Fast radio frequency quadrupole envelope computation for model based beam tuning

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Efficient tuning of complex accelerator chains requires automated procedures, themselves reliant upon beam physical models. The Isotope Separator and ACcelerator (ISAC) facility at TRIUMF requires frequent changes of beam species (isotope), mass to charge ratio and beam energy tailored to experiment requirements, which demands rapid beam tuning. In addition, emergent effects such as long term changes of energy or energy spread require beam optimization that must be based on a complete model of the accelerator. Using an envelope code to build an end-to-end simulation of the accelerator facility for operational purposes reduces computing times by 3 or 4 orders of magnitude, when compared to particle tracking codes, so that the requisite simulations may be carried out in real time, by polling control system data. Herein described is the second order Hamiltonian for an radio frequency quadrupole (RFQ), presented within the framework of the envelope code TRANSOPTR. To benchmark the TRANSOPTR model, envelope simulations of the TRIUMF-ISAC RFQ have been performed and compared with the multiparticle code PARMTEQ.

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I. INTRODUCTION

As the complexity and the intensity requirements of modern heavy ion accelerators have increased over the past decade, the community is working towards model based tuning approaches with beam measurement based refinements. This necessitates a detailed understanding of the different accelerator systems and beamline elements, itself requiring numerical models that describe these with sufficient accuracy. For accelerator physicists, the current toolkit notably includes particle tracking codes such as PARMTEQ and TRACK, both of which allow the simulation of accelerator particle dynamics, including space charge, for different types of accelerator structures such as radio frequency quadrupoles (RFQ) and drift-tube linacs (DTL). Such codes are particularly useful in the design of heavy ion accelerators, when variations in accelerator geometry and the resulting effects on beam dynamical behavior and losses are investigated. However, the aforementioned codes, and indeed much of the existing repository of RFQ simulations, rely upon the method of ray-tracing, tracking upwards of 10^5 particles through the time-varying fields of the accelerator, from which statistical quantities

such as the rms beam envelope may be extracted. This method and its variants pose a computational burden which results in total computation times generally on the order of several dozen seconds, if not minutes, particularly as the particle population increases to investigate effects like halo formation and beam losses. While this computational burden is not a critical issue during the design and testing phases, it does pose a problem if one wishes to implement a fast, nearly real-time simulation of an existing accelerator based upon current machine setpoints.

Such a requirement has emerged at ISAC (Isotope Separator and ACcelerator), TRIUMF's radioisotope beam (RIB) facility, whose heavy-ion postaccelerator consists of a 35.36 MHz CW RFQ, featuring external three-harmonic prebunching 5 m upstream [1], followed by a 106 MHz drift tube linac (DTL) [2]. Ongoing development of an integrated end-to-end simulation of the ISAC postaccelerator, enabling real-time beam simulations and the implementation of corrective feedback, has created the need for a computationally light, fast RFQ envelope simulation within the framework that has been developed at TRIUMF. In effect, for the former to be operationally useful in day-to-day activities, including tuning, troubleshooting and reoptimization by operators, there is a strict performance requirement. For instance, a comprehensive end-to-end model of the above described accelerator system using particle tracking codes would likely incur a considerable computational cost, requiring near-continuous simulations to be run with constantly evolving accelerator settings, making the development of a real-time tool difficult.

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The linear optics envelope code TRANSPORT [3] has been heavily used at TRIUMF since the early 80s for designing and modeling beam transfer lines and more recently also linear accelerators and in particular the new superconducting electron linac [4]. It offers an attractive option for such fast simulations. Desirous to implement a complete end-to-end model of the ISAC heavy-ion accelerator consisting of LEBT, RFQ, DTL and superconducting quarter-wave resonator linac, we lacked only the RFQ. This has now been developed and is the topic of the present paper. We discuss a subtlety in the interpretation of the Kapchinsky-Teplyaev potential function for an RFQ, which is crucial for implementation in a global integration code. We then provide a brief discussion on the matrix based Hamiltonian approach used in TRANSPORT. Next, we introduce a convenient second order expansion of the RFQ Hamiltonian in the case of a 2-term potential. With this in hand, we then produce the force matrix for the 2-term potential RFQ. Finally, we benchmark our TRANSPORT model by comparing its results with the particle-tracking code PARMTEQ, for the case of the ISAC-RFQ [5].

A. TRANSPORT: Some historical notes

TRANSPORT is a fully 6-dimensional beam envelope code. It integrates the equations of motion of the second moments of the particle beam. For a bunched beam, there are 21 possible second moments. This follows from the “ σ -matrix” formalism first developed in the 60s: the elements of the σ -matrix are essentially the beam’s second moments. So besides the usual (transverse position and momentum correlations, x - y coupling, energy-position or dispersion correlation) it can also handle longitudinal-transverse coupling or bunch tilt, with space charge, and elements like bunchers and rf deflectors. The early codes developed to calculate particle beams and design beamlines were TRANSPORT [6], GIOS [7], TRACE [8], and many more. A brief comparison between codes is shown in Table I. These were however not beam envelope integrators; instead they had stored the known analytic transfer matrices of standard elements such as hard-edged quadrupoles, dipoles, solenoids. This is how TRANSPORT originally functioned also. TRANSPORT was written to broaden the fitting capabilities of TRANSPORT [3]. This was accomplished by having the beam transport line coded directly into the computer language. The limitation to analytically integrable elements remained however, so that in either code, the only way to include space charge was to subdivide all elements into sufficiently small increments and interleave with artificial thin lenses, whose strengths depended upon the beam size. The option to integrate through spatially-varying fields was added in 1983 [9] in order to handle space charge in the manner developed by Sacherer [10]. This addition had the added benefit that elements such as quadrupoles and solenoids could be modeled in a more realistic soft-edged manner. Einzel

TABLE I. Various codes and their longitudinal coordinate definitions. The fifth column (EoM?) refers to whether the equations of motion are integrated as opposed to having stored transfer matrices. The rightmost column refers to whether the reference particle can be accelerated within an element. ($K \equiv (\gamma_0 - 1)mc^2$, $\Delta t \equiv t - t_0$).

