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High-order beam features and fitting quadrupole-scan data to particle-code models †

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Abstract. Quadrupole scans in the HEBT of the 6.7 MeV LEDA RFQ were analyzed to characterize the RFQ output beam. In previous work, profiles measured by the wire scanner were fit to models (beam parameterizations and HEBT simulations) to determine the transverse Courant-Snyder parameters α, β, and ε at the RFQ exit. Unfortunately, at the larger quadrupole settings, the measured profiles showed features that were not present in any of our simulations. Here we describe our latest analysis, which resulted in very good fits by using an improved model for the RFQ output beam. The model beam was generated by the RFQ simulation code TOUTATIS. In our fitting code, this beam was distorted by linear transformations that changed the Courant-Snyder parameters to whatever values were required by the nonlinear optimizer while preserving the high-order features of the phase-space distribution. No new physics in the HEBT was required to explain our quad-scan results, just an improved initial beam. High-order features in the RFQ output beam apparently make a significant difference in behavior downstream of the RFQ. While this result gives us increased confidence in our codes, we still have a mystery: exactly what high-order features in the beam are responsible for the the strange behavior downstream. Understanding this phenomenon may be helpful to understanding our halo-experiment data. We have begun to study this by comparing higher-order moments of the TOUTATIS distribution with other distributions.

1. Introduction

1.1. Quadrupole scans

During commissioning of the 6.7 MeV Low-Energy Demonstration Accelerator (LEDA) radio-frequency quadrupole (RFQ), we used a four-quadrupole high energy beam transport (HEBT) line to transport the beam from the RFQ exit to the beam stop. Quadrupole scans in the HEBT were used to characterize the transverse phase space at the RFQ exit. In this procedure, only the two quadrupoles immediately downstream of the RFQ exit were used. Quadrupole Q1 focuses in the *y*-direction and Q2 focuses in *x*. For characterizing the beam in the *x*-direction, Q2 was varied and the beam was observed at the wire scanner, which was about 2.5 m downstream, just before the beam stop. The strength of Q1 was fixed at a value that ensured that the beam was contained in both directions for all values of Q2. For characterizing the *y*-direction, Q1 was varied with Q2 fixed.

For both the *x*- and *y*-scans, as the quadrupole strength is increased from its minimum to its maximum value (we used about 10 settings in both cases), the beam size at the wire

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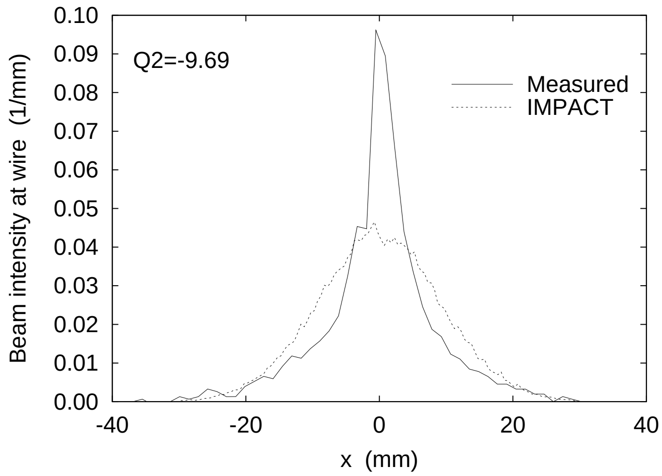

Figure 1. Comparison of a measured x-profile and an IMPACT simulation for Q2=−9.69 T/m. The initial beam for the simulation is a truncated Gaussian having Courant-Snyder parameters corresponding to the LINAC fit to the rms beam widths.

scanner goes through a minimum. At the minimum, the beam has a waist at the wire-scanner position. For larger quadrupole strengths, this waist occurs somewhere between the RFQ and the wire scanner. In this experiment, the wire-scanner profiles (beam intensities as functions of x or y) were recorded for each quadrupole setting. Although quad scans were done for several currents, we present results here for the highest current (nearly 100 mA) case.

