Simulation of Space-Charge Effects Using a Quantum Schrodinger Method

Ji Qiang

Lawrence Berkeley National Laboratory

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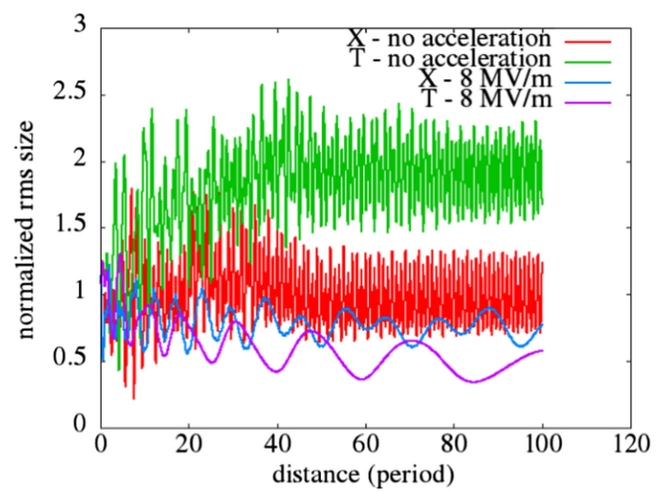
Outline

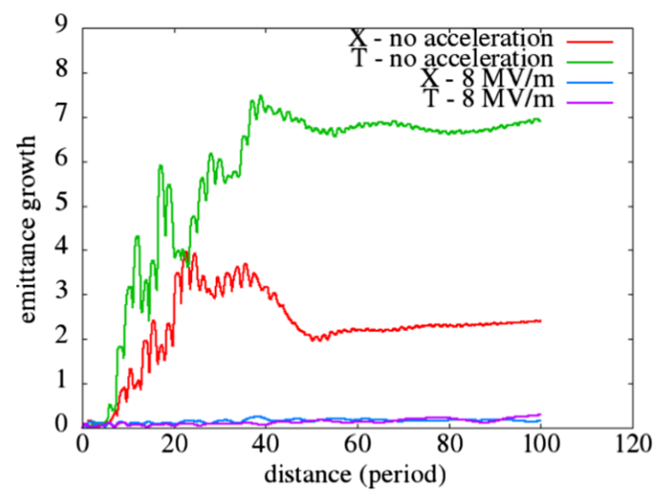
- Introduction
- Quantum Schrodinger space-charge model
- Test examples

Introduction

Nonlinear space-charge effects are important in high intensity accelerators by causing:

- **beam blow-up and emittance growth**
- **halo formation**
- **particle losses**





Space-Charge Dynamics Is Governed by Vlasov-Poisson Equations

$$\frac{\partial f}{\partial t} + [f, H] = 0,$$

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0},$$

$$\rho = \iiint f(r, p, t) d^3 p$$

Husimi Representation of Phase Space Distribution

$$\mathcal{F}(\mathbf{r}, \mathbf{p}, t) = |\bar{\Psi}(\mathbf{r}, \mathbf{p}, t)|^2$$

$$\Psi(\mathbf{r}, \mathbf{p}, t) = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \left(\frac{1}{2\pi\sigma^2}\right)^{3/4} \int d^3x \times \psi(\mathbf{x}, t) \exp\left(-\frac{|\mathbf{r}-\mathbf{x}|^2}{4\sigma^2} - i\frac{\mathbf{p}\cdot\mathbf{x}}{\hbar}\right)$$

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(x, y, z)\psi,$$

$$\frac{\partial\mathcal{F}}{\partial t} + [\mathcal{F}, H] = O(\hbar) + O(\hbar^2) + \cdots.$$

Schrodinger Equation of a Coasting Beam

Start with a z-dependent Hamiltonian of a particle in accelerator:

$$\bar{H}(z) = \frac{1}{2}(\bar{p}_x^2 + \bar{p}_y^2) + V(x, y, z), \quad \bar{p}_{x,y} = p_{x,y}/p_0$$

Rewrite the z-dependent Hamiltonian as t-dependent Hamiltonian:

$$H(t) = \frac{1}{2m\gamma_0}(p_x^2 + p_y^2) + p_0 v_0 V(x, y, z).$$

Replace the energy and momentum with corresponding operators:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m\gamma_0}\nabla^2\psi + p_0 v_0 V(x, y, z)\psi.$$

