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Title: Assessing the quantum physics impacts on future x-ray free-electron lasers

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Abstract

A new quantum mechanical theory of x-ray free electron lasers (XFELs) has been successfully developed that has placed LANL at the forefront of the understanding of quantum effects in XFELs. Our quantum theory describes the interaction of relativistic electrons with x-ray radiation in the periodic magnetic field of an undulator using the same mathematical formalism as classical XFEL theory. This places classical and quantum treatments on the same footing and allows for a continuous transition from one regime to the other eliminating the disparate analytical approaches previously used. Moreover, Dr. Anisimov, the architect of this new theory, is now considered a resource in the international FEL community for assessing quantum effects in XFELs.

Background and Research Objectives

Current x-ray free electron laser (XFEL) designs, constrained by increased facility costs and the ever increasing demand for high energy photons, are now approaching the quantum regime, where position and momentum uncertainty inherent in the quantum mechanical (QM) description of electrons will affect lasing efficiency. These effects are even more important for XFEL harmonic radiation generation (an important method for generating even shorter wavelength x-ray radiation from XFELs), necessitating the inclusion of QM effects for accurate predictions of XFEL performance. Quantum effects will become more prevalent as even higher energy XFEL sources, including the mission-critical MaRIE XFEL at LANL, come into being. Consequently, an XFEL theory that includes QM effects is needed to accurately design and optimize future XFEL facilities. The success of this work will increase the predictive capability for designing future XFELs and place LANL at the forefront of XFEL science.

The technical goals of including QM effects in the XFEL theory and accurately predicting MaRIE XFEL performance had the following research objectives:

1. Include the wave packet nature of quantum electrons in current 3D FEL codes that currently track classical electron trajectories. Investigate QM spreading of the electron wave packets as they propagate through the undulator (wiggler);
2. Use the electron wave functions to calculate the source current that excites the radiation and provide a self-consistent model for QM XFEL gain;
3. Include QM source terms for harmonic generation and quantify the expected production of higher harmonics with an emphasis on gamma ray production;
4. Verify and validate our new models by comparing their predictions in the high-gain regime with the results from existing classical physics codes and via comparison with current experimental data from the Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center (SLAC) and future data from the SACLA XFEL at the Spring-8 facility in Japan.

The expected result is a validated 3D FEL simulation code that includes QM spreading of the electron wave packets as they propagate through the wiggler, startup shot noise, QM dephasing of electrons in the exponential gain regime and QM electron de-trapping from the ponderomotive buckets in the saturation regime. These goals were achieved as described below.

Scientific Approach and Results

The proposed work has been divided into three areas:

(1) Develop a 1D quantum theory of XFEL operation
(2) Develop a QM simulation code based on the new theory
(3) Validate the QM code and use it to model existing and future XFEL sources.

A central theme of our scientific approach was to engage the international XFEL community from the start of the project. This has allowed us to determine the availability and assess the quality of the existing XFEL experimental data from the SACLA and LCLS XFEL facilities for comparisons with our quantum treatments. It has had the side benefit of advertising LANL's interest and expertise in developing and assessing quantum XFELs theories. In the process of executing this plan we discovered the following:

A. The quality of experimental data available was not sufficient for quantitative comparisons even with classical theory and there is no future development program in place to refine data acquisition in order to match classical predictions to the QM difference level.
B. There was a wide-spread lack of understanding of how relativistic electrons can be treated quantum mechanically (where the Comption wavelength is extremely small) within the limits of conventional XFEL theories.
C. There was consensus that a 1D quantum theory of XFEL operation would be a great starting point.
D. There was a strong desire to understand Bonifacio's proposals [ref] related to the development of a pure quantum x-ray free electron laser, yet there was no way to combine these efforts with classical XFEL treatments.
E. A fundamentally sound quantum mechanical treatment is needed before the codes can be improved by including these effects.

As a result of this feedback gathered from the scientific community, the development of a 1D quantum theory for XFELs was identified as the primary research objective for this work.

Research objective 1.