Code	Order	x_5	x_6	EoM?	$\beta_0(s)$?
COSY- ∞ [13]	∞	$-\frac{\beta_0 c \Delta t \gamma_0}{1 + \gamma_0}$	$\frac{\Delta E}{K}$	Yes	No
MARYLIE [14]	3	$-c \Delta t$	$\frac{\Delta E}{P_0 c}$	Yes	No
TRANSPORT [6]	Up to 3	$-(\beta_0 c t - \beta_0 c t_0)$	$\frac{\Delta P}{P_0}$	No	...
GIOS [7]	3	$\frac{\Delta t}{t_0}$	$\frac{\Delta E}{K}$	No	...
TRACE3D [8]	1	$-\beta_0 c \Delta t$	$\frac{\Delta P}{P_0}$	No	Impulses
TRANSPORT	1	$-\beta_0 c \Delta t$	$\frac{\Delta E}{\beta_0 c}$	Yes	Yes

lenses and static axial electric fields such as in acceleration columns [11] could also be coded simply. More recently, in order to simulate linear accelerators [4], we have added time-varying fields as well. A list of all features added since 1984 can be found in Ref. [12].

In order to integrate through accelerators as well as the usual optical elements, it is beneficial to be rigorous regarding the definitions of the six dependent particle coordinates. If they are canonical, then adding any kind of optical element is straightforward once the Hamiltonian is known. In order to compare different approaches to beam dynamics, let us introduce the 6-dimensional state vector $\mathbf{X} = (x_1, x_2, x_3, x_4, x_5, x_6)^T$. In common with most beam transport codes, TRANSPORT uses a Frenet-Serret coordinate frame that moves with the reference particle, with s , the distance along the reference trajectory, as the independent variable. For example, in SLAC-75 [15] Brown notes that the independent vector “*is not time but is the arc distance measured along the central trajectory*”. In this case, the Hamiltonian is not the energy but is $-P_s$. The transverse dependent coordinates are (x, P_x, y, P_y) , but the longitudinal coordinates x_5 and x_6 are time and energy. We nevertheless denote them as z and P_z , but they are defined as follows:

$$x_5 = z = -\beta_0 c(t - t_0) \quad (1)$$

$$x_6 = P_z = \frac{\Delta E}{\beta_0 c} \quad (2)$$

where $\beta_0 c$ is the reference particle’s speed and ΔE is the energy difference with respect to the reference particle (including the electrostatic potential energy), and

$$t_0 = \int_0^s \frac{ds}{\beta_0 c}, \quad (3)$$

the time of arrival of the reference particle at s . These are a canonically conjugate pair, as will be shown. In the general

case including accelerating elements, $\beta_0 = \beta_0(s)$ and so the canonical transformation $(t, E) \rightarrow (z, P_z)$ is not simply a scale change.

In TRANSOPTR, for the purposes of outputting transfer matrices in standard form, the generalized momenta (P_x, P_y, P_z) are renormalized. After every integration they are divided by the reference momentum P_0 . This effectively makes $x_2 = x' = P_x/P_0$ and $x_4 = y' = P_y/P_0$. In the absence of a scalar potential Φ , $x_6 = P_z/P_0 = \Delta P/P_0$ in common with the traditional beam transport codes, since $\Delta E = \beta_0 c \Delta P$. But if there is a scalar potential, we have in first order, $c^2 P \Delta P = (E - q\Phi) \Delta E$ instead of $c^2 P \Delta P = E \Delta E$.

In TRANSPORT, the 6-dimensional state vector is $\mathbf{X} = (x, \theta, y, \phi, l, \delta)^T$ where $\theta = x'$, $\phi = y'$ and $\delta = \Delta P/P_0$ and this is consistent with our notation, but l is the path length difference compared to the reference particle: $l = -\Delta(\beta c t) = c(\beta_0 t_0 - \beta t)$. On the other hand, the x_5 of TRANSOPTR is the difference of time of arrival at the position s , and the arrival of the reference particle at that position, scaled by speed to convert to a distance: $z = -\beta_0 c(t - t_0)$. For accelerating structures, the time of arrival relates directly to the rf phase so it is natural to use this coordinate rather than the $x_5 = l$ of TRANSPORT. For nonaccelerating elements, the difference between the TRANSPORT l and the TRANSOPTR z is trivial, requiring to adjust the 56 element of the transfer matrix by its length divided¹ by γ_0^2 . But for TRANSOPTR, where we accommodate elements that accelerate, this is not workable because γ_0 is changing continuously. Further, the longitudinal envelope, which is the rms of x_5 , namely $\sqrt{\langle z^2 \rangle}$, is the “bunch length” in the usual sense being the time of passage divided by its speed (not the actual length of the bunch in its own reference frame.) This bunch length is relevant to space charge calculations.

To be fair, it should be remembered that TRANSPORT was written only for “*designing charged particle beam transport systems*” [6]. It only had magnetic elements plus a “thin lens” acceleration. Further, excluding the dynamical part from x_5 had the simplifying effect that the encoded transfer matrices are purely geometric: the matrices include only the “momentum compaction” component of the net phase slip. Under these conditions, trajectories are not species-dependent: the only particle characteristic required for the transport calculation is the momentum. So the code was extremely simple and very fast, relying only on multiplying 6-dimensional matrices.