1.2. Fitting to model of beam and HEBT

To determine the phase-space properties of the beam at the RFQ exit, we have to fit our data to some model that describes the behavior of the beam in the HEBT under quad-scan conditions. A model consists of two parts: a representation of the beam at the RFQ exit and a means of computing the beam at the wire-scanner position, given this beam as input. The problem is to find an input beam that best fits our data. We used input beams parameterized by the Courant-Snyder parameters α, β, and ε in the three directions. The initial beam parameters for the longitudinal direction were taken from the RFQ simulations (there was little coupling between the three directions). For computing the evolution of the beam in the HEBT, we used various simulation codes.

2. Previous results

2.1. Fit to LINAC rms sizes

Using the LINAC code and a uniform-in-4-D input distribution as our model, we could find a set of α, β, and ε values that produced a good fit to the rms beam size as a function of quadrupole gradient[1, 2]. However, for the larger quadrupole gradients, for the situation in which the beam waist is upstream of the wire scanner, the simulated and the measured beam profiles look quite different. The measured profiles had shoulders (triangular tails) that did not appear in any of the simulations. The agreement was especially poor in the x-direction. Figure 1 compares the measured and simulated profiles for one of the larger Q2 values, Q2=−9.69 T/m. Because of the inability to reproduce the measured profiles, we did not believe fits to this model could be used to accurately determine the Courant-Snyder parameters of the RFQ beam.

2.2. Fit to IMPACT profile shapes

In an attempt to improve our fitting procedure, we made two changes. The first change was to use the IMPACT code[3] to determine the evolution of the beam in the HEBT. IMPACT is a 3-D particle-in-cell (PIC) code with nonlinear space charge. The input beam was a truncated Gaussian parameterized by the usual Courant-Snyder parameters. The second change was to use all the profile data, not just the rms widths. For the *x*-scans, for each of the 11 values of Q2 and for each of the 51 *x*-positions of the wire, the difference between the measured intensity and the simulated intensity at the wire positions was computed. It is the sum of the squares of these 561 differences that was minimized by varying the values of α_x, β_x, and ε_x of the input beam (beam at RFQ exit). Unfortunately, this improved fitting procedure still failed to reproduce the shoulders in the profiles at the wire scanner position for the larger quadrupole gradients[4].

The beams we were using in the fitting procedures described above were uniform or truncated Gaussians in 4-D phase space. We also did IMPACT simulations (no fitting) using collections of particles generated by the RFQ simulation code PARMTEQM[5], which was used to design this RFQ. In addition, we investigated various distortions of the input phase-space distributions. In no case did our simulations exhibit the shoulders on the profiles that were seen in the measurements for the larger quadrupole gradients.

3. Improved input-beam model

Our latest improvement, which finally got good fits to the profiles, consisted of using the RFQ output beam generated by the TOUTATIS code[6] as the input beam for the IMPACT simulations. In the new fitting code, this beam (a collection of coordinates in phase space) was distorted by linear transformations that changed the Courant-Snyder parameters to whatever values were required by the nonlinear optimizer, while preserving the high-order features of the original phase-space distribution. The transformation between the initial coordinates (x_i, x'_i) and the final coordinates (x_f, x'_f) was

$$\begin{pmatrix} x_f \\ x'_f \end{pmatrix} = \sqrt{\frac{\varepsilon_f}{\varepsilon_i}} \begin{pmatrix} \sqrt{\frac{\beta_f}{\beta_i}} & 0 \\ \frac{\alpha_i - \alpha_f}{\sqrt{\beta_i \beta_f}} & \sqrt{\frac{\beta_i}{\beta_f}} \end{pmatrix} \begin{pmatrix} x_i \\ x'_i \end{pmatrix}, \qquad (1)$$

where $(\alpha_i, \beta_i, \varepsilon_i)$ are the Courant-Snyder parameters of the initial beam and $(\alpha_f, \beta_f, \varepsilon_f)$ are those of the final beam.

