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A Study of the Transverse Coherence Properties of the LCLS

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Abstract

The LINAC Coherent Light Source (LCLS), an X-Ray free-electron laser(FEL) based on the self amplified spontaneous emission principle, has recently come on-line. For many users it is desirable to have an idea of the level of transverse coherence of the X-Ray beam produced. In this paper, we analyze the output of GENESIS simulations of electrons traveling through the FEL. We first test the validity of an approach that ignores the details of how the beam was produced, and instead, by assuming a Gaussian-Schell model of transverse coherence, predicts the level of transverse coherence simply through looking at the beam radius at several longitudinal slices. We then develop a Markov chain Monte Carlo approach to calculating the degree of transverse coherence, which offers a $\sim$100-fold speedup compared to the brute-force algorithm previously in use. We find the beam highly coherent. Using a similar Markov chain Monte Carlo approach, we estimate the reasonability of assuming the beam to have a Gaussian-Schell model of transverse coherence, with inconclusive results.

Contents

I. INTRODUCTION

The LINAC Coherent Light Source (LCLS) has recently come on-line. The LCLS is a free-electron laser (FEL) that works based on the self amplified spontaneous emission(SASE) principle.[1] The LCLS can create coherent X-Ray radiation, which will be able to be used for imaging very small objects, such as single proteins. Since the radiation produced by the LCLS is highly coherent, objects can be imaged through looking at the interference patterns produced. This is often more powerful than simply looking at absorption patterns as in the case, for example, with a conventional microscope.

The level of transverse coherence of the LCLS tells us a lot about its imaging capabilities. Therefore, it is desirable to have an accurate idea of the level of transverse coherence produced by the LCLS. Many diagnostics are being proposed and run to measure the properties of the beam produced. Traditionally, transverse coherence properties can be measured through setting up a double slit experiment and measuring the position and visibility of fringes produced. However, the LCLS is producing X-Rays, with wavelengths of $\sim$1.5 Angstroms, roughly the size an atom, so transverse coherence properties can not be easily measured through these standard techniques.

A. Transverse Coherence

Consider a flat surface of many light sources emitting monochromatic light of a wavelength much smaller than the size of the surface. We want to find how the light emitted depends on the level of coherence between the different light sources.

When the sources are in-phase and completely coherent, they will interfere to form a fairly straight beam pointed orthogonal to the surface. This is because when an observer is far away from the surface in the orthogonal direction, all of the sources are about the same distance apart and are in-phase. Therefore all sources positively interfere to create a high intensity orthogonal to the surface. However, if an observer is far away from the surface in a non-orthogonal direction, the observer is at a different distance from each source, therefore, most of the sources will destructively interfere. Therefore, the vast majority of the intensity will be concentrated in a coherent beam orthogonal to the surface, which will only be slightly divergent.

When the multiple sources are completely incoherent, the different sources have a random phase relative to each other. Therefore, the light produced by each source will not interfere with the light produced by other sources, as the random phase difference between sources remains a random phase difference regardless of the phase factor from differing distances between the sources and the observer. Therefore, light will emanate from our set of sources equally in all directions. Note that this is just a fancy way of describing something very intuitive-light produced by bulbs arranged on a surface will not spontaneously interfere to create a coherent beam.

We see that a completely coherent set of in-phase sources on a plane produces a beam that diverges very little. However, when the sources are made completely incoherent, they produce no beam at all, instead radiating equally in all directions. Viewing a continuous source as an infinite array of infinitesimally small point sources, we see that the level of transverse coherence will determine how quickly the resultant beam will diverge. A highly coherent source will produce a slightly divergent beam; a low-coherence source will produce a much more divergent beam. Armed with this notion, we now get a little more mathematical.

B. Mathematical Formulation

Many of the statistical properties of light can be described by the mutual coherence function.[23]

$$\Gamma(\mathbf{r}_1, \mathbf{r}_2, \tau) = \langle E(\mathbf{r}_1, t) E^*(\mathbf{r}_2, t+\tau) \rangle$$

Where $\mathbf{r}_1$ and $\mathbf{r}_2$ are positions, and $E(\mathbf{r}, t)$ is the complex-valued electric field at position $\mathbf{r}$ and time t.

