QUANTUM FEL II: MANY-ELECTRON THEORY

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Abstract

We investigate the emergence of the quantum regime of the FEL when many electrons interact simultaneously with the wiggler and the laser field. We find the Quantum FEL as the limit where only two momentum states are populated by the electrons. Moreover, we obtain exponential gain-perpass and start-up from vacuum.

INTRODUCTION

The recent years have seen rising interest in a possible novel regime of FEL operation: the so-called Quantum FEL. Bonifacio *et al.* [1] have proposed the implementation of this realm – despite experimental difficulties – because they expect better temporal coherence properties and a narrower linewidth of the radiation in SASE operation. Due to these prospects the Helmholtz-Zentrum Dresden-Rossendorf and Ulm University have started a collaboration to gain deeper insight into the emergence and the properties of the Quantum FEL. In a single-electron model we have identified the quantum regime of the FEL as an effective two-level system for the electron's momentum states [2] and have established a connection to the Jaynes-Cummings model [3].

In this article, we examine a situation where many electrons interact simultaneously with the laser and the wiggler field. Based on collective projection operators we develop a formalism which allows us to identify the two-level behaviour of the Quantum FEL. However, since we are dealing with many electrons, the suitable analogy is the Dicke [4] – describing a collection of two-level atoms interacting with a radiation field – rather than the Jaynes-Cummings model.

In the two-level approximation we find start-up from vacuum and exponential gain-per-pass in the short-time limit which are essential for SASE operation. Moreover, we calculate higher order corrections to this deep quantum regime and thus find analytical expressions which match the numerical results of [1].

MODEL

We start from the one-dimensional, quantized singlemode and many-particle Bambini-Renieri Hamiltonian [5,6]

$$\hat{H} \equiv \sum_{j=1}^{N} \frac{\hat{p}_{j}^{2}}{2m} + \hbar g \left(\hat{a}_{L} \sum_{j=1}^{N} e^{i2k\hat{z}_{j}} + \text{h.c.} \right)$$
(1)

where \hbar and *m* stand for the reduced Planck constant and for the electron mass, respectively and we already have eliminated the free dynamics of the laser field. The Bambini-Renieri frame - in which a nonrelativistic treatment of the FEL dynamics is possible - is defined by the condition that the wave numbers of the laser (subscript L) and the wiggler field (subscript W) are equal, i.e. $k_{\rm L} = k_{\rm W} \equiv k$ [5]. The position operator \hat{z}_i for the *j*-th of the N electrons and its conjugate momentum operator \hat{p}_i fulfill the canonical commutation relation $\left[\hat{z}_{j}, \hat{p}_{j}\right] = i\hbar$. While the laser field is quantized with the bosonic commutation relation $\left| \hat{a}_{\rm L}, \hat{a}_{\rm I}^{\dagger} \right| = 1$ for the photon annihilation and creation operators $\hat{a}_{\rm L}$ and $\hat{a}_{\rm I}^{\dagger}$, the wiggler is treated as an external classical field due to its high intensity. The coupling constant $g \equiv e^2 \mathcal{A}_{\rm L} \tilde{\mathcal{A}}_{\rm W} / (\hbar m)$ is given by the product of the amplitudes \mathcal{R}_L and $\tilde{\mathcal{R}}_W$ of the vector potentials of the laser and the wiggler field, respectively with *e* being the elementary charge.

An essential ingredient for recognizing the two-level behaviour of the Quantum FEL in the single-particle case is the occurrence of different time scales in the Schrödinger equation [2]. This feature stands out by expanding the state vector of the system in the scattering basis $|n + \mu, p - \mu q\rangle$ as introduced in [7] which is characterized by the number μ of scattered photons, that is, the number of times the electron experiences the quantum mechanical recoil $q \equiv 2\hbar k$ with n being the initial number of photons in the laser field and p the initial momentum of the electron.

This expansion is not possible in the many-particle case, since complicated entangled states are created by the Hamiltonian Eq. (1) as apparent from the case N = 2

$$\left(e^{2ik\hat{z}_1} + e^{2ik\hat{z}_2}\right)|p_1, p_2\rangle \sim |p_1 + q, p_2\rangle + |p_1, p_2 + q\rangle .$$
(2)

Therefore, we try to see the occurrence of the relevant time scales directly in the Hamiltonian and not from a particular representation of the state-vector. We achieve this goal by introducing the collective projection operators

$$\hat{\Upsilon}_{p',p''} \equiv \sum_{j=1}^{N} \hat{\sigma}_{p',p''}^{(j)} \equiv \sum_{j=1}^{N} |p'\rangle^{(j)} \langle p''|$$
(3)

where $|p\rangle^{(j)}$ is the momentum eigenstate of the *j*-th electron.