Figure 2 shows the data flow for the latest fitting code. Data files are represented by rectangular boxes and processes by boxes with rounded corners. The part of the figure inside the dashed lines correspond to a normal IMPACT simulation (no fitting to data). The initial particle file is *partcl_start.data*, which in the present case is the output of the TOUTATIS RFQ simulation. This distribution is transformed using equation (1) by the GENSIM code using new Courant-Snyder parameters stored in the file *beam.dat* to generate the file *partcl.data*, which is used by IMPACT as the initial beam. The optimizer process QSCANFIT looks at the final particle coordinates in file *fort.9*, which describes the beam at the wire-scanner location. This is done for all quadrupole settings. The error relative to the measured data is then determined. The nonlinear optimizer in the QSCANFIT process suggests new Courant-Snyder parameters, which are passed to the file *beam.dat* to use in the next iteration.

We started our new fitting calculation with a TOUTATIS beam having Courant-Snyder parameters determined by our previous LINAC fits to the rms widths. We found, to our

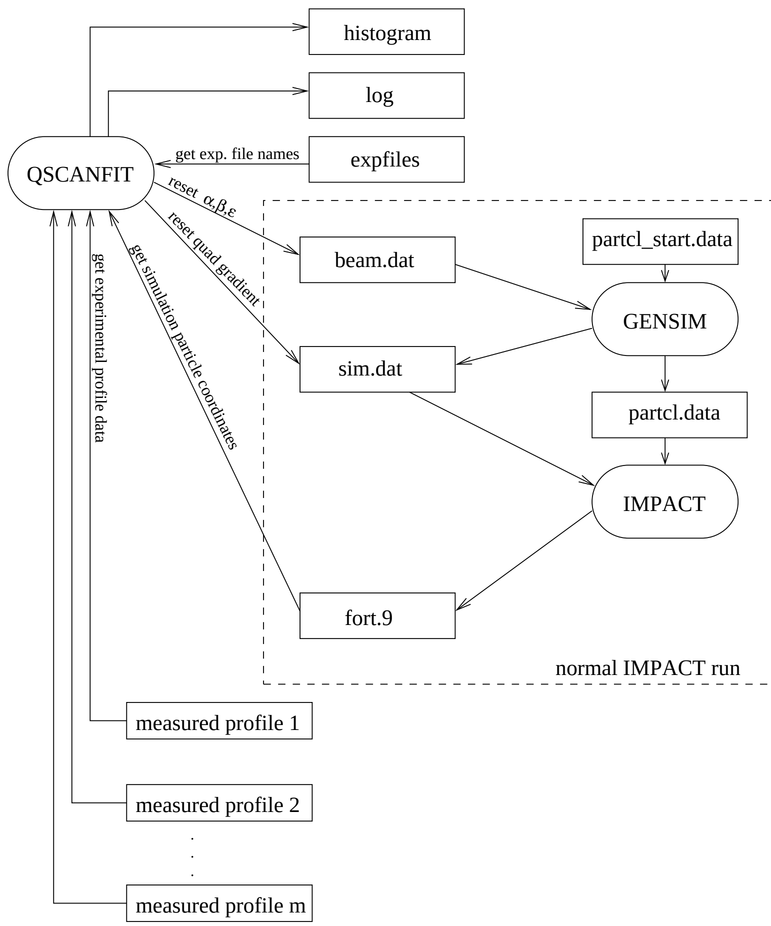

Figure 2. Data flow for fitting the quad-scan measured profiles to the TOUTATIS/IMPACT model. Data files are represented by rectangular boxes and processes by boxes with rounded corners.

surprise, that the optimizer could not find better Courant-Snyder parameters than this initial guess. The reason was that the simulation with this initial beam accurately reproduced all the structure of the measured profiles, including the shoulders on the profiles for the larger quad settings.