An electron in an XFEL has 3D particle dynamics, so we first addressed the question of whether every degree of freedom required a quantum treatment. In our assessment, the lack of the 3D coupling lead us to quantizing the longitudinal degree of freedom discussed by the classical XFEL theory. Such an approach is valid owing to the weak coupling between transverse and longitudinal degrees of freedom of an electron in an undulator. From a simulation standpoint, the widely used XFEL code Genesis calculates these perpendicular components independently. The transverse dynamics is expected to remain unaffected by the longitudinal quantum treatment owing to the predominantly forward emission of the x-ray photons.

The classical 1D theory is described by the pendulum equation for electrons and Maxwell's equation driven by the ensemble electron current. The wave packet nature of electrons affects the calculation of the classical current through the radiated field phase. The position uncertainty of the electrons resulted in a reduction of the driving term for x-ray radiation dependent upon the size of the wave packet. The corresponding change to the ponderomotive potential has been also implemented in order to conserve energy. The controlling equations are as follows.

$$\frac{dE_k}{dz} = \frac{1}{N}\sum_{\alpha=1}^{N} \langle e^{-ik\psi_\alpha}\rangle,$$

$$\frac{d\psi_\alpha}{dz} = \eta_\alpha,$$

$$\frac{d\eta_\alpha}{dz} = -2Re\big(E_k\langle e^{ik\psi_\alpha}\rangle\big).$$

Assuming a constant position uncertainty, the quantum reduction has been propagated through the calculations all the way to the expression for XFEL gain.

We have included the wave packet nature of quantum electrons in the current 3D FEL code, Genesis, which tracks classical electron trajectories. The quantum version of Genesis has demonstrated that it takes longer for electrons to start x-ray generation due to a quantum reduction of the current, yet the saturated power is still comparable to the classical prediction. We have also observed that emittance and energy spread exacerbated quantum gain reduction effects.

In order to include the QM spreading of electron wave packets as they propagate through the undulator for MaRIE parameters, we solved the classical 1D equations including quantum reduction effects numerically using a Runge-Kutta method. Quantum wave packet spreading due to free space dispersion was assumed. The results demonstrated that FEL operation at the fundamental wavelength is least affected which can have significant effects on harmonic generation. Therefore, one would have to suppress the generation of x-ray radiation at the fundamental wavelength to see the effect of the wave packet nature of electrons on harmonic gain.

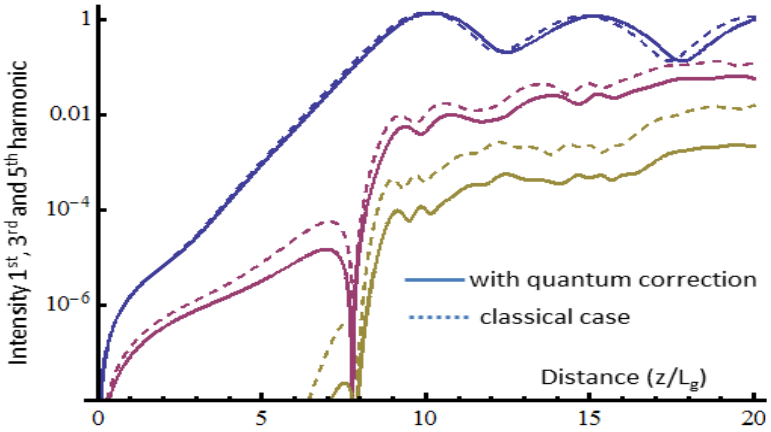

Figure 1 *The 1D theory does not capture beam effects but predicts quantum effects due to* $\langle e^{ik\psi_\alpha}\rangle = e^{-k^2\sigma^2/2}e^{ik\bar{\psi}_\alpha}$. *where* $d\sigma^2/dz = \frac{D^2 z}{2}$ *was added by hand in order to account for free space dispersion. It was later found that* $\sigma(z)^2 = \sigma(0)^2 + z^2/4\bar{\rho}^2\sigma(0)^2$ *where* $\bar{\rho} = \rho(mc\gamma/\hbar k)$ *is the quantum FEL parameter. Beam imperfection effects further exacerbate wave function spreading!*

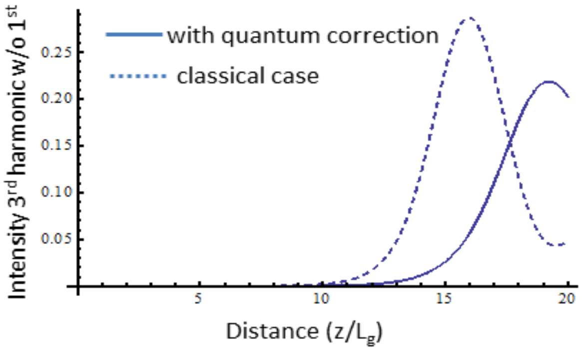

Figure 2 *Suppression of x-ray generation at the fundamental wavelength (labeled as 1st in Figure 1) results in a significant difference between the classical and quantum corrected cases.*

Research objective 2.