Numerical Solution of the Schrodinger Equation (1)

$$i\hbar \frac{\partial \psi}{\partial z} = -\frac{\hbar^2}{2p_0}\nabla^2 \psi + p_0 V(x,y,z)\psi$$

Lie-Trotter Splitting-Operator Method for Time Integration:

$$\psi(z+\tau) = e^{\frac{i\hbar\tau}{4p_0}\nabla^2} e^{-i\frac{p_0}{\hbar}V\tau} e^{\frac{i\hbar\tau}{4p_0}\nabla^2} \psi(z),$$

Spectral Method with Sine Function Representation in Spatial Dom.

$$\psi(x,y) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \psi_{lm} \; \sin(\alpha_l x) \; \sin(\beta_m y),$$

$$\psi_{lm} = \frac{4}{ab} \int_0^a \int_0^b \psi(x,y) \; \sin(\alpha_l x) \; \sin(\beta_m y) \, dxdy,$$

Numerical Solution of the Schrodinger Equation (2)

Wave Function Evolution for a Single Step:

$$\psi_{lm}(z+\tau/2) = e^{-\frac{i\hbar\tau}{4p_0}\gamma_{lm}^2}\psi_{lm}(z).$$

$$V = \frac{1}{2}k(z)(x^2 - y^2) + \frac{1}{2}K\phi,$$

$$\tilde{\psi}(z+\tau/2) = e^{-i\frac{p_0}{\hbar}V\tau}\psi(z+\tau/2).$$

$$\psi_{lm}(z+\tau) = e^{-\frac{i\hbar\tau}{4p_0}\gamma_{lm}^2}\tilde{\psi}_{lm}(z+\tau/2).$$

Numerical Solution of Poisson's Equation for Space-Charge Effects (1)

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -4\pi\rho,$$

$$\rho(x,y) = \int\int e^{-\frac{(x-x')^2}{2\sigma_x^2}} e^{-\frac{(y-y')^2}{2\sigma_y^2}} \psi(x',y')\psi^*(x',y')dx'dy',$$

Spectral Method with Sine Function Representation:

$$\rho(x,y) = \sum_{l=1}^{N_l}\sum_{m=1}^{N_m} \rho_{lm} \sin(\alpha_l x)\sin(\beta_m y)$$

$$\phi(x,y) = \sum_{l=1}^{N_l}\sum_{m=1}^{N_m} \phi_{lm} \sin(\alpha_l x)\ \sin(\beta_m y),$$

Numerical Solution of Poisson's Equation for Space-Charge Effects (2)

$$\rho_{lm} = \frac{4}{ab}\int_0^a \int_0^b \rho(x,y)\sin(\alpha_l x)\sin(\beta_m y)\,dxdy$$

$$\phi_{lm} = \frac{4}{ab}\int_0^a \int_0^b \phi(x,y)\;\sin(\alpha_l x)\sin(\beta_m y)\,dxdy,$$

$$\phi_{lm} = \frac{4\pi\rho_{lm}}{\gamma_{lm}^2},$$

Initial Condition and Diagnostics

Initial condition of wave function:

$$\psi(\mathbf{r},0) \propto \sum_{\mathbf{p}} \sqrt{f(\mathbf{r},\mathbf{p},0)}\, e^{i\mathbf{p}\cdot\mathbf{r}/\hbar + 2\pi\phi_{\mathrm{rand},\mathbf{p}}},$$

Beam properties from wave function:

$$\langle x^2\rangle = \int\int x'^2 \psi\psi^* dx' dy'$$

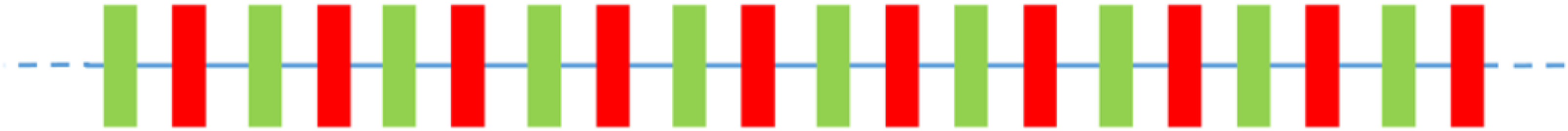
$$\langle p_x^2\rangle = \hbar^2 \int\int \frac{\partial\psi}{\partial x'}\frac{\partial\psi^*}{\partial x'} dx' dy'$$

$$\langle x p_x\rangle = \hbar\, \mathrm{Im}\left(\int\int x' \frac{\partial\psi}{\partial x'} \psi^* dx' dy'\right),$$