Figures 3 and 4 shows these results for the x-scan. We show the x-scans because it was this direction that gave the poorer fits in our previous work. The figure shows the measured and simulated profiles at the wire scanner for ten different Q2 values. We see how the beam width decreases as the strength of the quadrupole is turned up and then starts to increase again. At this point (see case for Q2=-7.70 T/m), shoulders (triangular tails) appear in the profiles. These tails were not present in any of our previous simulations that did not use the TOUTATIS beam as a starting point. Compare figure 1 to the third graph in figure 4. The old simulation did a very poor job of reproducing the shape of the distribution. It is important to remember that the only difference between the old and the new simulations is that the higher-order features of the initial beams are different. Both initial beams have exactly the same second moments (Courant-Snyder parameters). We repeated some of the TOUTATIS simulations with reduced and zero space charge. While this changed the beam size at the wire scanner substantially, the shoulders on the profiles remained. It is clear the behavior in the tails of the distribution is caused by the initial beam and not generated in the HEBT.

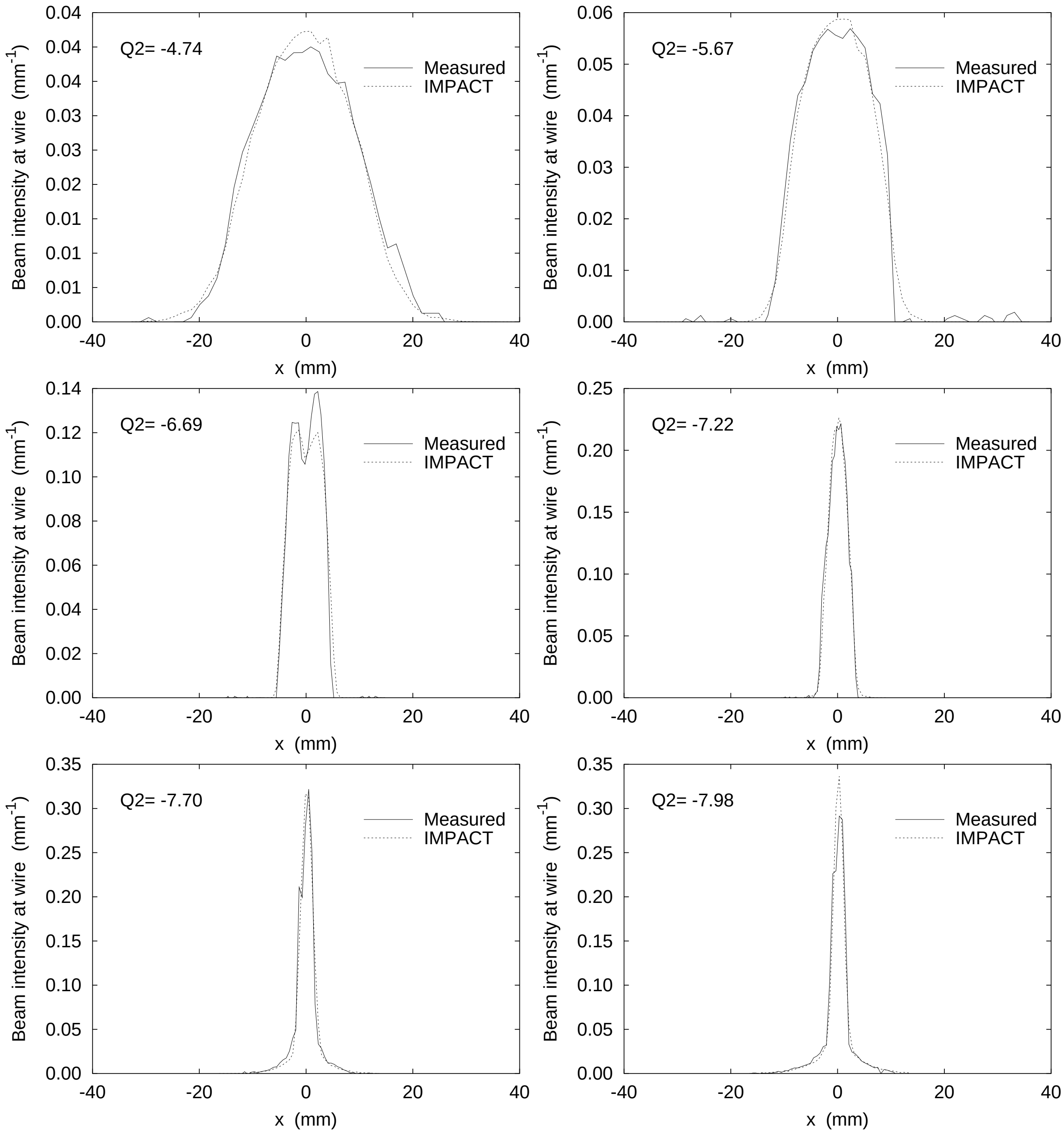

Figure 3. Comparison of measured profiles in the *x*-direction with IMPACT simulations for various values of Q2. The initial beam for all these simulations was an RFQ exit beam generated by TOUTATIS and distorted by a linear transformation to have Courant-Snyder parameters corresponding to those determined by fitting rms widths to LINAC simulations. Fitting by IMPACT to the details of the profiles did not improve these already good fits. Continued in figure 4.