In order to include the actual wave function dependence of an electron as it interacts with x-ray radiation while undergoing free-space dispersion, a quantum mechanical treatment for the XFEL from basic principles had to be derived. A bi-product of this effort was a canonical formulation of 1D quantum XFEL theory which, heretofore had been formulated from force equations instead of from the electron's Hamiltonian. Our new canonical formulation has the potential to improve the generality of current XFEL simulation codes. We are currently in discussions on ways to secure additional funding to support such an effort.

The main result of the quantum theory is that the classical XFEL variables for an electron – the ponderomotive phase, ψ, and the energy detuning from resonance, η, do not commute! The corresponding Heisenberg uncertainty principle for this pair of variables is

$$\Delta\psi\Delta\eta \geq \frac{1}{2\bar{\rho}}$$

where $\bar{\rho}$ is the quantum FEL parameter. It provides a measure of the number of photons emitted by an electron before saturation, or it can be interpreted as the ratio of XFEL bandwidth to photon recoil energy

$$\bar{\rho} = \rho(mc\gamma/\hbar k),$$

where ρ is the classical FEL parameter.

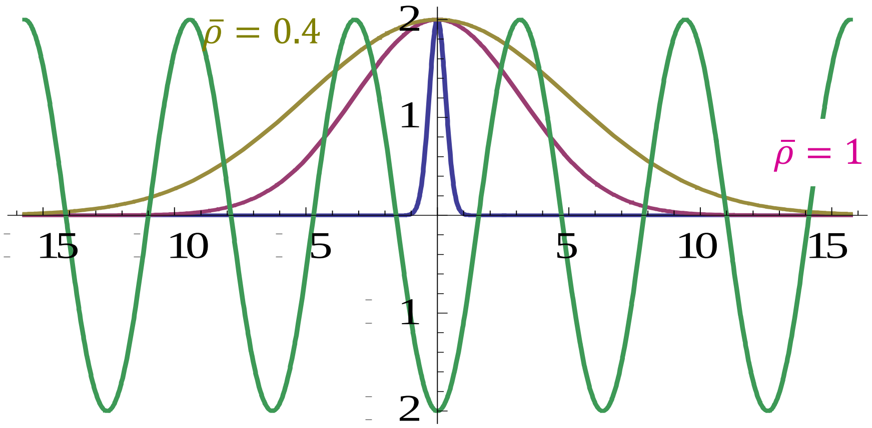

Figure 3 *Examples of the electron probability distribution for different values of the quantum FEL parameter.* $\bar{\rho} \gg 1$ *(i.e.* $\sigma \ll \pi$ *) the classical case (blue);* $\bar{\rho} = 1$ *(i.e.* $\sigma = \pi$ *) the classical-to-quantum transition (red);* $\bar{\rho} = 0.4$ *(i.e.*$\sigma = 5$*) the quantum case where the XFEL spectrum makes a transition from continuous to discrete.*

The quantum state evolution is described by Schrodinger's equation

$$i\frac{\partial\Psi}{\partial\tau} = \left\{-\frac{1}{2\bar{\rho}}\frac{\partial^2}{\partial\theta^2} + 2\bar{\rho}\Im\left[A(\tau)e^{i\theta}\right]\right\}\Psi(\theta,\tau)$$

where the $-\frac{1}{2\bar{\rho}}\frac{\partial^2}{\partial\theta^2}$ term is responsible for free space evolution such that $\sigma^2(\tau) = \sigma^2(0) + \frac{\tau^2}{4\bar{\rho}^2\sigma^2(0)}$ and the $+2\bar{\rho}\Im\left[A(\tau)e^{i\theta}\right]$ term describes the ponderomotive potential created by the undulator and the generated radiation. The solution has the form

$$A(\tau) = \frac{A(0)}{3}\sum_{n=1}^{3} e^{\lambda_n\tau} \text{ for } \lambda_{1,2} = \frac{i\pm\sqrt{3}}{2} \text{ and } \lambda_3 = -i.$$