With the help of the completeness relation

$$\sum_{p'} |p'\rangle^{(j)} \langle p'| = \mathbb{1}$$
(4)

we rewrite the Hamiltonian Eq. (1) in terms of these collective operators as

$$\sum_{j=1}^{N} \hat{p}_{j}^{2} = \sum_{p'} p'^{2} \hat{\Upsilon}_{p',p'} \quad \text{and} \quad \sum_{j=1}^{N} e^{\pm i2k\hat{z}_{j}} = \sum_{p'} \hat{\Upsilon}_{p'\pm q,p'}$$
(5)

where we have made use of $_{(j)} \langle p' | \hat{p}_j^2 | p'' \rangle_{(j)} = p'^2 \delta_{p',p''}$ and $_{(j)} \langle p' | e^{\pm i2k\hat{z}_j} | p'' \rangle_{(j)} = \delta_{p',p''\pm q}$. Note that we do not sum over the particles any longer, but over the momenta, which in our formalism are numbers instead of operators.

In order to further simplify our approach we note that due to the discreteness of the recoil μq each electron can only be in momentum states separated by the recoil q. Assuming that initially all electrons have the same momentum p, i.e. $|\Psi(t = 0)\rangle = |p, p, ..., p\rangle \otimes |n\rangle$ (with the laser field being initially in the Fock state with photon number n) we can change the summation index in Eq. (5) to the integer number μ according to $p' \rightarrow p - \mu q$ (with p fixed) so that $\hat{\Upsilon}_{p'\pm q,p'} \rightarrow \hat{\Upsilon}_{\mu\mp 1,\mu}$.

The last step in recognizing the different time scales is to transform the Hamiltonian into the interaction picture which yields the expression

$$\hat{H}_{\text{Int}} = \epsilon \left(\hat{a}_{\text{L}} e^{i\Delta\tau} \sum_{\mu} \hat{\Upsilon}_{\mu,\mu+1} e^{-i2\mu\tau} + \text{h.c.} \right).$$
(6)

Here, we have introduced the scaled time $\tau \equiv \omega_{\rm r} t$, the coupling constant $\epsilon \equiv g/\omega_{\rm r}$, the recoil frequency $\omega_{\rm r} \equiv q^2/(2m\hbar)$ and the momentum deviation from resonance $\Delta \equiv p/(q/2) - 1$. Moreover, we have made the transformation to the interaction picture with the help of the commutation relation

$$\left[\hat{\Upsilon}_{\mu,\nu},\hat{\Upsilon}_{\rho,\lambda}\right] = \delta_{\nu,\rho}\,\hat{\Upsilon}_{\mu,\lambda} - \delta_{\lambda,\mu}\,\hat{\Upsilon}_{\rho,\nu} \tag{7}$$

which can be easily verified using the definition Eq. (3). We emphasize that we have defined the resonant electron momentum at p = q/2, which is the reasonable definition for the Quantum FEL [2] as we will see in the next section.

DEEP QUANTUM REGIME

The Hamiltonian Eq. (6) consists of terms oscillating with integer multiples of the recoil frequency ω_r and a contribution due to the deviation Δ from resonance. When we choose

FEL Theory

the initial momentum p of the electrons in the vicinity of the quantum resonance q/2, i.e. $\Delta \ll 1$, the terms $e^{\pm i\Delta \tau}$ will be slowly varying. In contrast, the phase factors with $e^{i\mu\tau}$ are rapidly oscillating for $\mu \neq 0$ and we can neglect them in the weak-coupling limit performing a rotating-wave-like approximation. This quantum regime is determined by the quantum parameter [2]

$$\alpha \equiv \epsilon \sqrt{N} = \frac{g \sqrt{N}}{\omega_{\rm r}} \tag{8}$$

given by the ratio of the coupling and the recoil frequency and has to be small to fulfill the weak-coupling condition, i.e. $\alpha \ll 1$.