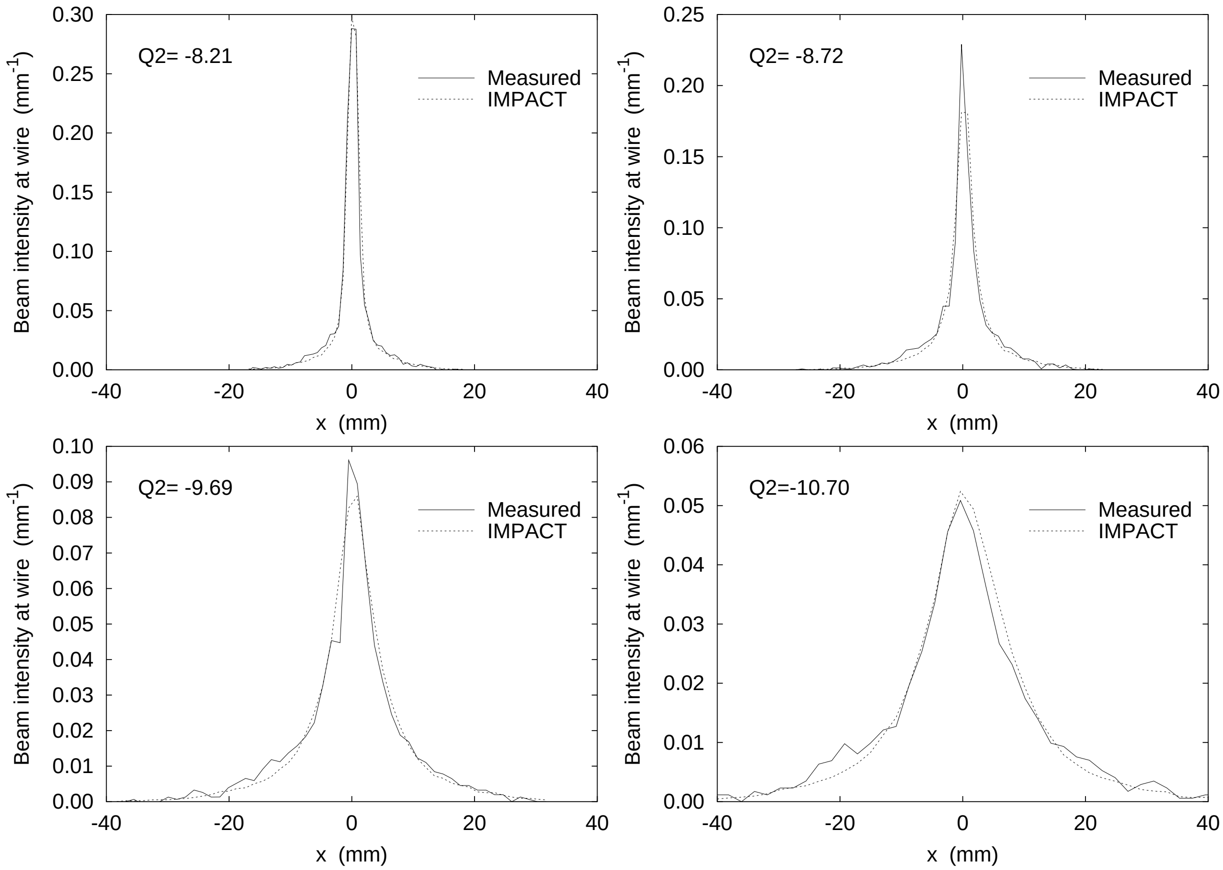

Figure 4. Continuation of figure 3. Some more Q2 values.

Table 1. Courant-Snyder parameters at the RFQ exit (unnormalized).

	α_x	β_x (mm/mrad)	ε_x (mm·mrad)	α_y	β_y (mm/mrad)	ε_y (mm·mrad)
Prediction (PARMTEQM)	1.59	0.398	2.03	-2.74	0.726	2.04
Prediction (TOUTATIS)	1.99	0.464	1.68	-3.63	0.904	1.75
Measured (LINAC rms fit)	1.79	0.358	2.11	-2.48	0.892	2.62

Table 1 shows the Courant-Snyder parameters for the LINAC rms fit. Also shown are the predictions from the PARMTEQM and TOUTATIS codes.

4. Discussion

In summary, we have seen that using a TOUTATIS beam as the basis for the input-beam model correctly reproduces the previously mysterious shoulders in the wire-scanner profiles. We have also seen that there is little feed-down from higher order. Our older rms fits generated good values for the second moments (Courant-Snyder parameters) even though those simulations got the higher-order features wrong.

The beam from the TOUTATIS simulation of the RFQ contains higher-order features that are not in the uniform, truncated Gaussian, or even the PARMTEQM output beams. It appears that features of the beam seen in the HEBT have their origins in the RFQ or