It is of course not essential to choose the particular longitudinal coordinates in Eqs. (1), (2). Other choices are given in Table I. In the COSY- ∞ case, x_6 is the energy

¹This can be seen as follows. From the x_5 in Table I, we see the faster particle arrives early by length $\Delta\beta(ct) = \frac{\Delta\beta}{\beta_0} L = \frac{L}{\gamma_0^2} \frac{\Delta P}{P_0}$, where L is the accumulated length.

deviation, normalized by a parameter $K = (\gamma_0 - 1)mc^2$ that is often called the “kinetic” energy. MARYLIE along with others as commonly taught at recent accelerator schools, e.g., Ryne [16], Wolski [17], normalize the energy deviation with $P_0 c$: $x_6 = \frac{\Delta E}{P_0 c} = \frac{E}{P_0 c} - \frac{1}{\beta_0}$. Typically, then t_0 is given as $\frac{s}{\beta_0 c}$ and this is not applicable (or canonical) when β_0 is a function of s as we will see below.

TRACE3D deserves a special mention in the context of this paper since it already has an “RFQ cell.” Since it is a stored-matrix code, it can describe an RFQ as a series of such cells, having stored transfer matrices for impulses applied 18 times per half cell. This is similar to the way in which it applies space charge: as impulses. TRANSOPTR integrates equations of motion using adaptive Runge-Kutta and so can handle space charge in a compute-optimized manner, and as will be described, can model an RFQ in the same way.

II. HAMILTONIAN DYNAMICS

If the independent variable is s , the distance along the path taken by the reference particle, the Hamiltonian is $-P_s$, the canonical momentum in the direction of the reference trajectory. For an RFQ, this trajectory is straight so the Hamiltonian of a charged particle experiencing a time-dependent electric field can be written as

$$H_s(x, P_x, y, P_y, t, E; s) = -\sqrt{(E - q\Phi)^2/c^2 - m^2c^2 - P_x^2 - P_y^2}. \quad (4)$$

Φ is the scalar potential while q is the particle’s charge. As is usual for RFQs, the vector potential is not included as the rf magnetic fields have negligible effect on the dynamics compared with the electric fields.

A. RFQ spatial phase

In the present study, we confine ourselves to the simplest, “two-term” scalar potential for the RFQ (e.g., Wangler [18], Staples [19])

$$\Phi(x, y, s, t) = \frac{V_0}{2} [A_{10} \cos(ks) I_0(kr) + A_{01} (x^2 - y^2)] \sin(\omega t + \phi), \quad (5)$$

where I_0 is the modified Bessel function and $r^2 = x^2 + y^2$. The potential features both the accelerating and focusing efficiencies, respectively defined as:

$$A_{10} = \frac{m^2 - 1}{m^2 I_0(ka) + I_0(mka)} \quad (6)$$

$$A_{01} = \frac{1 - A_{10} I_0(ka)}{a^2}. \quad (7)$$

The parameters k , A_{10} , A_{01} are usually tabulated, one value per halfcell, versus s . This potential is used in codes such as PARMTEQ and TRACE3D which calculate through only one half cell at a time. In that case s would be reset to zero at each halfcell start. But we would like the ODE solver to run s from the beginning of the RFQ to its exit, choosing its own stepsize for accuracy and efficiency, while spline-interpolating the three parameters k , A_{10} , A_{01} . Thus Eq. (5) is incorrect for our purposes: the spatial modulation to the point s is not ks but $\int_0^s k(\zeta)d\zeta$.

In a perfect RFQ, $k(s) = \frac{2\pi}{\beta(s)\lambda} = \frac{\omega}{\beta c} = \omega \frac{dt}{ds}$, or $k(s)ds = \omega dt$, we integrate, arbitrarily using the initial condition $s = 0$ at $t = 0$ to define phase, and find $\int_0^s k(\zeta)d\zeta = \omega t$. In other words, as time t progresses, the particle experiencing the potential (5) will not stay synchronous unless the argument of the cosine is

$$\psi(s) = \int_0^s k(\zeta)d\zeta \quad (8)$$

rather than ks :

$$\Phi(x, y, s, t) = \frac{V_0}{2} [A_{10} \cos \psi I_0(kr) + A_{01}(x^2 - y^2)] \sin(\omega t + \phi). \quad (9)$$

B. The on-axis reference particle

In order to transform from (t, E) to (z, P_z) as per Eqs. (1) and (2), we need to first find time t_0 and energy E_0 of the reference particle. We find time t_0 from Eq. (4) as:

$$\frac{dt_0}{ds} = -\frac{\partial H}{\partial E} = \frac{E_0 - q\Phi}{c\sqrt{(E_0 - q\Phi)^2 - m^2c^4}} = \frac{\gamma}{c\sqrt{\gamma^2 - 1}} = \frac{1}{\beta c}. \quad (10)$$

(This is essentially the definition of β and γ ; from here on, unsubscripted β and γ refer to the reference particle and both are functions of s .)

We find the energy of the on-axis reference particle now as follows:

$$\frac{dE_0}{ds} = \frac{\partial H}{\partial t} = \frac{1}{\beta c} \frac{\partial \Phi}{\partial t}. \quad (11)$$

As above, energy E_0 is not directly γmc^2 because the scalar potential in an RFQ is not zero on axis. In fact, $\gamma mc^2 = E_0 - q\Phi$, so:

$$mc^2\gamma' = \frac{d(E_0 - q\Phi)}{ds} = \frac{1}{\beta c} \frac{\partial \Phi}{\partial t} - q \left(\frac{\partial \Phi}{\partial s} + \frac{\partial \Phi}{\partial t} \frac{dt}{ds} \right) = -q \frac{\partial \Phi}{\partial s}. \quad (12)$$

This can be identified as the longitudinal electric field. Performing the derivative of Eq. (9) above for on-axis,

$$mc^2\gamma' = \frac{qV_0}{2} k A_{10} \sin \psi \sin(\omega t_0 + \phi_s), \quad (13)$$

and this agrees with standard references [18], except that the argument of the sine function is ψ rather than ks .