Schrodinger's equation replaces the pendulum equations for an electron and indicates that free space dispersion dominates the wave packet evolution for the 75% of the undulator length before saturation. The effect of the ponderomotive potential on the quantum state evolution becomes noticeable in the last 25% of the undulator length before saturation.

The calculation of the source current that excites the radiation involves quantum averaging over the wave packet and averaging over the classical ensemble of electrons. Our analysis shows that the classical ensemble averaging dominates the quantum effects as long as $\bar{\rho} > 1$. For the MaRIE XFEL, the relevant quantum FEL parameter is $\bar{\rho} = 50$ such that no significant performance degradation is expected.

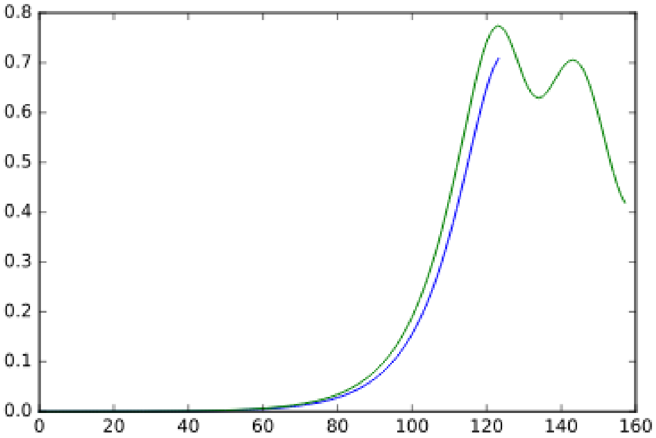

***Figure 4** The classical source current (green) vs the quantum source current (blue) as a function of undulator length in arbitrary units for MaRIE relevant parameters where* $\bar{\rho} = 50$.

1D linear gain for a quantum FEL

The analysis of the FEL instability in the quantum regime can be performed based on the system of equations describing the change of the amplitude of the radiation field A and the Wigner function W. These equations were used in earlier research, e.g. Ref. [1]. In the course of this project it has been shown that these equations have higher a degree of accuracy than previously believed and they are capable of describing FELs in the strong quantum regime.

$$\frac{\partial}{\partial t}A(t)-i\delta\omega A(t)=\int e^{-i\theta}W(\theta,p)d\theta dp, \qquad (1)$$

$$\frac{\partial}{\partial t}W(\theta,p,t)+\frac{p}{M}\frac{\partial}{\partial\theta}W(\theta,p,t)=\frac{2M}{\hbar}\mathrm{Re}\left(Ae^{i\theta}\right)\left[W\left(\theta,p+\frac{\hbar}{2},t\right)-W\left(\theta,p-\frac{\hbar}{2},t\right)\right] \qquad (2)$$

Here $\delta\omega$ describes the frequency shift of the radiation from the exact resonant condition defined by the average beam energy in a given undulator. Eq. (2) describes the evolution of the Wigner function including radiation recoil. In the classical limit, $\hbar\to 0$, Eq. (2) transforms into classical Vlasov equation describing the change of the electron distribution function in the field of the wave.

This set of equations (1) - (2) describing the SASE FEL instability in the quantum regime is similar to the Maxwell-Vlasov equations describing waves in a plasma. The linear analysis of such a system can be performed in the same way as the linear analysis of the eigen-modes in plasmas, i.e. through a dispersion relation. We linearize the set of equations describing the 1D SASE quantum FEL growth assuming that the field amplitude and the correction to the Wigner distribution function are small. Analyzing the instability assuming a Gaussian distribution of the initial electron beam with an rms energy spread of $\sigma_p{}'$, results in the dispersion relation

$$\omega-\delta\omega=\frac{\bar{\rho}}{\sigma_p'}\left[Z\left(\frac{\omega+1/(2\bar{\rho})}{\sigma_p'}\right)-Z\left(\frac{\omega-1/(2\bar{\rho})}{\sigma_p'}\right)\right], \qquad (3)$$

where

$$Z(\varsigma) = \frac{1}{\sqrt{\pi}} \int\limits_{\substack{Landau\\contour}} \frac{e^{-t^2}}{t-\varsigma} dt = i\sqrt{\pi} e^{-\varsigma^2} \left[1 - erf(-i\varsigma)\right]. \tag{4}$$