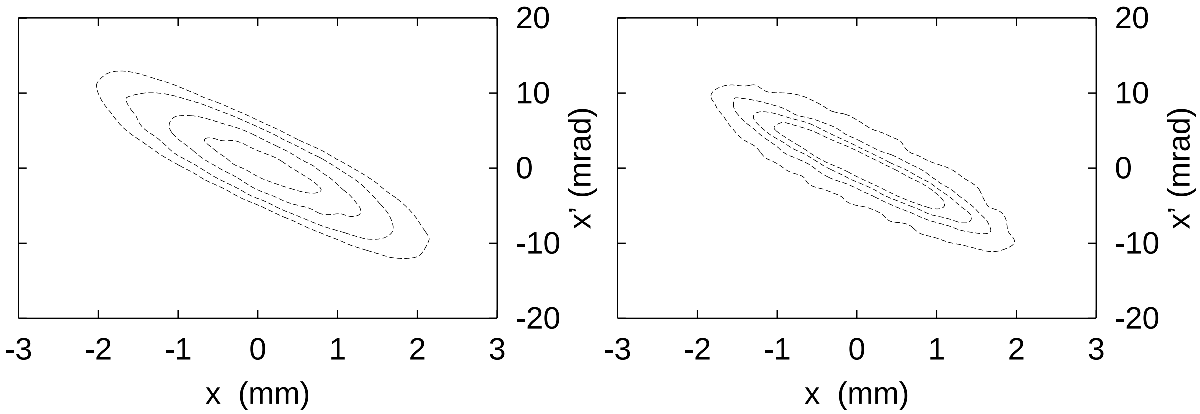

Figure 5. Contours of equal density in phase space for the PARMTEQM (left) and the TOUTATIS (right) RFQ exit distributions in the *x*-direction. Both of these beams have the same second moments.

perhaps even upstream of the RFQ. The practical consequence of this is that we have to be careful in preparing beams because high-order features can significantly influence behavior downstream. The good news is that no new physics was required to explain our quad-scan results, just a better input beam. The simulation codes accurately reproduce our experimental results. Although the quad-scan procedure differs from the ordinary HEBT operation or beam transport in a linac, the physics regime is still similar. We felt it was important that the beam behavior we observed in the experiment be seen in the simulations. We now believe we have a believable characterization of the RFQ output beam, but this is of secondary importance (quad scans are probably not a good way to measure the LEDA RFQ beam properties). The fact that the simulation codes correctly predict beam behavior increases our confidence in the design work that is based on our codes.