We can also consider the coherency between two points limited to a single frequency basis, which is called the cross-spectral density function.

$$W(\mathbf{r}_1, \mathbf{r}_2, \omega) = \int_{-\infty}^{\infty} \Gamma(\mathbf{r}_1, \mathbf{r}_2, \tau) e^{-i\omega\tau} \delta\tau$$

We also care about the mutual intensity function

$$J(\mathbf{r}_1, \mathbf{r}_2) = \Gamma(\mathbf{r}_1, \mathbf{r}_2, 0)$$

When we are dealing with light that is close to monochromatic, we can assume that all of the light is close to the frequency ω_0, and we make the assumption:

$$J(\mathbf{r}_1, \mathbf{r}_2) \propto W(\mathbf{r}_1, \mathbf{r}_2, \omega_0)$$

C. The Gaussian-Schell model

The Gaussian-Schell model is a model of transverse coherence of a beam moving along the z-axis. At $z = 0$, the source point of the beam,

$$W(\mathbf{r}_1, \mathbf{r}_2, z = 0, \omega = \omega_0) = A^2 exp[-\frac{(\mathbf{r}_1^2 + \mathbf{r}_2^2)}{4\sigma_S^2}] exp[-\frac{(\mathbf{r}_1 - \mathbf{r}_2)^2}{2\sigma_G^2}]$$

A is the amplitude

$\mathbf{r}_2, \mathbf{r}_2$ are two-dimensional vectors representing transverse positions

σ_S is equal to the beam radius at the source, σ_G is equal to the transverse coherence length at the source

We are making a quasi-monocromatic approximation, $J \propto W(\omega_0)$ so we can say:

$$J(\mathbf{r}_1, \mathbf{r}_2, z = 0) \propto exp[-\frac{(\mathbf{r}_1^2 + \mathbf{r}_2^2)}{4\sigma_S^2}] exp[-\frac{(\mathbf{r}_1 - \mathbf{r}_2)^2}{2\sigma_G^2}]$$

We can see that the intensity at the source, $I \propto J(\mathbf{r}, \mathbf{r}, z = 0) \propto exp[\frac{-\mathbf{r}^2}{2\sigma_S}]$, so at the source, there is a beam of Gaussian intensity, where σ_S is the beam radius.

The correlation coefficient between the field at any two points is

$$\frac{J(\mathbf{r}_1, \mathbf{r}_2)}{(\sqrt{J(\mathbf{r}_1, \mathbf{r}_1) J(\mathbf{r}_2, \mathbf{r}_2)})} = exp[-\frac{(\mathbf{r}_1 - \mathbf{r}_2)^2}{2\sigma_G}]$$

We can see that the correlation coefficient decays as a Gaussian with the distance between $\mathbf{r}_1$ and $\mathbf{r}_2$, where σ_G is the transverse coherence length

Now we want to see what the properties of the beam are away from the source point. At points away from the source, $z > 0$, the beam propagates as:

$$J(\mathbf{r}_1, \mathbf{r}_2, z) \propto \frac{1}{\Delta(z)^2} exp[-\frac{(\mathbf{r}_1^2 + \mathbf{r}_2^2)}{4\sigma_S^2[\Delta(z)]^2}] exp[-\frac{(\mathbf{r}_1 - \mathbf{r}_2)^2}{2\sigma_G^2[\Delta(z)]^2}] exp[-\frac{ik(\mathbf{r}_1^2 - \mathbf{r}_2^2)}{2R(z)}]$$

where $\Delta(z)$ is the expansion coefficient

$$\Delta(z) = \sqrt{1 + (z/k\sigma_S\delta)^2}$$

,

$$\frac{1}{\delta^2} = \frac{1}{(2\sigma_S)^2} + \frac{1}{\sigma_G^2}$$

$$R(z) = z[1 + (\frac{k\sigma_S\delta}{z})^2]$$

where k is the wavenumber of the frequency ω_0.

The first exponential term is related to the beam radius, as it is the only term that doesn't go to 1 as $\mathbf{r}_1 \to \mathbf{r}_2$. The second term is related to the transverse coherence length, whose magnitude scales as a Gaussian of the distance between $\mathbf{r}_1$ and $\mathbf{r}_2$. The third term is a phase difference due to the slightly different lengths of $\mathbf{r}_1$ and $\mathbf{r}_2$ from the source. We can see that the both beam radius and the transverse coherence length increase proportionally to the expansion coefficient, $\Delta(z)$.