Here Z is the plasma dispersion function widely used in plasma physics. This dispersion relation describes the 1D SASE growth rate in the quantum regime for arbitrary values of the FEL parameter, relative energy spread and the quantum energy recoil. Therefore, it can describe both the classical and quantum regimes. This is the first time a dispersion relation describing quantum FEL growth rate for an arbitrary energy distribution in the electron beam has been derived.

We can benchmark the dispersion relation (3) – (4) in the classical limit $\hbar \to 0$ or $\bar{\rho} \to \infty$ to find the thermal corrections to the growth rate caused by the nonzero energy spread. Focusing on the growing branch of the dispersion curve $\mathrm{Im}(\omega)<0$ simplifies the expression for the Z-function since the growing mode satisfies the causality principle allowing the Landau contour to coincide with the real axis in the complex plane in Eq. (4). The Z-function can then be expanded as

$$Z(\varsigma) \approx -\frac{1}{\varsigma}\left(1 + \frac{1}{2\varsigma^2} + \frac{3}{4\varsigma^4} + \ldots\right), \qquad \varsigma >> 1 \tag{5}$$

The growth rate for the instability in this regime results in

$$\mathrm{Im}(\omega) \approx -\frac{\sqrt{3}}{2}\left(1 - \frac{(\sigma_p^{'})^2}{2}\right), \tag{6}$$

which matches the 1D growth rate which can be obtained from the classical Ming-Xie scaling [1] in the 1D limit when the radiation diffraction and beam emittance terms can be neglected. Next, we benchmark the dispersion relation (3) – (4) in the cold quantum regime where the thermal energy spread of the beam can be neglected, $\sigma_p{}' \to 0$ but the quantum recoil correction is included. In this regime the dispersion relation becomes

$$(\omega - \delta\omega)\left(\omega^2 - \frac{1}{(2\bar{\rho})^2}\right) = 1. \tag{7}$$

This dispersion relation describing three FEL modes matches previously obtained results [2]. Benchmarking our results shows that the dispersion relation (3) – (4) describes the 1D growth rate of an FEL in two previously studied regimes. Therefore, we conclude that our expression is general and can describe the 1D instability in any regime of interest including quantum correction to any degree of accuracy. The accuracy of the description of quantum effects follows from the general form of the fluid equation describing the evolution of the Wigner distribution function in Eq. (2). The recoil effect in that equation is included accurately without assumptions of it being small. Then the dispersion relation describing SASE growth rate of a quantum FEL including thermal corrections can be approximated as

$$(\omega - \delta\omega)\left(\omega^2 - \frac{1}{(2\bar{\rho})^2}\right) = 1 + \frac{(\sigma_p^{'})^2 \bar{\rho}}{2} \cdot \frac{\left(\omega + \frac{1}{2\bar{\rho}}\right)^3 - \left(\omega - \frac{1}{2\bar{\rho}}\right)^3}{\left(\omega^2 - \frac{1}{(2\bar{\rho})^2}\right)^2}, \qquad \sigma_p^{'} << 1. \tag{8}$$

The analysis of the FEL dispersion relation described with Eqs. (4) and (8) indicates that quantum effects are insignificant until $\bar{\rho} < 1$ when the recoil relative energy reaches the relative bandwidth of the FEL so that electrons become off-resonant after a single emission or absorption event. The main difference between the quantum and classical regimes for an FEL is the bandwidth of the instability. The classical regime allows instability at any large detuning from the resonance, $\delta\omega>0$. At the same time, the quantum FEL limits the bandwidth of the instability to some finite region. This effect is demonstrated in Fig. 5 which compares the dispersion curves in strongly classical and moderately quantum regimes.