If we perform this rotating-wave-like approximation, we arrive at the Quantum FEL Hamiltonian

$$\hat{H}_{\text{QFEL}} \equiv \epsilon \left\{ \hat{a}_{\text{L}} \, e^{+i\Delta\tau} \, \hat{\Upsilon}_{0,1} + \hat{a}_{\text{L}}^{\dagger} \, e^{-i\Delta\tau} \, \hat{\Upsilon}_{1,0} \right\} \tag{9}$$

which governs the dynamics of the FEL in the deep quantum regime. Here, the electrons can only have the momenta p and p - q and we observe the same two-level behaviour as in the single-particle case [2]. This limit is analogous to the Jaynes-Cummings model [3] in quantum optics, which describes the dynamics of a *single* two-level atom interacting with a quantized radiation field.

However, the algebra of the collective operators $\hat{\Upsilon}_{\rho,\lambda}$ with $\rho, \lambda = 0, 1$ is more complicated and therefore richer than that of the Pauli matrices which appear in the Jaynes-Cummings Hamiltonian. This distinctive difference originates from the fact that the collective operators create entangled superposition states as exemplified by Eq. (2) and products of these operators cannot be cast in a closed form. Indeed, the Hamiltonian Eq. (9) is equivalent to the Dicke Hamiltonian [4] which describes the simultaneous interaction of a *collection* of two-level atoms with a quantized electromagnetic field. Thus, the projection operators $\hat{\Upsilon}_{\rho,\lambda}$ are equivalent to the pseudo angular momentum operators of the Dicke model.

The time evolution of the system follows from the Heisenberg equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\hat{O} = \mathrm{i}\left[\hat{H}_{\mathrm{QFEL}},\hat{O}\right] \tag{10}$$

for an operator \hat{O} and we obtain a system of coupled nonlinear differential equations, for which no analytical solution is known. However, for short times we can linearize this set of equations in the parametrical approximation [8].

For this purpose, we notice the appearance of the operator $\hat{\Upsilon}_z \equiv \hat{\Upsilon}_{0,0} - \hat{\Upsilon}_{1,1}$ in the equations for $\hat{\Upsilon}_{1,0}$ and \hat{a}_L . This operator describes a kind of inversion of the number of electrons in the excited and ground state denoted by p and p-q, respectively. For an initial state $|p, p, ..., p\rangle \otimes |n\rangle$, with all electrons in the excited state, the expectation value of $\hat{\Upsilon}_z$ gives the number of electrons $N \gg 1$. We assume that for short times comparatively few electrons change to the ground state and we can replace $\hat{\Upsilon}_z$ by its expectation value at $\tau = 0$, i.e. $\hat{\Upsilon}_z \approx \langle \hat{\Upsilon}_z \rangle_0 = N$. Thus, we arrive at the

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Figure 1: Mean number of photons $\langle n_L \rangle$ for the Quantum FEL as a function of the scaled time τ according to Eq. (13) with $\alpha = 0.3$ - for resonance $\Delta = 0$ (blue line), $\Delta = 0.3$ (red dashed line) and $\Delta = 0.5$ (green dashed/dotted line).

linearized set of equations

$$i\frac{d}{d\tau}\begin{pmatrix}\tilde{\Upsilon}_{1,0}\\\tilde{a}_{L}\end{pmatrix} = \alpha \begin{pmatrix} 0 & -1\\ 1 & \kappa \end{pmatrix} \begin{pmatrix}\tilde{\Upsilon}_{1,0}\\\tilde{a}_{L}\end{pmatrix}$$
(11)

for the operators $\tilde{\Upsilon}_{1,0} \equiv \hat{\Upsilon}_{1,0} / \sqrt{N}$ and $\tilde{a}_{\rm L} \equiv \hat{a}_{\rm L}$. Here, we have already transformed to a frame where the time dependence due to the detuning $\Delta \equiv \kappa \alpha$ has been eliminated.

Searching for a solution of the kind $\sim e^{-i \mathcal{\lambda} \tau}$ we easily find the frequencies

$$\lambda_{\pm} = \frac{\kappa \alpha}{2} \pm i\alpha \sqrt{1 - (\kappa/2)^2} . \tag{12}$$

The non-vanishing imaginary part – which has its maximum at resonance – leads to an exponential gain-per-pass. Indeed, the time evolution of the mean photon number

$$\langle \hat{n}_{\rm L}(\tau) \rangle = \frac{1}{1 - (\kappa/2)^2} \, \sinh^2 \left[\alpha \tau \sqrt{1 - (\kappa/2)^2} \right] \quad (13)$$

with the photon number operator $\hat{n}_{L} \equiv \hat{a}_{L}^{\dagger} \hat{a}_{L}$ confirms this claim, where we have started with the laser field in vacuum, i.e. n = 0. Hence, with the start-up from vacuum and the exponential gain-per-pass we have obtained two important ingredients for the realisation of a SASE-FEL [9]. In Fig. 1 we show the photon number versus time τ for different detunings from resonance q/2. We note that the photon number grows more slowly, the further away the electrons are from resonance.