C. Hamiltonian in (z, P_z)

This follows the technique developed for the axially symmetric linac [4]. The Hamiltonian (4) with the potential (9) is transformed to new longitudinal coordinates

$$z = -\beta(s)c(t - t_0(s)) \quad \text{and} \quad P_z = \frac{E - E_0(s)}{\beta(s)c}, \quad (14)$$

where $t_0(s) = \int \frac{ds}{\beta c}$. The transformation is most easily understood if done in two steps: first transforming from $(t, -E)$ to $(-\Delta t, \Delta E)$. The generating function that accomplishes this is [20]:

$$G_1 = -\left(t - \int \frac{ds}{\beta c}\right)(\Delta E + E_0). \quad (15)$$

This produces the Hamiltonian-added terms:

$$\frac{\partial G_1}{\partial s} = \frac{\Delta E + E_0(s)}{\beta c} - \Delta t E'_0. \quad (16)$$

Next, we transform once more from $(-\Delta t, \Delta E)$ to $[-\beta c \Delta t, \Delta E/(\beta c)]$, accomplished by using a second generating function [20]:

$$G_2 = -\beta c \Delta t P_z, \quad (17)$$

thus adding

$$\frac{\partial G_2}{\partial s} = \frac{\beta'}{\beta} z P_z = \frac{\gamma'}{\beta^2 \gamma^3} z P_z \quad (18)$$

to the Hamiltonian (4).

D. Hamiltonian for linear motion

We then substitute Eq. (14) into the Hamiltonian (See Appendix for detailed derivation.) Since we are only interested in the linear motion, we expand the resulting Hamiltonian to second order in the 6 canonical variables (using the abbreviation $P \equiv \beta \gamma mc$):

$$H(x, P_x, y, P_y, z, P_z) = \frac{E_0}{\beta c} - P + \frac{P_x^2}{2P} + \frac{P_y^2}{2P} + \frac{P_z^2}{2\gamma^2 P} + \frac{\mathcal{A}_+}{2} x^2 + \frac{\mathcal{A}_-}{2} y^2 + \frac{\mathcal{C}}{2} z^2 + \mathcal{B} z P_z \quad (19)$$

where

$$\mathcal{A}_{\pm} = \frac{qV_0 \sin(\omega t_0 + \phi)(k^2 A_{10} \cos \psi \pm 4A_{01})}{4\beta c}, \quad (20)$$

$$\mathcal{B} = \frac{qV_0 A_{10} \{k \sin \psi \sin(\omega t_0 + \phi) + [\omega/(\beta c)] \cos \psi \cos(\omega t_0 + \phi)\}}{2\beta^2 \gamma^3 m c^2}, \quad (21)$$

$$\mathcal{C} = \frac{qV_0 (\omega/(\beta c))^2 A_{10} \cos \psi [qV_0 A_{10}/(\beta^2 \gamma^3 m c^2) \cos \psi \cos^2(\omega t_0 + \phi) - 2 \sin(\omega t_0 + \phi)]}{4\beta c}. \quad (22)$$

There are no terms first order in the six dependent coordinates, confirming that the reference particle's coordinates are invariant.

E. Implementation in TRANSOPTR

The phase-space representation of an arbitrary particle is the column vector

$$\mathbf{X} = (x, P_x, y, P_y, z, P_z)^T. \quad (23)$$

The equations of motion are written in the form

$$\mathbf{X}' = \mathbf{F}\mathbf{X} \quad (24)$$

where $\mathbf{X}$ is the particle's state vector $(x, P_x, y, P_y, z, P_z)^T$, so $\mathbf{F}$ is simply the matrix of second derivatives of the Hamiltonian evaluated for the reference particle:

$$\mathbf{F}(s) = \begin{pmatrix} \frac{\partial^2 H}{\partial P_x \partial x} & \frac{\partial^2 H}{\partial P_x^2} & \cdots & \frac{\partial^2 H}{\partial P_x \partial P_z} \\ -\frac{\partial^2 H}{\partial x^2} & -\frac{\partial^2 H}{\partial x \partial P_x} & \cdots & -\frac{\partial^2 H}{\partial x \partial P_z} \\ \frac{\partial^2 H}{\partial P_y \partial x} & \frac{\partial^2 H}{\partial P_y \partial P_x} & \cdots & \frac{\partial^2 H}{\partial P_y \partial P_z} \\ -\frac{\partial^2 H}{\partial y \partial x} & -\frac{\partial^2 H}{\partial y \partial P_x} & \cdots & -\frac{\partial^2 H}{\partial y \partial P_z} \\ \frac{\partial^2 H}{\partial P_z \partial x} & \frac{\partial^2 H}{\partial P_z \partial P_x} & \cdots & \frac{\partial^2 H}{\partial P_z^2} \\ -\frac{\partial^2 H}{\partial z \partial x} & -\frac{\partial^2 H}{\partial z \partial P_x} & \cdots & -\frac{\partial^2 H}{\partial z \partial P_z} \end{pmatrix} \quad (25)$$

The total transfer matrix $\mathbf{M}$ can be found by integrating (24) starting with columns of the identity matrix.

A particle beam is a collection of particles. Choosing N as the number of particles, we can find the “envelope” of the beam as the second moments of the distribution given by

$$\sigma \equiv \frac{1}{N} \sum_{i=1}^N \mathbf{X} \mathbf{X}^T. \quad (26)$$

For example, $\sigma_{11} = \langle x^2 \rangle$, $\sigma_{12} = \langle x P_x \rangle$, $\sigma_{13} = \langle xy \rangle$, etc. For a distribution of particles so dense that we do not see

graininess on any scale of our diagnostics, the sums go over into integrals. By direct substitution of $\mathbf{X}_f = \mathbf{M}\mathbf{X}_i$ into the definition of σ , we find

$$\sigma_f = \mathbf{M} \sigma_i \mathbf{M}^T, \quad (27)$$

and this can be used to find σ_f as is done in the matrix codes. But this will not apply when there are space charge forces because the defocusing is added to $\mathbf{F}$ and causes a recursive dependence on σ . (See Appendix B for the space charge contribution to $\mathbf{F}$.) Moreover even for zero space charge it will not give envelope sizes at intermediate points along the element.