The degree of transverse coherence is:

$$\zeta(z) = \frac{\int |J_{12}|^2 \delta\mathbf{r}_1 \delta\mathbf{r}_2)}{(\int J_{11}\delta\mathbf{r}_1)^2}$$

$$J(\mathbf{r}_1, \mathbf{r}_2, z) = \langle E(\mathbf{r}_1, z) E^*(\mathbf{r}_2, z) \rangle$$

Where $J_{12} = J(\mathbf{r}_1, \mathbf{r}_2, z)$, and $J_{11} = J(\mathbf{r}_1, \mathbf{r}_1, z)$

For the GSM, evaluating the degree of transverse coherence analytically shows that it depends on the ratio between the beam radius and the transverse coherence length, and is independent of z

$$\zeta_{GSM} = \frac{\sigma_G^2}{\sigma_G^2 + (2\sigma_S)^2}$$

The appeal of assuming a GSM is that we can predict all coherence properties through simply measuring the beam radius for several values of z (Possible experimentally or through a computer simulation) without ever considering the details of how the beam was actually produced. Then, through knowing the expansion coefficient, we can calculate all transverse coherence properties of the beam produced. The question is, of course, whether the actual beam properties are close enough to the GSM to make this approximation reasonable. Another issue when assuming a GSM for an FEL is where to assume the beam source to be; unlike in a conventional source, the radiation from a FEL originates at all points within the undulators.

II. NUMERICAL METHODS

A. Curve Fitting

1. *Finding the beam radius*

One way we can find the beam radius is by finding the root-mean-square of the beam intensity.

$$\text{Beam Width}^2 = \frac{1}{2}\frac{\int J(\mathbf{r},\mathbf{r})\mathbf{r}^2}{\text{Power}^2}$$

The factor of $\frac{1}{2}$ is because we are integrating over a two-dimensional vector.

Another way we can find the beam radius is through fitting. Since both the simulated beam intensity profile and a Gaussian beam intensity profile are functions over the same space, we can treat them as vectors, and try to minimize the angle between them.

$$cos(\theta) = \frac{I_{Measured} \cdot I_{Gaussian}}{|I_{Measured}||I_{Gaussian}|}$$

This is equivalent to maximizing the quantity,

$$\frac{(I_{Measured} \cdot I_{Gaussian})^2}{|I_{Measured}|^2|I_{Gaussian}|^2}$$

2. *Fitting beam radius to the GSM*

If we know the location of the beam source, then all we need to know is δ and σ_S to know all of the properties of the beam. Therefore, we assume a source point, which is a somewhat unsafe assumption, as the radiation produced comes from the total length of the undulators. Having assumed a source point, we assume σ_S to be the beam radius at the source point. We can then simply fit δ with a least-squares fit. This approach has the advantage in that it can be done simply through looking at the beam radius at various points without ever considering the details of how the beam was produced. The same approach was used to model the properties of FLASH(Free electron LASer at Hamburg), a FEL at DESY operating under the SASE principle.[4]

B. Calculating the Degree of Transverse Coherence

Using data produced by the GENESIS code[5], which performs simulations of electrons traveling through the undulators, we can measure the electric field at all points in time at every position along the z-axis. Since in a simulation, unlike in experiment, we can observe everything, we can make calculations we could not otherwise make.

One quantity of interest is the degree of transverse coherence, which is

$$\zeta(z) = \frac{\int\int |J_{12}|^2 \delta\mathbf{r}_1 \delta\mathbf{r}_2}{(\int J_{11}\delta\mathbf{r}_1)^2}$$

where $J_{12} = J(\mathbf{r}_1, \mathbf{r}_2, z)$, $J_{11} = J(\mathbf{r}_1, \mathbf{r}_1, z)$.

Note that J_{11} is equal to the intensity at $\mathbf{r}_1$; Therefore, $\int J_{11}\delta\mathbf{r}_1 \propto$ Beam Power. We can replace the term in the denominator with the total power squared, giving us:

$$\zeta = \frac{\int\int |J_{12}|^2 \delta\mathbf{r}_1 \delta\mathbf{r}_2}{\text{Power}^2}$$

ζ is difficult to calculate explicitly, as the integration area is very large. To do this, we need to integrate over all pairs of points $(\mathbf{r}_1, \mathbf{r}_2)$ along the axis. For example, if your electric field is 100 cells wide, then you have 10,000 values of $\mathbf{r}$. Therefore, you have to calculate $10,000^2 = 100$ million quantities for J_{12}(One for each pair $(\mathbf{r}_1, \mathbf{r}_2)$): Note-You can get it down to 50 million using the Hermitian propertiy of the J matrix, as $J(\mathbf{r}_1, \mathbf{r}_2) = J(\mathbf{r}_2, \mathbf{r}_1)^*$, but it's still a fairly unwieldy calculation.