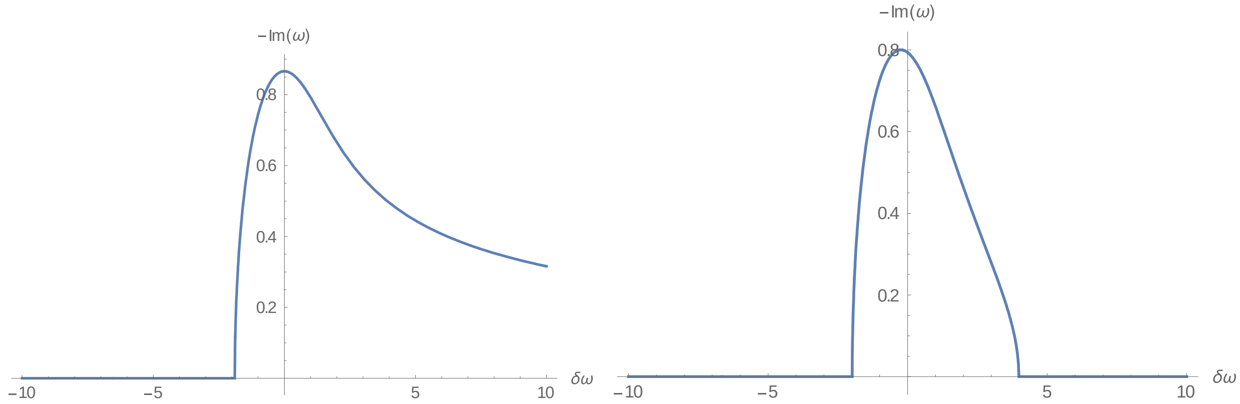

Figure 5. *Dispersion curves from the quantum FEL formulation corresponding to the parameters of the MaRIE XFEL design with* $\bar{\rho} = 50$ *(left plot) and for the highly relativistic regime of* $\bar{\rho} = 1$ *(right plot).*

Research objective 3.

The canonical formulation of the 1D FEL theory self-consistently includes the physics of harmonic radiation. Applying this treatment to XFELs in the MaRIE regime, we do not see a noticeable degradation in XFEL performance.

In collaboration with Prof. Schleich of Ulm, we are working on studying the squeezing properties of the XFEL Hamiltonian derived here.

Anticipated Impact on Mission

The results of this project provide scientifically-based knowledge that confirm that the classical physics-based design of the MaRIE 1.0 project, a future signature facility for LANL, is sound. From our analysis, the MaRIE XFEL will not be degraded by quantum effects owing to the ensemble averaging of the electron source term provided the driving electron bunches. Our analysis removes any doubts that these effects might prevent the design from reaching its performance objectives. We are confident that quantum effects at the fundamental wavelength or lower harmonics are not going to reduce the expected MaRIE XFEL performance.

This work has strengthen the Laboratory’s modeling capabilities and improved our understanding of fundamental FEL physics. We are working with the group and division leadership to maintain this expertise in support of the future MaRIE Project..

Conclusion

The work performed under this ER has placed LANL at the forefront of the understanding of quantum effects in XFELs. Dr. Anisimov is now a resource in the international FEL community for assessing quantum effects in XFELs. The quantum treatment of XFELs developed under this ER provides a foundation for the performance assessment of FELs in the short wavelength X-ray regime. The results of this work have been presented in references [3-9].

This work proves that quantum effects will not produce a significant degradation of the fundamental and harmonic emission of XFELs in the MaRIE parameter regime. Thus, this ER research has strengthened the technical validity of the MaRIE XFEL design while simultaneously increasing both the theoretical FEL expertise at LANL and the technical stature of LANL in the international XFEL community.

As we wait for the MaRIE Project CD0 to move forward, Dr. Anisimov is exploring collaborations to use this newly developed modeling capability. For example, our treatment can be applied to single-electron systems, e.g. the operation of the Iota storage ring at Fermi National Laboratory, under single-electron conditions to probe the quantum nature of relativistic electrons and their interaction with radiation at the single photon level. It can also model an XFEL with a sheered wave front undulator, currently planned at Helmholtz-Zentrum Dresden-Rossendorf as a stepping stone on a path to creating a fully quantum-effects-dominated free electron laser.

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