TRANSOPTR [9] instead integrates directly the equation of motion of the σ -matrix [10] found by differentiating equation (26):

$$\sigma' = \mathbf{F}\sigma + \sigma\mathbf{F}^T. \quad (28)$$

With space charge included, this can be shown to reduce to the Kapchinsky-Vladimirsky envelope equations for the simpler case of a coasting unbunched uncoupled beam.

From the Hamiltonian (19) we find directly the $\mathbf{F}$ -matrix:

$$\mathbf{F} = \begin{pmatrix} 0 & \frac{1}{P} & 0 & 0 & 0 & 0 \\ -\mathcal{A}_+ & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{P} & 0 & 0 \\ 0 & 0 & -\mathcal{A}_- & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathcal{B} & \frac{1}{\gamma^2 P} \\ 0 & 0 & 0 & 0 & -\mathcal{C} & -\mathcal{B} \end{pmatrix}. \quad (29)$$

For the full 6D case, it represents 21 equations (the σ -matrix is symmetric), but in the present case 12 of these are trivial because there is no coupling between the 3 planes. A Runge-Kutta integrator is used to solve Eq. (28), simultaneously while integrating $\psi' = k$ (8), t'_0 (10), and γ' (13). Space charge is included if needed by augmenting the $\mathbf{F}$ -matrix with the appropriate linear space charge defocusing terms [4,9] (see Appendix B).

In TRANSPORT a global input data file contains beam initial parameters plus the element parameters one is free to vary. A subroutine describing the transport system optical elements (quads, drifts, solenoids, linacs, etc.) are called in order, or in do loops if they are periodic. The RFQ element is called via the new subroutine RFQ which reads the file containing the table of (s, A_{01}, A_{10}, k) , and has as arguments the phase and amplitude of the RFQ, and a length scale.

III. APPLICATION RESULTS

In this section we introduce our own ISAC-RFQ, compare and benchmark the TRANSPORT envelope calculation with the PARMTEQ calculation, and show as a use case how the new possibility of end-to-end TRANSPORT calculation refines the match to the RFQ.

A. The ISAC-RFQ

Heavy rare isotope beams at the ISAC postaccelerator initially encounter a three-harmonic prebuncher, which modulates the energy to create a longitudinal focus 5 m downstream, at the RFQ's entrance. This unique separated prebuncher design shortens the RFQ and reduces its power consumption [21]. As such, the RFQ operates without an internal bunching section. The buncher operates at 11.8 MHz and so fills only every third bucket. The ISAC-RFQ accepts beams in the range $1 \leq A/q \leq 30$, with an injection energy of 2.06 keV per atomic mass unit and output energy of 153 keV per atomic mass unit. A constraint of this design is that the longitudinal time focus at the RFQ entrance provided by the buncher is sensitive to the effects of space charge, as shown in Fig. 1. This limits the maximum time averaged current to roughly $2 \mu\text{A}$.

The parameters (A_{01}, A_{10}) were computed from Eqs. (6) and (7), using the machine parameters (a, m, k) for the ISAC-RFQ, though TRANSPORT can also directly accept the latter. The table of (s, A_{01}, A_{10}, k) for the ISAC-RFQ, shown in Fig. 2, was fed into TRANSPORT. For the purposes of this simulation, the $s = 0$ coordinate is defined at the entrance ground wall of the RFQ vacuum tank. The parameter k , as supplied to TRANSPORT, represents the value at the half-cell. A cubic spline produces a smooth interpolation, from which the function $\psi(s)$ is computed at each iteration through the linac. Figure 3 shows two separate cases, corresponding to a well matched, and a slightly mismatched $^{14}\text{N}^+$ beam, injected into the ISAC-RFQ, with parameters shown in Table II. In both cases, beam is injected at $E_i = 2.06$ keV per atomic mass unit and accelerated through the RFQ to 0.153 MeV per atomic mass unit. The slightly off-nominal case highlights betatron oscillations in the transverse envelope.

Input beam parameters can be optimized not only for a good match in the linac, but also through a sequence of elements that both precedes and follows the accelerator.

FIG. 1. PARMELA multiparticle simulation of the effects of space charge on the longitudinal ISAC-RFQ time focus, for a mass 30 beam, corresponding to the upper limit of RFQ mass to charge acceptance. The three-harmonic modulation, which defines the time focus after a 5 m drift from prebuncher to RFQ, begins to degrade as the bunch exceeds roughly $1 \mu\text{A}$ in beam intensity, with a $2 \mu\text{A}$ simulation shown for clarity. X-axis units are degrees at 35.36 MHz, the ISAC-RFQ operating frequency.

In the case of Fig. 3, the adaptively determined optimum step size, as chosen by TRANSPORT's Runge-Kutta engine, produced 2×10^4 steps, to meet a user specified Runge-Kutta relative error tolerance of 10^{-4} . This simulation, run on a conventional dual core desktop PC, was executed in less than ~ 0.1 second. The rapid computing time has important implications for troubleshooting and machine tuning from an operational standpoint where real-time simulations can assist operators in visualizing machine behavior, and for enabling development of automated tuning methods.

FIG. 2. ISAC-RFQ parameters A_{01} (red), A_{10} (purple), and k (green) used for TRANSPORT simulation. The parameters A_{01} and A_{10} are dimensionless, while k is in cm^{-1} . A radial matching section, starting 8.88 cm after the RFQ vacuum tank wall, occupies the first 8 cm of the vanes, followed by a transition cell and 195 accelerating cells. A high-energy transition cell finally gives way to a short unmodulated vane segment at the high energy end.

FIG. 3. 2-term TRANSOPTR simulation of the ISAC-RFQ, showing 2 rms envelopes on the left-hand vertical axis, with the y-envelopes shown as negative values for clarity. The simulation runs from the start of the RFQ tank at $s = 0$. Two separate envelopes are shown, corresponding to a matched and a mismatched case, in the transverse dimensions, with values from Table II. The mismatched case highlights the betatron oscillation and is shown in color including the longitudinal envelope. The beam energy is shown on the right-hand vertical axis. The transversely matched envelope is shown in light grey.