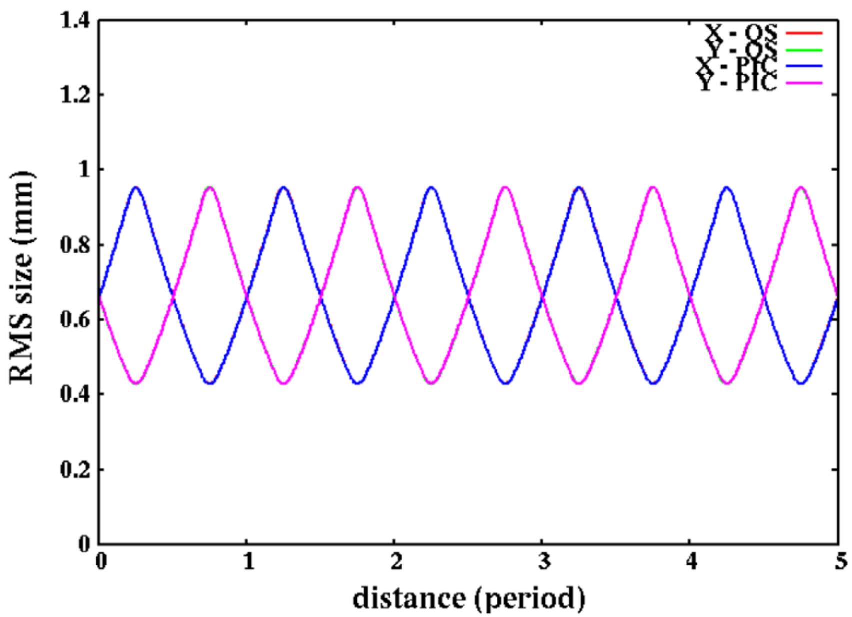
$$\epsilon_x = \sqrt{\langle x^2\rangle\langle (p_x/p_0)^2\rangle - \langle x(p_x/p_0)\rangle^2}$$

$$\epsilon_y = \sqrt{\langle y^2\rangle\langle (p_y/p_0)^2\rangle - \langle y(p_y/p_0)\rangle^2}.$$

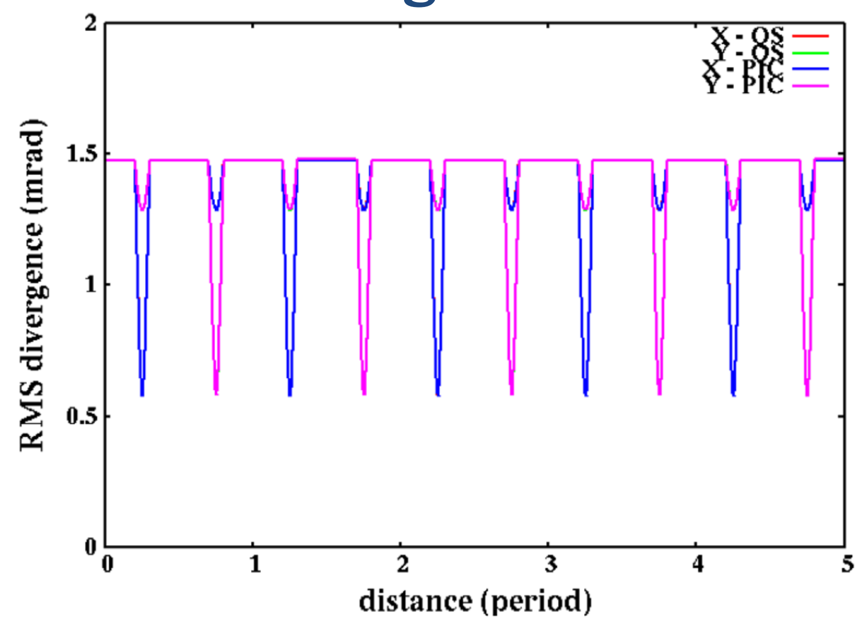
Test Case 1: No Space-Charge Effects (1)



