Hamiltonian of Eq. (1). After some manipulation, the result may be expressed as:

$$\left(\frac{E - q\phi S(t)}{c} \right)^2 - \frac{2qTS(t)}{c}\left(\frac{E - q\phi S(t)}{c} \right) + \mathcal{O}(x^4, y^4) \tag{19}$$

Terms of fourth order in (x,y) are small and neglected from here on since they do not contribute to the linear optics. With this done, the remainder of Eq. (19) is now purely expressed in terms of the longitudinal component $\phi(s)$, while a mixed transverse-longitudinal first order contribution remains as a perturbation. We may now insert this, together with the partial derivative terms from the generating functions of Eqs. (6) and (8) into the of Eq. (1):

$$H_s = \frac{\partial G_1}{\partial s} + \frac{\partial G_2}{\partial s} - \sqrt{\left(\frac{E - q\phi S(t)}{c} \right)^2 - \frac{2qTS(t)}{c}\left(\frac{E - q\phi S(t)}{c} \right) - m_0^2c^2 - P_x^2 - P_y^2} \tag{20}$$

The Hamiltonian must now be expanded, which will render the F-matrix computation more straightforward. First, from the square root term in Eq. (20), it is now possible to extract a quantity that we identify as the time and energy perturbed total momentum:

$$H_S = \frac{\partial G_1}{\partial s} + \frac{\partial G_2}{\partial s} - P\sqrt{1 - \frac{P_x^2 + P_y^2}{P^2}} \tag{21}$$

with:

$$P = \sqrt{\left(\frac{E + \Delta E - q\phi S(t+\Delta t)}{c}\right)^2 - \frac{2qTS(t+\Delta t)}{c}\left(\frac{E + \Delta E - q\phi S(t+\Delta t)}{c}\right) - m_0^2 c^2} \tag{22}$$

The time expansion of $S(t)$ was noted in Eq. (11) which, together with the energy expansion are inserted into the total momentum expression of Eq. (22), which grows considerably. Terms are however truncated to second order [1] in Δt and ΔE. After manipulation and simplification, the momentum expression becomes:

$$P = \sqrt{\left(\frac{E_0 - q\phi(s)S_0}{c}\right)^2 - \frac{2qTS_0}{c}\left(\frac{E_0 - q\phi S_0}{c}\right) - m_0^2 c^2 + \epsilon} \tag{23}$$

with perturbation parameter:

$$\begin{aligned}\epsilon = 2E_0\Big(\Delta E + \frac{1}{2}q\phi(s)(\omega\Delta t)^2 S_0 - q\phi(s)(\omega\Delta t)C_0\Big) \\ + \Delta E\Big(\Delta E - 2q\phi S_0 - 2q\phi(\omega\Delta t)C_0\Big) \\ + q^2\phi(s)^2(\omega\Delta t)\Big((\omega\Delta t)(C_0^2 - S_0^2) + 2C_0 S_0\Big).\end{aligned} \tag{24}$$

A reference momentum may now be extracted from Eq. (23):

$$P = P_0\sqrt{1 - \frac{2qTS_0}{cP_0^2}\left(\frac{E_0 - q\phi S_0}{c}\right) + \frac{\epsilon}{P_0^2}} \tag{25}$$

where:

$$P_0 = \sqrt{\left(\frac{E_0 - q\phi S_0}{c}\right)^2 - m_0^2 c^2} \tag{26}$$

The reference momentum in Eq. (26) depends only on the longitudinal component of the potential, and carries the normal relativistic definition $P_0 = \beta\gamma m_0 c$. This is expected, as the reference particle is assumed to be perfectly synchronous ($\Delta t = \Delta E = 0$) and on-axis ($x = y = 0$), where the transverse potential components are zero. The total momentum in Eq. (25) may itself be expanded to second order:

[1] This means up to Δt^2, ΔE^2 or $\Delta t\Delta E$.

$$P \approx P_0\left(1 - \frac{qTS_0}{cP_0^2}\left(\frac{E_0 - q\phi S_0}{c}\right) + \frac{\epsilon}{2P_0^2} - \frac{\epsilon^2}{8P_0^4}\right). \tag{27}$$

With this, the Hamiltonian of Eq. (21) can now be expressed as:

$$H_s = \frac{\partial G_1}{\partial s} + \frac{\partial G_2}{\partial s} - P_0 - \frac{\epsilon}{2P_0} + \frac{\epsilon^2}{8P_0^3} + \frac{qTS_0}{cP_0}\left(\frac{E_0 - q\phi S_0}{c}\right) + \frac{P_x^2 + P_y^2}{2P}. \tag{28}$$

We observe that the terms in P_x and P_y in Eq. (28) are scaled by the momentum P, which is approximated as P_0. This transverse momentum approximation will only be correct near-axis, where higher order terms are negligeable. The generating function terms are explicitly substituted in the Hamiltonian of Eq. (28). The second term in the contribution of G_1 from Equation (6) may be found by evaluating one of Hamilton's equations:

$$\frac{\partial G_1}{\partial s} = \left(\frac{\Delta E + E_0}{\beta c}\right) - \frac{q\phi\omega\Delta t}{cP_0}\left(\frac{E_0 - q\phi S_0}{c}\right)C_0 \tag{29}$$