B. Comparison to PARMTEQ

The TRANSOPTR model was verified through comparison with the particle tracking code PARMTEQ, itself used in 1995 for the design of the ISAC-RFQ [1] and for subsequent studies of its performance [22]. In the present study, a Monte Carlo method was used to produce a PARMTEQ input file with 10^4 particles, consisting of three independent Gaussian distributions in (x, x') , (y, y') and (ϕ, E) . TRANSOPTR was supplied with only the initial rms values for emittances and Twiss parameters, as shown in Fig. 4.

It should be noted that from the longitudinal standpoint, the aforementioned input conditions do not emulate the reality of ISAC prebunching, which generates a modulated time-focus which includes high and low energy tails, as was introduced in Fig. 1. However, strictly for the purpose of model comparison, using such a realistic scenario in PARMTEQ would result in a broader longitudinal envelope, given the effects of rf filamentation, absent in TRANSOPTR. Further, both models were run with a purposely mismatched input, with corresponding Twiss parameters shown in Table II. This exaggerates the transverse and longitudinal oscillations visible on the envelope, shown in Fig. 5.

The emergent effects of longitudinal filamentation may already be seen in Figs. 4 and 5, where hints of bunch deformation in the longitudinal phase space are visible in the PARMTEQ distribution, resulting in a systematically broader longitudinal envelope. Running the same input parameters, but tripling the longitudinal emittance renders explicit the disagreement between models, with the resulting output distributions shown in Fig. 6. While both show excellent transverse phase space agreement, TRANSOPTR's second order Hamiltonian approach cannot include nonlinearities and as such does not simulate filamentation. Nevertheless, for well matched beams, one can still appreciate that the longitudinal envelope calculated by TRANSOPTR contains the core of the beam distribution.

Particle losses in PARMTEQ also represent an important consideration when comparing models. Being an rms

envelope code, TRANSOPTR does not track particle transmission losses and assumes conservation of normalized longitudinal emittance. On the other hand, the PARMTEQ RFQ model, under mismatched beam injection conditions will lose particles as phase-space trajectories become unstable and particles are ultimately intercepted by the RFQ vane, or drop out of the main bucket. As particles are lost along the linac, discrete variations in the rms beam parameters are expected. As no such constraint exists in TRANSOPTR, which places no constraint on the size of the second moments of the beam distribution, this does not arise. However, while tracking TRANSOPTR envelopes, it is a simple matter to detect when the envelope exceeds the aperture.

Simplicity of use is another advantage: the TRANSOPTR model is lightweight, requiring only an ascii formatted input file, containing a mapping of (s, A_{01}, A_{10}, k) , shown in Fig. 2. The main body of RFQ cells does not require more

TABLE II. TRANSOPTR RFQ simulation parameters as used in Fig. 3, for the matched and unmatched cases, both with ^{14}N . The transverse emittance ϵ_{xy} is used as an input emittance for both x and y dimensions. Twiss parameters for the longitudinal dimension have a subscript z . Starting coordinate $s = 0$ corresponds to the inner surface of the RFQ vacuum tank, 8.8 cm before the vanes.

Parameter	Matched	Mismatched
V_0 (kV)	35.200	35.200
E_i (keV/nucleon)	2.06	2.06
m_0 (MeV/ c^2)	13041.020	13041.020
α_x	2.390	2.300
β_x (cm/rad)	31.500	28.500
α_y	2.700	2.300
β_y (cm/rad)	33.600	28.500
ϵ_{xy} (cm rad)	3.0×10^{-3}	3.0×10^{-3}
α_z	-2.00	-2.00
β_z (rad/MeV)	2900.000	2900.000
ϵ_z (rad MeV)	10^{-4}	10^{-4}

FIG. 4. PARMTEQ normalized particle density distribution overlaid with TRANSOPTR ellipse of area $4\pi\epsilon_{rms}$, corresponding to 86% containment for Gaussian distributed beam. Input distributions in x - P_x , y - P_y , and t - E shown at top and output shown at bottom. The input and output locations are defined at the outer edges of the RFQ vacuum tank, 16.86 cm before and 15.83 cm after the RFQ vanes, respectively.

than one point per cell, since the smooth profile of the parameters (A_{01} , A_{10}) make the cubic spline interpolation adequate. For a more faithful simulation, a higher local density of points (10) was defined for both the low-energy transition cell, between radial matching section and first

accelerating cells, likewise for the high-energy transition cell. This avoided causing artificial variations arising by forcing the spline to locally conform to the transition cell geometry. As a comparison, the PARMTEQ simulation of the ISAC-RFQ requires externally generated electric field

FIG. 5. ISAC-RFQ envelope simulation of a $^{14}\text{N}^+$ beam, with injection parameters as shown in Table II and accelerated to 2.15 MeV. PARMTEQ rms envelope values are shown as black dots. TRANSOPTR transverse envelopes are shown in continuous red lines with dimensions on the left-hand vertical axis. The y -envelope is shown with negative values, and the x -envelope positive. The longitudinal envelopes for both codes are shown in the bottom half with dimensions shown on the right-hand vertical axis, with TRANSOPTR in continuous blue.

FIG. 6. PARMTEQ normalized particle density distribution compared to TRANSOPTR ellipse of area $4\pi\epsilon_{\text{rms}}$, corresponding to 86% containment for Gaussian distributed beam. Profiles for x - P_x , y - P_y , and t - E , taken at the RFQ vacuum tank exit, 15.83 cm downstream of the vanes. Input longitudinal emittance has been tripled with respect to that used in Fig. 4.

maps for the low and high energy transition regions, obtained using the code RELAX3D [1,23]. In total, there are 298 lines to the input TRANSOPTR mapping.