RMS Size Evolution



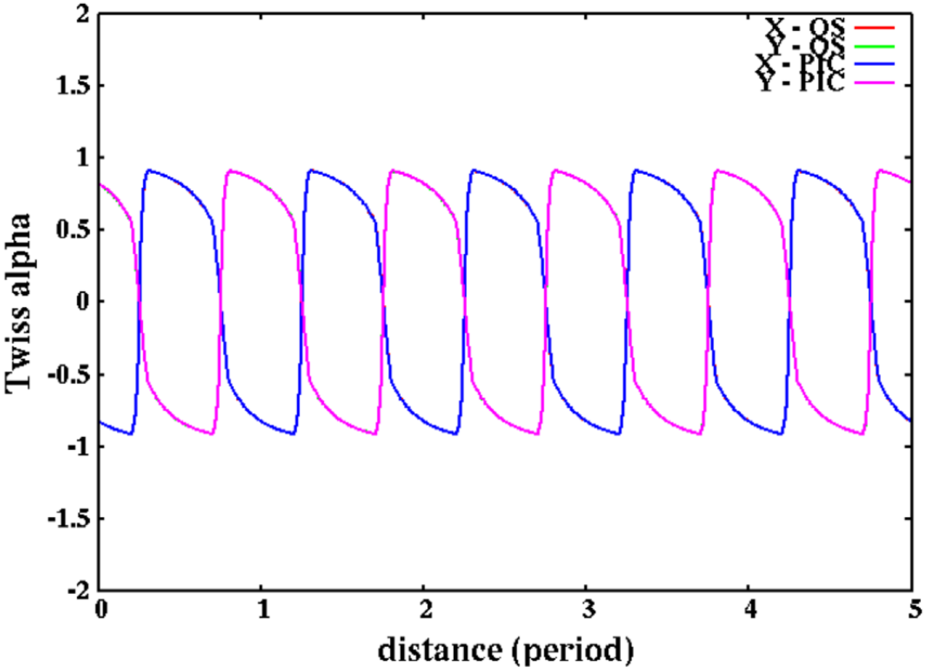
RMS Divergence Evolution



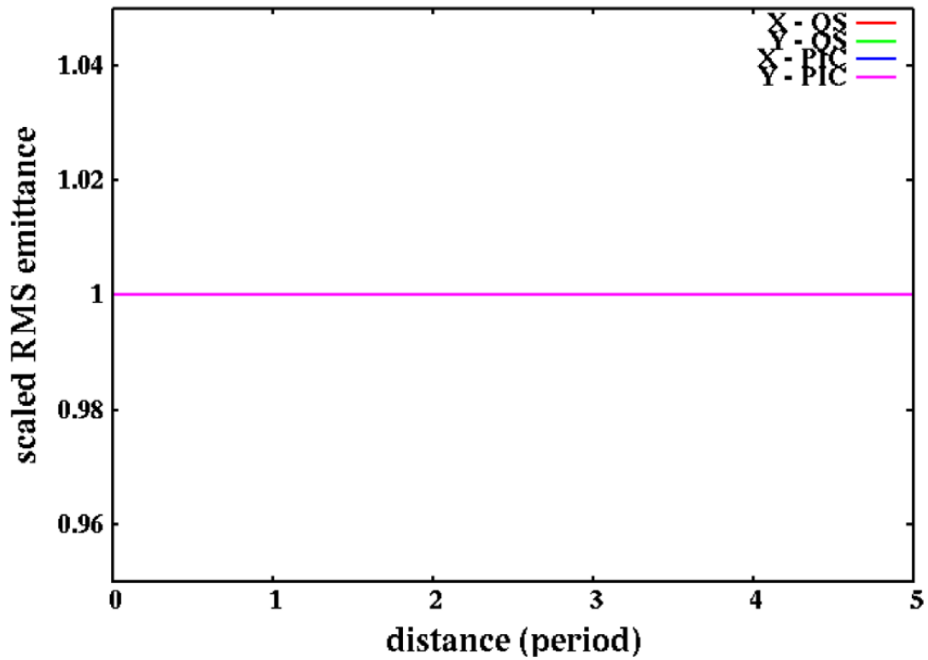
- **Good agreement between the PIC simulation and the quantum Schrodinger simulation.**

Test Case 1: No Space-Charge Effects (2)