Fortunately, we can make the degree of transverse coherence susceptible to Markov chain Monte Carlo techniques by rewriting the degree of transverse coherence as:

$$\zeta(z) = \int \frac{|J_{12}|^2}{\text{Power}^2} = \int \frac{|J_{12}|^2}{J_{11}J_{22}} \frac{J_{11}J_{22}}{\text{Power}^2} = \int f(\mathbf{r}_1, \mathbf{r}_2) P(\mathbf{r}_1, \mathbf{r}_2)$$

Where $P(\mathbf{r}_1, \mathbf{r}_2) = \frac{J_{11}J_{22}}{\text{Power}^2}$ and
$f(\mathbf{r}_1, \mathbf{r}_2) = \frac{|J_{12}|^2}{J_{11}J_{22}}$

We can treat $P(\mathbf{r}_1, \mathbf{r}_2)$ as a probability, as $\int(P(\mathbf{r}_1, \mathbf{r}_2)) = \frac{\int J_{11} \int J_{22}}{\text{Power}^2} = \frac{\text{Power}^2}{\text{Power}^2} = 1$. Therefore, we can estimate it by sampling $f(\mathbf{r}_1, \mathbf{r}_2)$ with probability $P(\mathbf{r}_1, \mathbf{r}_2)$, which we can do through using a random weighted walk through the state space. In this case, a state α represents a pair of transverse points $(\mathbf{r}_1, \mathbf{r}_2)$.

We use a weighted random walk through the state space. Each state α has a certain probability distribution of states α' it can transition to during each iteration. The pseudocode for the algorithm is straightforward and is shown below:

State α

State $\alpha' = \text{randomNeighboringState}(\alpha)$

$$\text{if}\left(\text{rand}() < \frac{\text{Probability}(\alpha')}{\text{Probability}(\alpha)}\right)$$

$\alpha \leftarrow \alpha'$

Sample f(α)

where rand() returns a random number from zero to 1.

It can be proven that, as long as, for all (α_1, α_2), the probability of α_2 being proposed as a transition from α_1 is equal to the probability of the opposite, the correct probability distribution is generated by this set of transition probabilities. Markov chain Monte Carlo algorithms have the significant advantage over other Monte Carlo algorithms in that most of the time is spent sampling from the most important parts of the summation. This makes a Monte Carlo approach faster.

Initial states of the random walk are determined through rejection sampling, where we propose states with uniform probability, and then only accept them with probability proportional to $P(\alpha)$. This algorithm will return the correct distribution of α. Since for our implementation, $P(\alpha) = P(\mathbf{r}_1)P(\mathbf{r}_2)$, values of $\mathbf{r}_1$ and $\mathbf{r}_2$ can be generated independently from each other, speeding up the algorithm significantly.

C. Estimating the Similarity of the Emitted Radiation to the GSM

One way to see how well our model fits is to estimate the difference between $J(\alpha)$ and $G(\alpha)$. In doing so, we neglect the phase term of the GSM, as it depends on the source point, which we don't exactly know. This might not be a safe assumption.

Since both $J(\alpha)$(measured from simulation data) and $G(\alpha)$(our GSM based on the calculated beam radius and measured degree of transverse coherence) are functions over the same space, we can treat them both as vectors and find the "angle" between the two.

$$cos(\theta) = \frac{J \cdot G}{|J||G|}$$

$$cos(\theta)^2 = \frac{(J \cdot G)^2}{(J \cdot J)(G \cdot G)}$$

$$J \cdot G = \int_\alpha J(\alpha) G^*(\alpha)$$

$$J \cdot G = \int_\alpha \frac{J(\alpha)G^*(\alpha)}{J_{11}(\alpha)J_{22}(\alpha)} J_{11}(\alpha)J_{22}(\alpha) = \text{Power}^2 \int_\alpha \frac{J(\alpha)G^*(\alpha)}{J_{11}(\alpha)J_{22}(\alpha)} \frac{J_{11}(\alpha)J_{22}(\alpha)}{\text{Power}^2}$$

$$= \text{Power}^2 \int_\alpha f_{JG}(\alpha) P(\alpha)$$

Where $f_{JG}(\alpha) = \frac{J(\alpha)G^*(\alpha)}{J_{11}(\alpha)J_{22}(\alpha)}$, and $P(\alpha)$ is still $\frac{J_{11}(\alpha)J_{22}(\alpha)}{\text{Power}^2}$