C. ISAC-RFQ injection tune correction

The addition of an RFQ subroutine opens the door to a more complete simulation capability for the envelope code. An example of such use is the refinement of the RFQ injection tune for the ISAC-low energy transport beamline (IRA), which matches the low energy transport from the target ion source to the RFQ. This matching section consists of 4 quadrupoles; their settings had been calculated based on match conditions that had been calculated from the RELAX3D field at the start of the RFQ vanes [24], and were always known to be in some sense approximate. This can be remedied now that we can optimize the match

directly observing the beam envelope in the RFQ. Figure 7 shows two simulations: the original IRA-RFQ injection match setting, as computed in 1997 in the upper plot, and the rematched case calculated using TRANSOPTR's internal optimizer. The quadrupole settings differ in these two cases by roughly 10%.

D. Other example uses

The availability of a fast envelope simulation and optimizer, able to continuously simulate acceleration through an RFQ or other linac, also opens the door to the development of on-line tuning methods. At TRIUMF, we have developed a graphical user interface that allows operators to choose sections of beamlines, which may include a linac, and using sliders that represent tuning parameters, explore their effect upon the envelope.

FIG. 7. Transverse beam envelopes for ISAC-RFQ injection. The top figure shows the original IRA-RFQ tune, computed 1997, prior to RFQ installation. The IRA electrostatic quadrupoles are numbered on both plots and their relative strength functions are shown in black, in arbitrary units. In the bottom figure, the RFQ injection has been recomputed using TRANSOPTR's RFQ subroutine, providing an optimized match through the accelerator.

The calculation is sufficiently fast that the output envelope plot can change continuously as (for example) a quadrupole strength or a cavity phase or amplitude is changed. As well, fitting goals can be built into the calculations that allow TRANSOPTR to calculate new tunes to, for example, change the final focus spot size. As the RFQ vane voltage and phase can be treated by the optimizer as any other tuneable element, both can now be incorporated into these computations.

Further operational developments include the coupled use of the envelope simulation, together with feedback diagnostic systems, such as quadrupole scan tomography, to provide the model with realistic input conditions. The fast execution time means the resulting envelopes can be used by control system applications intended to aid operators in optimizing tunes through the RFQ. Such a scheme is presently being developed at TRIUMF, which notably aims to use TRANSOPTR as part of a feedback coupled control system for operators to tune beamlines and accelerators, yielding a more controlled and reproducible tuning methodology and significantly reducing tuning overhead time.

IV. CONCLUSION

In this paper the second order Hamiltonian of an RFQ has been presented using the two first terms of Kapchinsky and Teplyaev's series solution to Laplace's equation for a modulated quadrupole accelerator. This Hamiltonian is the generator of the "two-term" linear part of the motion in the RFQ and has been implemented into the framework of TRANSOPTR. Simulations of the beam dynamics of the TRIUMF ISAC-RFQ with TRANSOPTR have been benchmarked with PARMTEQ. This implementation represents a novel application for the envelope code TRANSOPTR, now capable of simulating RFQ acceleration near-axis with sub-second computation times. The Hamiltonian of equation (19) also provides a handy, easily manipulable form with which the elementary dynamics of RFQ accelerators may be considered.

From a practical standpoint, the ability to include RFQ beam envelope computations with minimal computation time means TRANSOPTR can now be used to assist in the study and operation of a heavy-ion linac facility such as TRIUMF-ISAC. This development can help operators troubleshoot or optimize tunes through an RFQ accelerator, including accounting and correcting for space charge effects.

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APPENDIX A: DETAILED DERIVATION OF HAMILTONIAN FOR LINEAR MOTION

The Hamiltonian (4) with the added terms from the generating function can now be expanded to second order as appropriate for the description of only the linear motion. We have

$$\begin{aligned} H_s(x, P_x, y, P_y, z, P_z; s) \\ = -\sqrt{(E - q\Phi)^2/c^2 - m^2c^2 - P_x^2 - P_y^2} \\ + P_z + \frac{\beta'}{\beta} z P_z + \frac{z E'_0 + E_0}{\beta c}, \end{aligned} \quad (\text{A1})$$

excluding terms not dependent upon the 6 dependent variables, and implicitly assuming the substitutions:

$$E = \beta c P_z + E_0 \quad (\text{A2})$$

$$E_0 = \gamma m c^2 + q\Phi_0 \quad (\text{A3})$$

$$\begin{aligned} \Phi = \frac{V_0}{2} (A_{10} \cos \psi [(k^2/4)(x^2 + y^2) + 1] \\ + A_{01} [x^2 - y^2]) \sin(\omega t + \phi) \end{aligned} \quad (\text{A4})$$

$$\Phi_0 = \frac{V_0 A_{10}}{2} \cos \psi \sin(\omega t_0 + \phi) \quad (\text{A5})$$

$$E'_0 = \frac{q V_0 \omega}{2 \beta c} A_{10} \cos \psi \cos(\omega t_0 + \phi) \quad (\text{A6})$$

$$t = t_0 - \frac{z}{\beta c} \quad (\text{A7})$$

$$\beta' = \frac{\gamma'}{\beta \gamma^3} \quad (\text{A8})$$

$$(\text{A9})$$

E_0 , E'_0 , Φ_0 , t_0 , and β , γ are functions only of s . During numerical Runge-Kutta integration of equations of motion, ψ , t_0 , and $\gamma - 1$ are found by simultaneously integrating the following equations. (We track $\gamma - 1$ rather than γ , to avoid computational loss of precision at low energies.)

$$t'_0 = \frac{1}{\beta c} \quad (\text{A10})$$

$$\psi' = k \quad (\text{A11})$$

$$mc^2\gamma' = \frac{qV_0}{2}kA_{10}\sin\psi\sin(\omega t_0 + \phi) \quad (\text{A12})$$

As the reference particle, $(x, P_x, y, P_y, z, P_z) = (0, 0, 0, 0, 0, 0)$ will retain these null values during motion along s , all the first partial derivatives evaluated at null coordinates, must be zero. This is obvious for x, P_x, y, P_y since these variables are quadratic under the square root sign. This leaves only $z, P_z, \frac{\partial H}{\partial P_z}|_0$ will be zero because the term P_z after the square root will cancel a term coming from $\frac{\partial E}{\partial P_z}$ from the derivative of the square root term. Similarly, the fourth term gives a $\frac{\partial H}{\partial z}$ that is canceled by a term coming from $\frac{\partial \Phi}{\partial z}$ from the derivative of the square root term through the t -dependence in Φ . This result simply confirms that the canonical transformation of H from (t, E) to the differential coordinates with respect to the reference particle (z, P_z) is correct.