Twiss Parameter Alpha Evolution



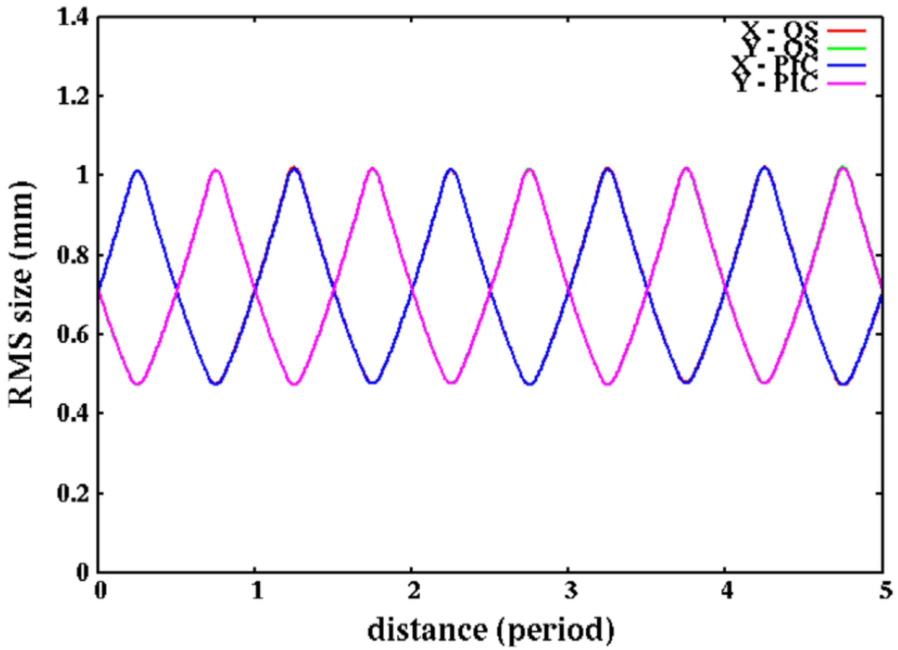
RMS Emittance Evolution



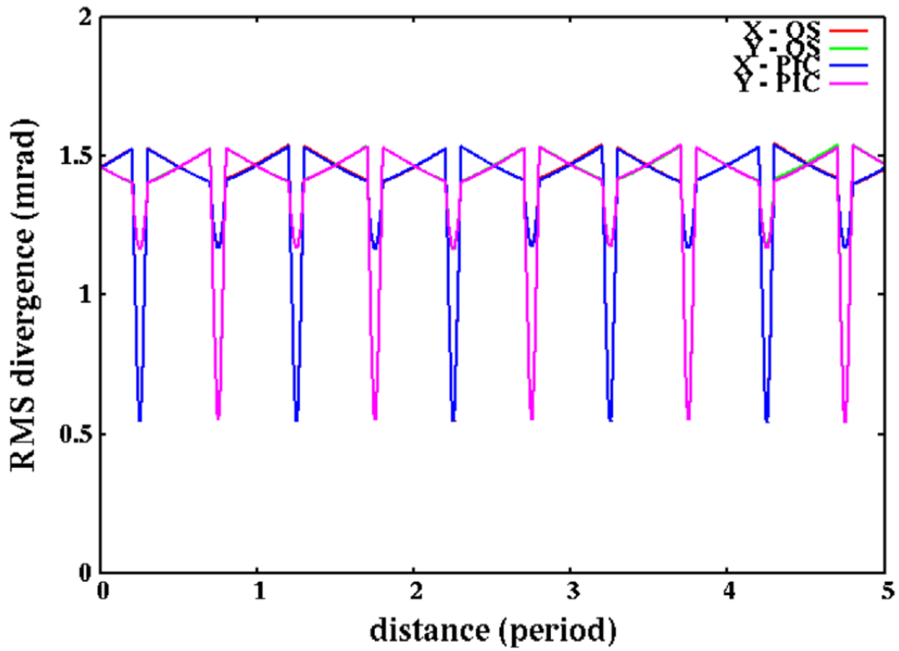
- Both methods agree with each other well and show no emittance growth without the space-charge effects.