We use the same scheme for $J \cdot J$ and $G \cdot G$:
$J \cdot J = \text{Power}^2 \int_\alpha P(\alpha) f_{JJ}(\alpha)$, where $f_{JJ}(\alpha) = \frac{|J(\alpha)|^2}{J_{11}(\alpha)J_{22}(\alpha)}$
$G \cdot G = \text{Power}^2 \int_\alpha P(\alpha) f_{GG}(\alpha)$, where $f_{GG}(\alpha) = \frac{|G(\alpha)|^2}{J_{11}(\alpha)J_{22}(\alpha)}$

$$cos(\theta)^2 = \frac{(J \cdot G)^2}{(J \cdot J)(G \cdot G)} = \frac{(\text{Power}^2 \int_\alpha P(\alpha) f_{JG}(\alpha))^2}{\text{Power}^2 \int_\alpha P(\alpha) f_{JJ}(\alpha) \text{Power}^2 \int_\alpha P(\alpha) f_{GG}(\alpha)}$$

$$= \frac{(\int_\alpha P(\alpha) f_{JG}(\alpha))^2}{\int_\alpha P(\alpha) f_{JJ}(\alpha) \int_\alpha P(\alpha) f_{GG}(\alpha)}$$

We estimate each of the three quantities($J \cdot G$, $J \cdot J$ and $G \cdot G$) using the same Markov chain. By doing this, we cause the uncertainties in each measurement to be correlated to each other, significantly reducing the error.

1. Monte Carlo error estimation

We estimate $J \cdot G$, $J \cdot J$ and $G \cdot G$ using the same set of statistically independent Markov Chains. We have enough statistically independent branches (400) to provide a good estimate of the distribution of measured ($J \cdot G$, $J \cdot J$, $G \cdot G$). Therefore, what we do is randomly select N estimations out of our N Markov chains (Some being selected multiple times and some not at all). This will give us an estimate of the distribution of calculations we were

likely to make. Therefore, from doing this multiple times, we can find the error bar of our calculation. This is a much more straightforward method than explicitly calculating all of the standard deviations and correlations between the three quantities estimated.

D. Implementation

I implemented the algorithms in MATLAB. All random walks were executed in parallel using MATLAB's array functionality.

III. RESULTS AND DISCUSSION

A. Curve Fitting

Having 84 meters of undulators, we first naively assume the source of the GSM to be at the end of the undulators, and fit the measured growth of the beam radius to that predicted by the GSM. [Fig. 1]

This doesn't work very well at all. The expansion coefficient of the GSM starts off with a quadratic regime and then goes to a linear regime. However, the beam radius increases fairly linearly, which causes a poor fit. We therefore assume the source to be located inside the undulators at 64 meters, which is approximately where saturation is reached and the beam power plateaus. [Fig. 2]. This gives us somewhat better results, but still leaves much to be desired.

B. Analyzing Transverse Coherence Properties

The Markov chain Monte Carlo approach works about 100 times faster than the brute force algorithm, and converges to within a reasonable error bar within 45 seconds. This is much better than the hour and a half runtime that the brute-force algorithm takes[Fig. 4], and will be a very useful for analyzing future simulations.

Analyzing the degree of transverse coherence[Fig. 5], we can see that the degree of transverse coherence peaks at approximately 70 meters, which is about the same point where the beam power plateaus. Transverse coherence peaks at almost 90%, which is very

good. We can either estimate the beam radius as the (root mean square) rms of intensity, or by fitting the intensity profile to a Gaussian. We compare the agreement between these two approaches. [Fig. 6] We see that we get a somewhat better agreement when we find the beam radius through fitting rather than through a rms calculation. Finding a value of the beam radius through fitting gives a somewhat smaller value [Fig. 7]. This is because the intensity profile is mostly Gaussian, but has a non-Gaussian "Halo", which "contaminates" the rms calculation of the beam radius. Knowing the beam radius (both found through rms and fitting) and the degree of transverse coherence, we can propose a GSM and see how well the mutual intensity function J fits the predictions of the GSM. We ignore the phase factor of the GSM, as it depends on the location of the source. [Fig. 8].

This is somewhat close, but certainly not close enough to consider the GSM to be the end-all model for transverse coherence of the LCLS. To see how much better the agreement might be if we were to have picked the right source point which produced the right phase factor, we test the agreement between the magnitude of the GSM and the magnitude of the mutual intensity function [Fig. 9]. This provides an upper-bound on any possible agreement, as different phase factors between the two can only make the agreement worse. The agreement in this case is extremely good at some points, which suggests that the GSM might still be the correct model of transverse coherence if we chose a reasonable source point.

IV. CONCLUSION

I have devised and written a Markov Chain Monte Approach which will quickly analyze the transverse coherence, performing $\sim$100 times faster than the brute force algorithm previously in use. I have found the GENESIS simulation code to predict a very high level of transverse coherence for the LCLS, which is encouraging. One interesting result I have found is that the transverse coherence declines significantly after saturation, which suggests that users who want a high degree of coherence might be better off using the LCLS without the full length of the undulators, sacrificing some intensity in exchange for greater coherence. A comparison of the emitted radiation and beam divergence to that predicted by the GSM is somewhat inconclusive. Certainly one problem of the GSM model of transverse coherence is that it requires a single source point, which is not the case for an FEL. The LCLS has only recently come online, and the prediction of it's properties is ongoing work.