The contribution from the G_2 term from Equation (8) is:

$$\frac{\partial G_2}{\partial s} = -\frac{\beta'}{\beta}\Delta t\Delta E \tag{30}$$

This procudes the final, second order, $s-$independent Hamiltonian for a two-term RFQ potential field, which is found by explicitly writing the generating functions (29) and (30), in addition to the the perturbation polynomial ϵ of Eq. (24) in the Hamiltonian (28), then re-arranging terms and substituting the quantities $(\beta c\Delta t,\ \Delta E/(\beta c)) = (z, P_z)$. Finally, the separated potential terms $\phi(s)$ and $T(x, y, s)$, from Eqs. (16) and (17) are explicitly written, producing to second order:

$$H_s = \left(\frac{E_0}{\beta c} - P_0\right) + \frac{P_x^2}{2P_0} + \frac{P_y^2}{2P_0} + \frac{P_z^2}{2\gamma^2 P_0} + \frac{\mathcal{T}_1(s)}{2}x^2 + \frac{\mathcal{T}_2(s)}{2}y^2 + \mathcal{B}(s)zP_z + \frac{\mathcal{C}(s)}{2}z^2 \tag{31}$$

with:

$$\mathcal{T}_1(s) = \frac{qV_0}{4\beta c}\left(4A_{01} + A_{10}k^2\cos(\psi)\right)\sin(\omega t_0 + \theta) \tag{32}$$

$$\mathcal{T}_2(s) = \frac{qV_0}{4\beta c}\left(-4A_{01} + A_{10}k^2\cos(\psi)\right)\sin(\omega t_0 + \theta) \tag{33}$$

$$\mathcal{B}(s) = \frac{qV_0 A_{10}}{2\beta^2\gamma^3 mc^2}\left(\frac{\omega}{\beta c}\cos(\psi)\cos(\omega t_0+\theta) + k\sin(\psi)\sin(\omega t_0+\theta)\right) \tag{34}$$

$$\mathcal{C}(s) = \frac{A_{10}\omega^2\cos(\psi)}{4\beta^5\gamma^3 mc^5}\left(q^2V_0^2A_{10}\cos(\psi)\cos(\omega t_0+\theta)^2 - 2qV_0\beta^2\gamma^3 mc^2\sin(\omega t_0+\theta)\right) \tag{35}$$

The perturbation and expansion procedure has allowed us to remove all square root dependencies and has also separated transverse and longitudinal coordinates, rendering the evaluation of second partial derivatives much easier. Thus, obtention of the F-matrix for the RFQ is simply a matter of evaluating second order partial derivatives with respect to each of the canonical coordinates upon the Hamiltonian (31). It is expressly reiterated that the coordinate z is not equivalent to s. Rather, the canonical pair are ($t-t_0$,$E-E_0$) or (Δt, ΔE), not (l,$\Delta P/P$). The reason choosing the latter usually works is by applying a trick: If we scale by $\beta_0 c$, we can make them match the proper canonical choice, since $\beta_0 c\Delta t = z$, and in magnetic elements, $\Delta E/(\beta_0 c) = \Delta P$, but this is only true of magnetic elements, and leads the analysis astray when there are electric fields. We use this same trick because then coordinate 6 only deviates from the usual $\Delta P/P$ in regions where electric potential $\Phi = 0$. Further, the coordinate 5 is not "path length difference" as stated by Brown in [4], but the time difference with respect to the reference particle, scaled by the reference particle's speed.

RFQ F-Matrix

Evaluating the set of second partial derivatives of the Hamiltonian (31), one obtains the 2-term RFQ F-matrix:

$$\mathbf{F_2}(s) = \begin{pmatrix} 0 & \frac{1}{P_0} & 0 & 0 & 0 & 0 \\ \mathcal{T}_1(s) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{P_0} & 0 & 0 \\ 0 & 0 & \mathcal{T}_2(s) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathcal{B}(s) & \frac{1}{\gamma^2 P_0} \\ 0 & 0 & 0 & 0 & \mathcal{C}(s) & -\mathcal{B}(s) \end{pmatrix}$$

The above provides `TRANSOPTR` with a complete description of an RFQ, as described by a 2-term potential expansion. A distinct advantage of the two-term potential lies with the focusing and accelerating terms, A_{10} and A_{10}, respectively. These standard RFQ parameters may easily be computed directly from the vane aperture and modulation parameters, in addition to the design wavenumber. Thus, by simply providing a mapping of (s, a, m, k) in the form of an ascii-formatted input file, `TRANSOPTR` will provide a near-axis description of RFQ dynamics.

References

[1] R. Baartman. *Fast Envelope Tracking for Space Charge Dominated Injectors.* In *Proceedings of LINAC 2016 Conference*, pages 1017–21, 2016.

[2] T.P. Wangler. *RF Linear Accelerators, 2nd Edition.* Wiley-VCH, 2008.

[3] Goldstein H., Poole C.P., and Safko J.L. Classical Mechanics. Addison Wesley, 2002.

[4] Karl L Brown, Frank Rothacker, David C Carey, and F Christoph Iselin. Transport: a computer program for designing charged-particle beam-transport systems. Technical Report SLAC-R-91-REV-3, Stanford Linear Accelerator Center, Calif., 1980.