Case 2: with Space-Charge and Initial Matched Beam (1)

RMS Size Evolution



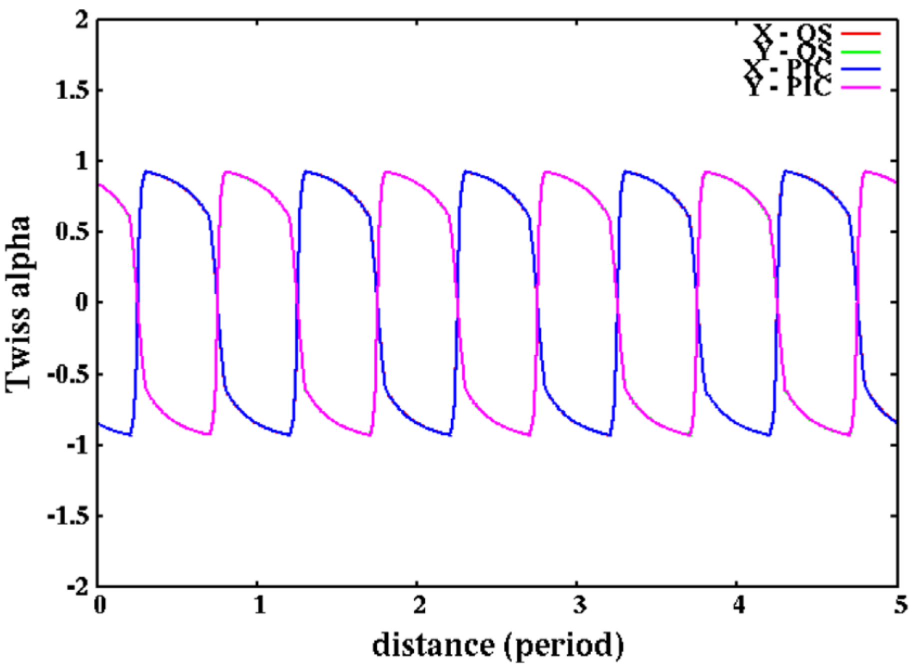
RMS Divergence Evolution



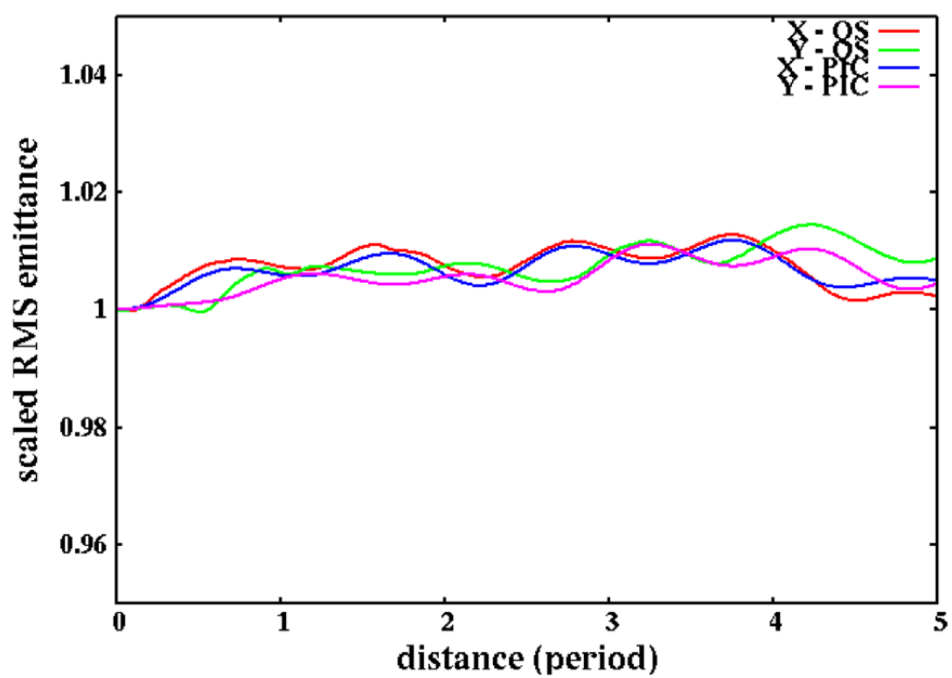
- Good agreement between the PIC simulation and the quantum Schrodinger simulation with space-charge effects and an initial matched beam.