My work will provide a useful tool for predicting the degree of transverse coherence, and I have made my code easily extensible to predict the accuracy of any proposed models of transverse coherence.

Acknowledgments

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TABLE I: Parameters of the Electrons Entering the Undulators

Slice Emittance : 0.4 μm
Peak Current: 3 kA
Slice Energy Spread: 0.01%

V. FIGURES

A. Fitting for Simulated FEL Having 84 Meters of Undulators

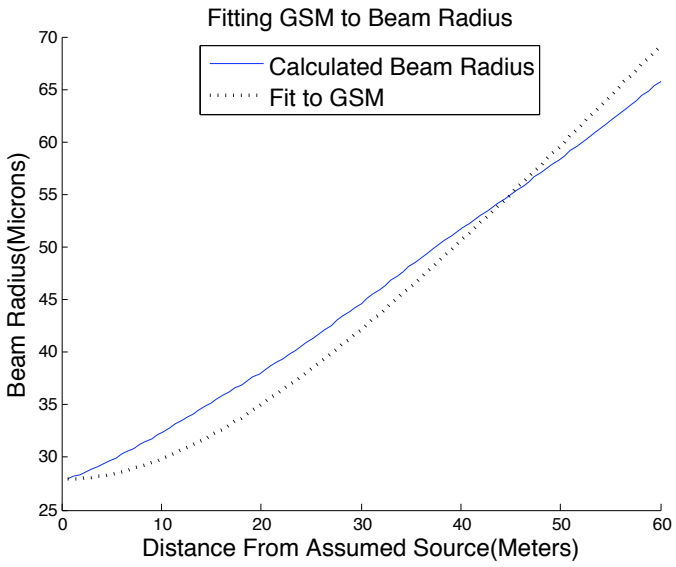

FIG. 1: Curve fit of beam radius to GSM assuming a point source at 84 meters(end of the last undulator).

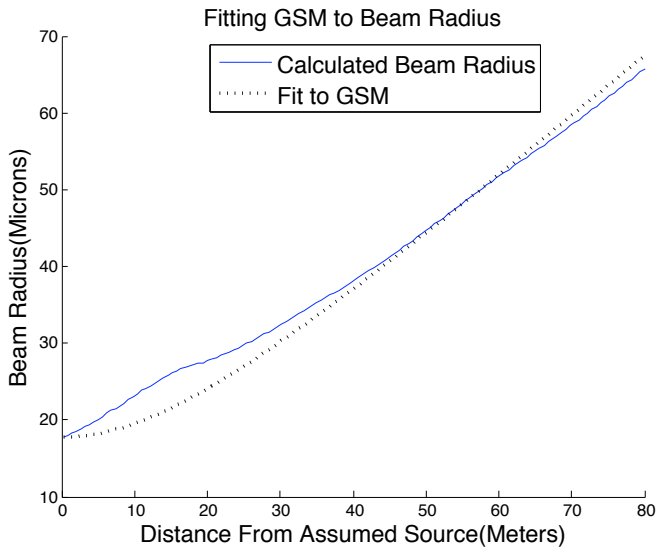

FIG. 2: Curve fit of beam radius to GSM assuming a point source at 64 meters(around the saturation point).

B. Analysis of Fields for FEL with 100 meters of undulators

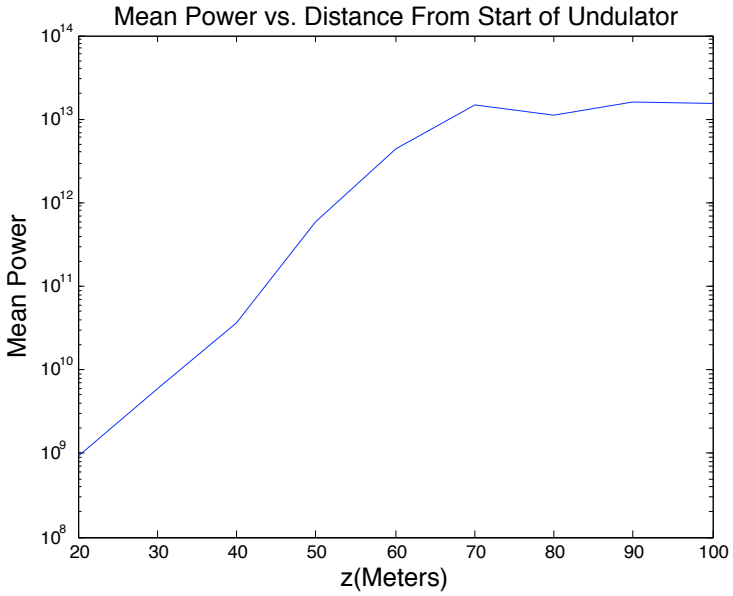

FIG. 3: Beam power, note that saturation occurs at about 64 meters.