Of course, there is still a mystery. Exactly what high-order features in the RFQ output beam are causing the shoulders in the wire-scanner profiles? This should be investigated because it may be related to halo generation in linacs having its origin upstream of the RFQ exit. In particular, an understanding of this phenomenon may help us better understand our halo-experiment data[7].

In the TOUTATIS code, the space charge and external (rf) electric fields are calculated numerically with a multigrid finite-difference method using the actual vane geometry. This provides a more accurate representation of the fields in the region outside a cylinder of radius equal to the minimum aperture than the expansions used in PARMTEQM. Also, TOUTATIS uses the actual vane geometry to determine which particles are lost by striking the walls instead of the circular cylinder used in PARMTEQM. (The latter feature has been incorporated into the latest version of PARMTEQM and the resulting beams are now more similar to the TOUTATIS results.) Apparently, the details of the motion of particles in the RFQ near the periphery of the beam are responsible for the interesting behavior we observed in the quadrupole-scan experiments in the LEDA HEBT.

Figure 5 compares the PARMTEQM and TOUTATIS beams at the RFQ exit. Both beams have been distorted to have the Courant-Snyder parameters α, β, and ε to correspond to that of the LINAC rms fit. The contours shown for both beams are for phase-space densities of 0.005, 0.015, 0.030, and 0.050 $(\mathrm{mm}\cdot\mathrm{mrad})^{-1}$. The PARMTEQM distribution is smoother than the TOUTATIS distribution because it has more particles (93k particles compared to 27k). There is no obvious feature that explains why only the TOUTATIS beam leads to the shoulders in the profiles at the wire scanner.

One way to analyze the high-order features of the beam is by higher moments. One well-

Table 2. Invariant kurtosis for some distributions.

Distribution	k_2
uniform	2.31
Gaussian	3.46
PARMTEQM	2.96
TOUTATIS	4.46

known technique for 1-D distributions is to look at the kurtosis k, which is the fourth moment of the distribution, normalized by the square of the second moment:

$$k = \frac{<x^4>}{<x^2>^2}. \tag{2}$$

This quantity has value 2 for a uniform distribution, 3 for a Gaussian distribution, and higher values for more peaked distributions. Often, the kurtosis is defined with a 3 subtracted from the ratio above making the kurtosis zero for a Gaussian distribution.

For phase space (x, p), we have two dimensions for one degree of freedom. If we want to extend the definition of kurtosis to phase space we need to also account for correlations between x and p. A reasonable definition is something like the halo variable in reference [8]

$$k_2 = \frac{\left(<x^4><p^4> - 4<x^3p^{>}<xp^3> + 3<x^2p^2>^2\right)^{1/2}}{<x^2><p^2> - <xp>^2}. \tag{3}$$

The numerator and denominator are both moment invariants, which are functions of moments that are preserved for linear motion. The denominator is the square of the usual rms emittance. Other moment invariants exist and may also possibly be useful for describing halo. The advantage of a definition like that of (3) is that its value is the same anywhere in a beamline where the motion is linear. Thus the halo cannot hide just by being observed at some particular point in the beamline. (Of course, this is only approximate if nonlinearities are involved.) Because of this property, we can think of k_2 as some kind of invariant kurtosis. Table 2 shows the value of k_2 for some distributions. Notice that the TOUTATIS distribution has a fairly high value of the invariant kurtosis. It may be useful to study if high kurtosis is an indicator of susceptibility to halo generation.

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