Case 2: with Space-Charge and Initial Matched Beam (1)

Twiss Parameter Alpha Evolution



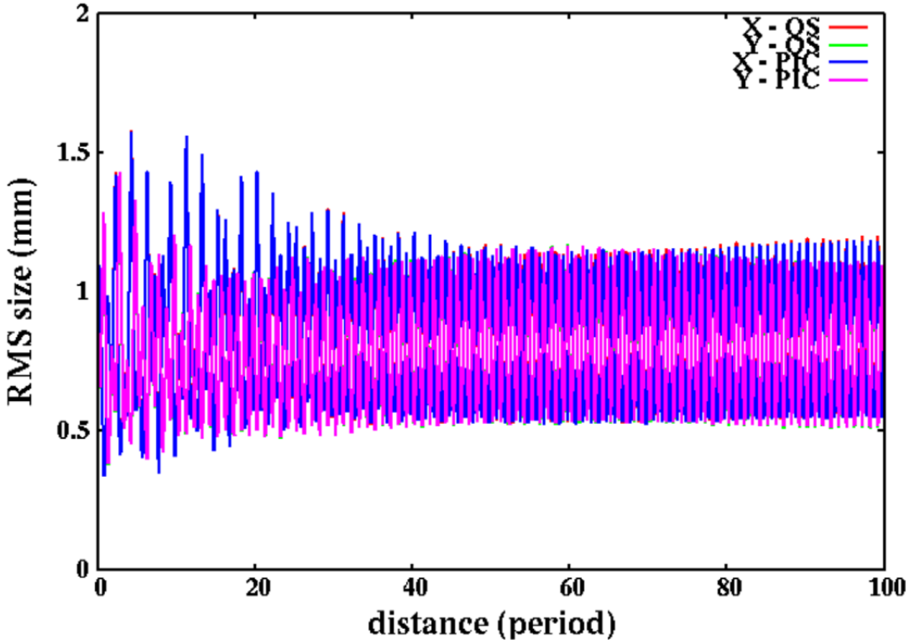
RMS Emittance Evolution



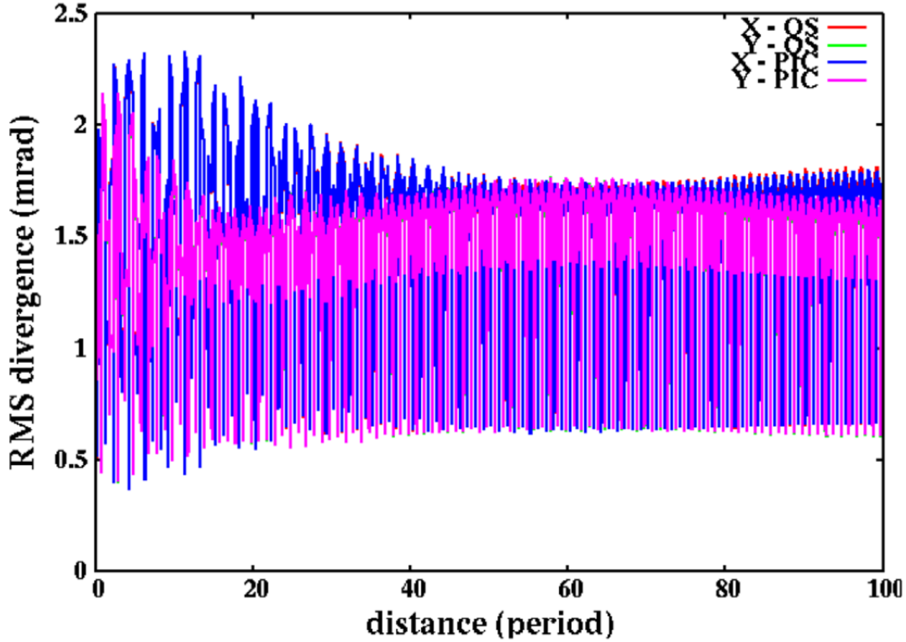
- Both methods show good agreement and small emittance growth due to the space-charge effects.

Case 3: with Space-Charge and Initial Mismatched Beam (1)