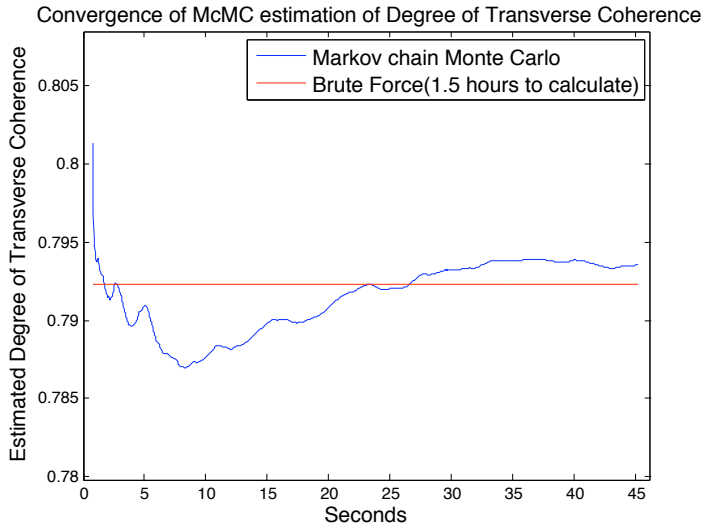

FIG. 4: The Markov chain Monte Carlo algorithm quickly converges to the correct value.

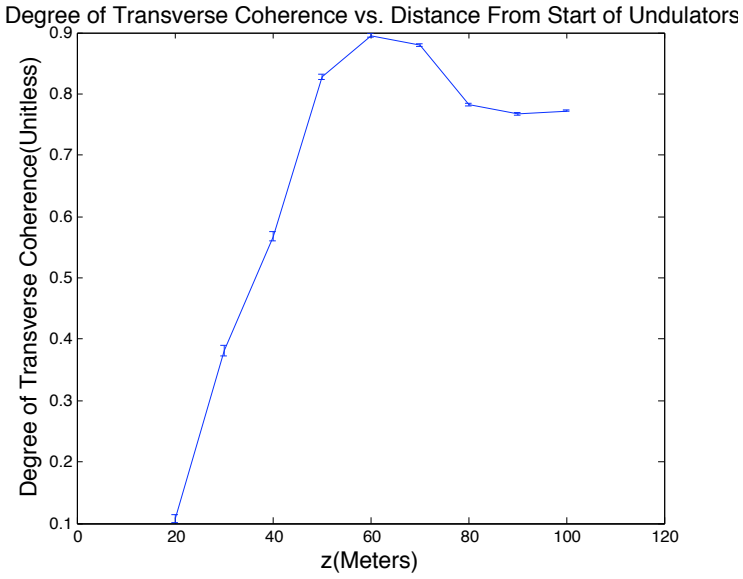

FIG. 5: Degree of transverse coherence as a function of z.

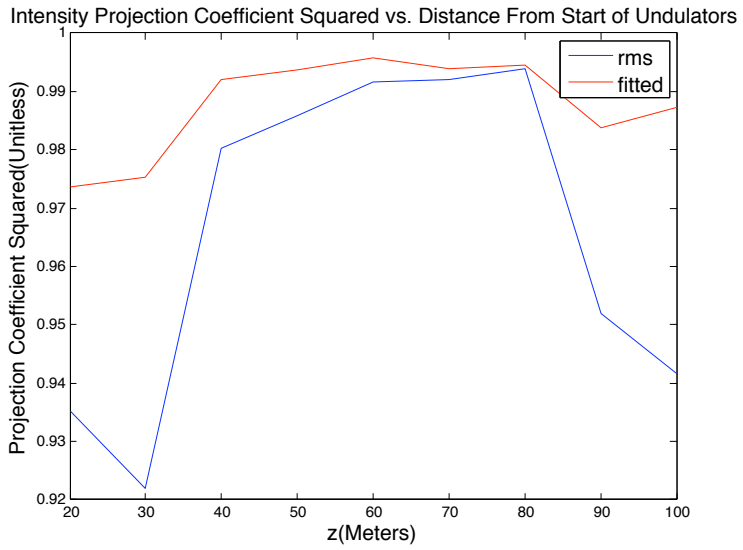

FIG. 6: Agreement of measured intensity with Gaussian model.