Of zeroth order second derivatives, only those listed below are nonzero. Evaluated for the reference particle, the square root in Eq. (A1) is the reference momentum $P = \beta\gamma mc$. Using this abbreviation, we find:

$$\begin{aligned} \frac{\partial^2 H}{\partial x^2}|_0 &= \frac{\partial}{\partial x} \frac{E - q\Phi}{\sqrt{\dots}} q \frac{\partial \Phi}{\partial x} \\ &= \frac{qV_0}{4\beta c} (k^2 A_{10} \cos\psi + 4A_{01}) \sin(\omega t_0 + \phi) \end{aligned} \quad (\text{A13})$$

$$\frac{\partial^2 H}{\partial P_x^2}|_0 = \frac{\partial}{\partial P_x} \frac{E - q\Phi}{\sqrt{\dots}} P_x = \frac{1}{P} \quad (\text{A14})$$

$$\begin{aligned} \frac{\partial^2 H}{\partial y^2}|_0 &= \frac{\partial}{\partial y} \frac{E - q\Phi}{\sqrt{\dots}} q \frac{\partial \Phi}{\partial y} \\ &= \frac{qV_0}{4\beta c} (k^2 A_{10} \cos\psi - 4A_{01}) \sin(\omega t_0 + \phi) \end{aligned} \quad (\text{A15})$$

$$\frac{\partial^2 H}{\partial P_y^2}|_0 = \frac{\partial}{\partial P_y} \frac{E - q\Phi}{\sqrt{\dots}} P_y = \frac{1}{P} \quad (\text{A16})$$

$$\begin{aligned} \frac{\partial^2 H}{\partial z^2}|_0 &= \frac{\partial}{\partial z} \frac{E - q\Phi}{\sqrt{\dots}} q \frac{\partial \Phi}{\partial z} \\ &= -\frac{qV_0}{2\beta c} A_{10} \cos\psi \left(\frac{\omega}{\beta c}\right)^2 \sin(\omega t_0 + \phi) \\ &\quad + \frac{(qV_0 \omega A_{10} \cos\psi \cos(\omega t_0 + \phi))^2}{4\beta^5 \gamma^3 mc^5} \end{aligned} \quad (\text{A17})$$

$$\frac{\partial^2 H}{\partial P_z^2}|_0 = -\beta c \frac{\partial}{\partial P_z} \frac{E - q\Phi}{\sqrt{\dots}} = \frac{1}{\gamma^2 P} \quad (\text{A18})$$

$$\begin{aligned} \frac{\partial^2 H}{\partial z \partial P_z}|_0 &= \frac{\beta'}{\beta} - \beta c \frac{\partial}{\partial z} \frac{E - q\Phi}{\sqrt{\dots}} \\ &= \frac{qV_0 A_{10}}{2\beta^3 \gamma^3 mc^3} [k\beta c \sin\psi \sin(\omega t_0 + \phi) \\ &\quad + \omega \cos\psi \cos(\omega t_0 + \phi)] \end{aligned} \quad (\text{A19})$$

and this results in the Hamiltonian of Eq. (19) upon which the TRANSOPTR calculation is based.

APPENDIX B: SPACE CHARGE

TRANSOPTR includes the effects of space charge on bunched beams by augmenting the **F**-matrix with a set of linear space charge defocusing terms [4]:

$$\mathbf{F}_{\text{SC}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ K_{\text{XSC}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & K_{\text{YSC}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & K_{\text{ZSC}} & 0 \end{pmatrix} \quad (\text{B1})$$

where [10]:

$$K_{\text{XSC}} = \frac{Q}{4\pi\epsilon_0(mc^2/e)\beta^2\gamma^3} \frac{1}{(5\sigma_{11})^{3/2}} g\left(\frac{\sigma_{33}}{\sigma_{11}}, \frac{\gamma^2\sigma_{55}}{\sigma_{11}}\right) \quad (\text{B2})$$

$$K_{\text{YSC}} = \frac{Q}{4\pi\epsilon_0(mc^2/e)\beta^2\gamma^3} \frac{1}{(5\sigma_{33})^{3/2}} g\left(\frac{\gamma^2\sigma_{55}}{\sigma_{33}}, \frac{\sigma_{11}}{\sigma_{33}}\right) \quad (\text{B3})$$

$$K_{\text{ZSC}} = \frac{Q}{4\pi\epsilon_0(mc^2/e)\beta^2\gamma^3} \frac{1}{(5\gamma^2\sigma_{55})^{3/2}} g\left(\frac{\sigma_{11}}{\gamma^2\sigma_{55}}, \frac{\sigma_{33}}{\gamma^2\sigma_{55}}\right) \quad (\text{B4})$$

here, Q is the integrated bunch charge. The function g is defined as:

$$g(u, v) = \frac{3}{2} \int_0^\infty (1+s)^{-3/2} (u+s)^{-1/2} (v+s)^{-1/2} ds \quad (\text{B5})$$

belonging to the family of Carlson elliptic integrals [25]. These integrals are strictly correct only for uniform charge density inside an ellipsoid. However, as shown by Sacherer [10], they are still correct, within a few percent, for describing the linear part of the space charge force, for other distributions as well, as long as the distribution has ellipsoidal symmetry. A more detailed, relativistically-correct derivation is given by Fubiani [26].

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