RMS Size Evolution



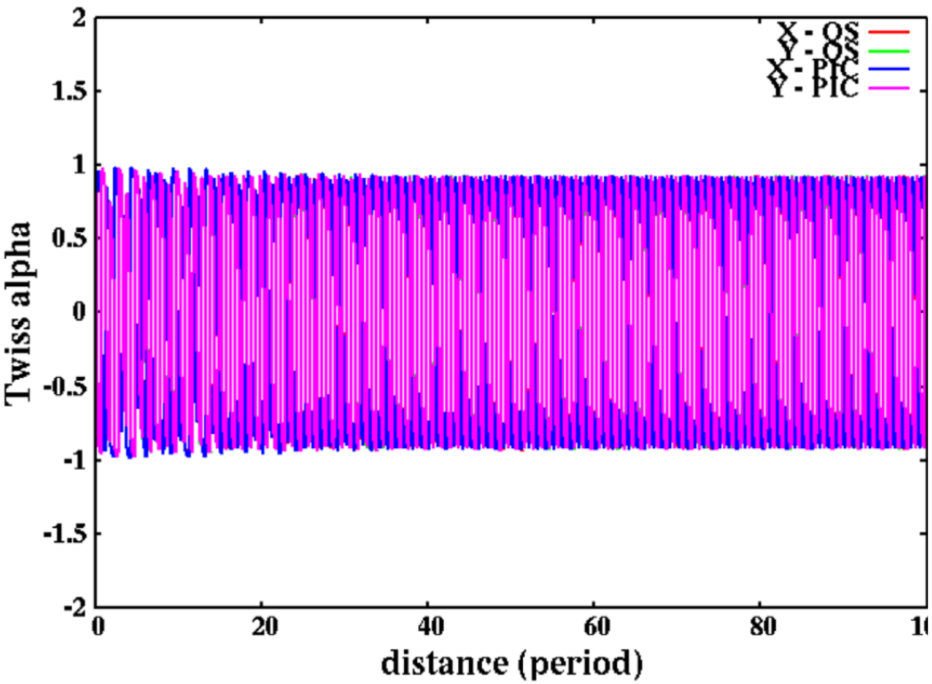
RMS Divergence Evolution



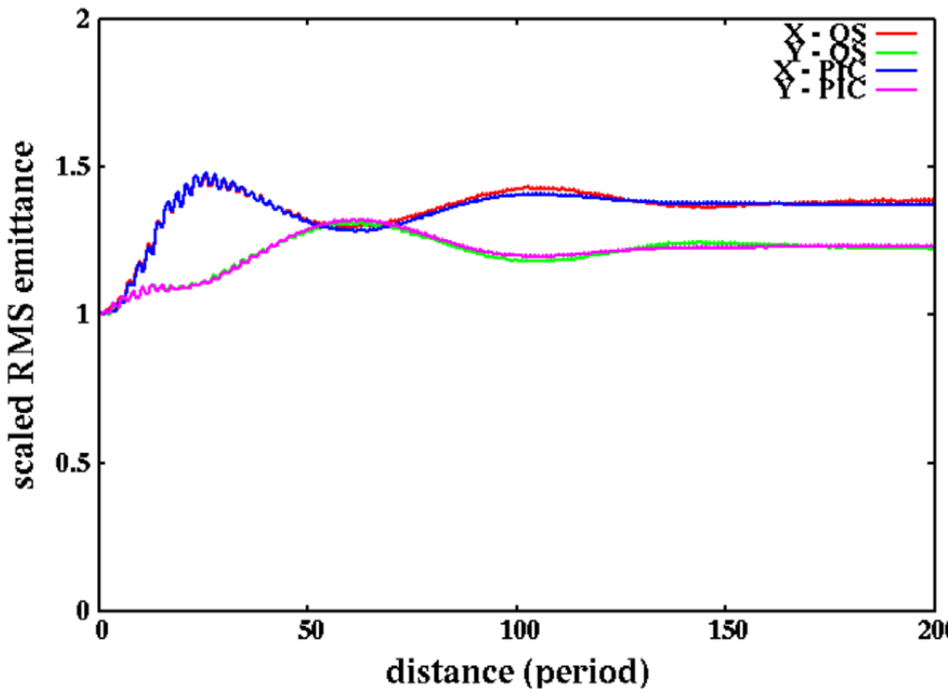
- Both the PIC and the quantum Schrodinger methods show initial beam size growth due to mismatched space-charge effects.

Case 3: with Space-Charge and Initial Mismatched Beam (2)

Twiss Parameter Alpha Evolution



RMS Emittance Evolution



- Both methods show large emittance growth due the mismatched space-charge effects.

Summary slide, 5th ICFA mini-workshop on Space Charge
Theme: Bridging the gap in space charge dynamics

In 1-2 sentences, summarize the content of this presentation

This presentation proposed a new method to simulate space-charge effects based quantum Schrodinger equation. This method might open the possibility to do classic beam dynamics simulation on quantum computers.

From your perspective, where is the gap regarding space charge effects? (understanding/control/mitigation/prediction/?)

The gap is to simulate long-term space-charge effects with controlled numerical errors.

What is needed to bridge this gap?

New advanced computation method is needed.