At resonance, the photon number increases exponentially with $e^{2\alpha\omega_r t}$, thus we find the gain length

$$L_{\rm g}^{\rm (q)} = \frac{c}{2\alpha\omega_{\rm r}} \tag{14}$$

for the Quantum FEL where we have used $t \approx z/c$ with *c* being the speed of light.

We have to keep in mind that the length given by Eq. (14) is measured in the co-moving reference frame and we have to include the effects of relativistic length contraction to

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compute the gain length in the laboratory frame. Note that the scaling with α^{-1} is not very different from the classical regime where $L_{\rm g}^{\rm (cl)} \sim \alpha^{-2/3}$ [10]. However, since in the quantum regime $\alpha \ll 1$ the gain length $L_{\rm g}^{\rm (q)}$ is very large. Hence, the suggestion of an optical undulator in [11], where more undulator periods can be passed within the same absolute wiggler length, seems reasonable.

We note that the connection between the Quantum FEL and the Dicke model – at least for exact resonance – was already found in [12] starting from a second-quantized Hamiltonian [13]. The link to our model can be established by applying Schwinger's representation [14] of angular momentum $\hat{\Upsilon}_{1,0} = \hat{c}_1^{\dagger} \hat{c}_0$, where \hat{c}_1^{\dagger} and \hat{c}_0 are bosonic operators. In the next section we present the first proof for the two-level behaviour of the Quantum FEL within a many-electron model, at least in the linearized regime.

HIGHER ORDER CORRECTIONS

A very useful technique to treat Hamiltonians of the type Eq. (6) is the Bogoliubov-Mitropolskii method of averaging [15] which is well-known in non-linear mechanics and has recently found its application in the field of atomic Bragg diffraction [16]. Since we now apply this method to the Hamiltonian and not to the equations of motion, we use a variation of the original technique: the so-called "Canonical Averaging" [17].

For this purpose we first cast our Hamiltonian in the form

$$\hat{H}'(\tau) = \epsilon \sum_{\mu} \hat{H}_{\mu} e^{i2\mu\tau}$$
(15)

with

$$\begin{cases} \hat{H}_{0} \equiv \hat{a}_{L} \hat{\Upsilon}_{0,1} + \hat{a}_{L}^{\dagger} \hat{\Upsilon}_{1,0} - \kappa \sqrt{N} \, \hat{n}_{L} \\ \hat{H}_{\mu} \equiv \hat{a}_{L} \hat{\Upsilon}_{-\mu,-\mu+1} + \hat{a}_{L}^{\dagger} \hat{\Upsilon}_{\mu+1,\mu} \end{cases}$$
(16)

where we have already eliminated the time-dependence due to the detuning $\Delta = \kappa \alpha$ which again is assumed to be small, i.e. $\Delta \ll 1$.

Following the procedure of [17] we search for a transformation of the density operator $\hat{\rho}(\tau)$ in the form of $e^{\hat{A}(\tau)}\hat{\rho}(\tau)e^{-\hat{A}(\tau)}$ where $\hat{A}(\tau)$ itself can be expanded into a power series of ϵ and every term of this series again is expressed as a Fourier series similar to Eq. (15). Using the Liouville equation

$$i\frac{d}{d\tau}\hat{\rho}(\tau) = \left[\hat{H}'(\tau), \hat{\rho}(\tau)\right]$$
(17)

we choose $\hat{A}(\tau)$ in such a way that all secular growing terms vanish order by order and we arrive at a time-independent effective Hamiltonian

$$\hat{H}_{\rm eff} = \epsilon \hat{H}_{\rm eff}^{(1)} + \epsilon^2 \hat{H}_{\rm eff}^{(2)} + \epsilon^3 \hat{H}_{\rm eff}^{(3)} + \dots .$$
(18)