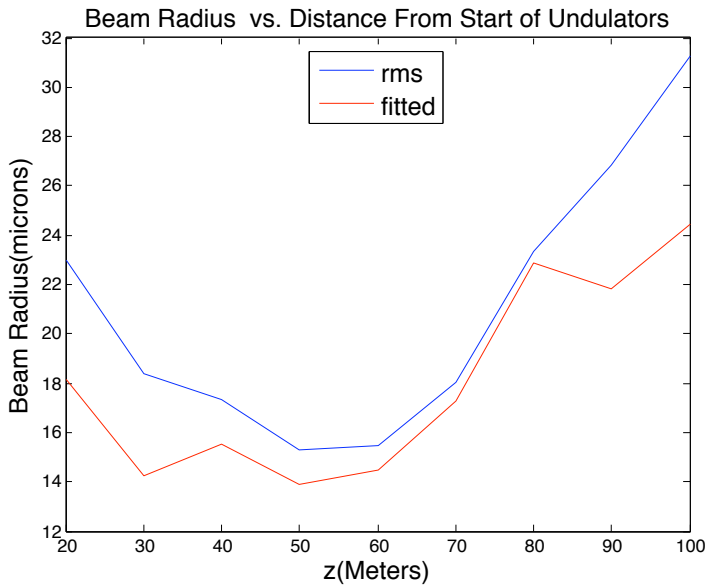

FIG. 7: Beam radius, both found by rms calculation and fitting.

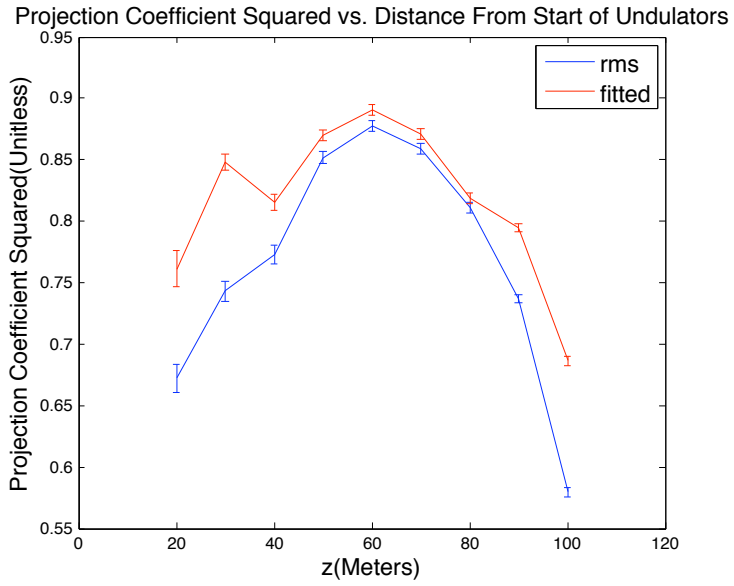

FIG. 8: Projection of mutual intensity function onto phase-less GSM model.

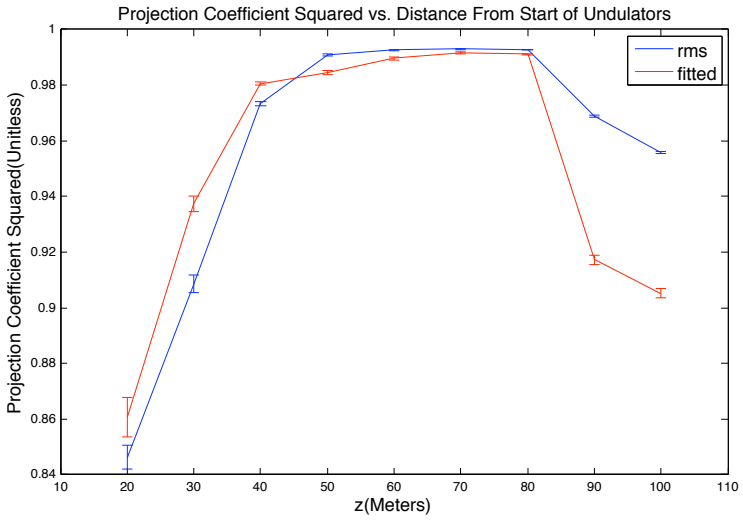

FIG. 9: Projection of magnitude of mutual intensity function onto GSM model, neglecting phase differences.

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