The first order gives $\hat{H}_{\text{eff}}^{(1)} = \hat{H}_0$ in accordance with the discussion of the preceding section. We do not want to show the cumbersome expressions [17] for the higher orders. Instead we sketch the procedure: After calculating the Heisenberg

equations of motion for $\hat{\Upsilon}_{1,0}$ and \hat{a}_L up to third order in ϵ we again linearize these equations by setting $\hat{\Upsilon}_{0,0} \approx N$. Here, the largest terms behave as $\epsilon^k N^{k/2} = \alpha^k$ for the *k*-th order. Keeping only these contributions we arrive at the linear set of equations

$$i\frac{d}{d\tau}\begin{pmatrix}\tilde{\Upsilon}_{1,0}\\\tilde{a}_{L}\end{pmatrix} = \alpha \ \boldsymbol{M}\begin{pmatrix}\tilde{\Upsilon}_{1,0}\\\tilde{a}_{L}\end{pmatrix}$$
(19)

with the matrix

$$\boldsymbol{M} \equiv \begin{pmatrix} 0 & -\left(1 - \frac{\alpha^2}{8}\right) \\ 1 - \frac{\alpha^2}{8} & -\left(\kappa + \frac{\alpha}{2} - \frac{\kappa\alpha^2}{4}\right) \end{pmatrix}.$$
 (20)

Using again the ansatz $e^{-i\lambda\tau}$ we find the expression

$$Im\lambda = \pm \alpha \sqrt{1 - \frac{\kappa^2}{4}} \left[1 - \frac{\kappa/2}{1 - \frac{\kappa^2}{4}} \frac{\alpha}{4} - \frac{5 - 3\kappa^2 + \kappa^4/2}{\left(1 - \frac{\kappa^2}{4}\right)^2} \frac{\alpha^2}{32} \right]$$
(21)

for the imaginary part of the frequency which is responsible for the exponential gain. For $\alpha \ll 1$ terms of higher order yield only small corrections to Eq. (12). Note, that for exact resonance $\kappa = 0$ the second order term vanishes and we have to go to the next higher order to see the corrections.

At last we compare our results for the Quantum FEL with the ones of Bonifacio *et al.* in [1]. Starting from a description in terms of collective bunching operators, they have derived the cubic equation

$$\left(\lambda^2 - 1\right)\left(\lambda + 1 + \Delta\right) - 2\alpha^2 = 0 \tag{22}$$

for the frequencies λ , which for $\alpha \gg 1$ give asymptotically the correct results for the classical high-gain FEL [9].

We now study Eq. (22) in the quantum regime $\alpha \ll 1$ by expanding λ in powers of α , that is

$$\lambda = \lambda^{(0)} + \alpha \lambda^{(1)} + \alpha^2 \lambda^{(2)} + \alpha^3 \lambda^{(3)} + \dots$$
 (23)

and solve the resulting equations order by order. Here, we have set $\Delta = \kappa \alpha \ll 1$. Indeed, we obtain – apart from an unimportant rapidly oscillating solution – two solutions whose imaginary part match with Eq. (21).

Hence, we have found a perfect correspondence between our solution for the Quantum FEL and the one of [1], at least up to third order in α and a small momentum detuning Δ . This agreement is shown in Fig. 2 where we compare our analytical results with the numerical solution of Eq. (22) for two different values of α . Moreover, we see that the maximum of Im λ is shifted from p = q/2 to the left for increasing α . This feature is in accordance with the fact that for the classical high-gain FEL the resonance is at p = 0 [10].



Figure 2: Imaginary part Im λ of the scaled frequency λ , which governs the dynamics of the Quantum FEL vs. the initial momentum p of the electrons in units of q/2. Our results, first order in the quantum parameter α , Eq. (12), (black line), and third order in α , Eq. (21), (red line), are compared with the numerical solution of the cubic equation Eq. (22) of [1] (blue dashed line) for $\alpha = 0.1$ (above) and $\alpha = 0.5$ (below).

CONCLUSION

We have proposed a many-electron theory of the Quantum FEL based on collective projection operators. This analysis brings out most clearly that the underlying dynamics is not governed by the Jaynes-Cummings but the Dicke Hamiltonian. In particular, the linearized Heisenberg equations of motion for the lowest collective electron operator and the annihilation operator of the field predict an exponential gain starting from the vacuum. This result is crucial for the realization of the SASE-FEL. Moreover, the method of canonical averaging has allowed us to calculate higher order corrections which are in complete agreement with the results of Ref. [1]. A more detailed study of the quantum properties of the radiation of the Quantum FEL is in preparation.

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