RAPID COMMUNICATIONS

PHYSICAL REVIEW A VOLUME 43, NUMBER 6 15 MARCH 1991

Effective density matrix for free-electron-laser radiation

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(Received 14 December 1990)

The effective density matrix of the radiation field in the free-electron laser is computed under realistic initial conditions for the electrons and photons. The field is predicted to be a superposition of a coherent state and a chaotic state. The width of the distribution in the coherent-state expansion is given by the sum of classical and quantum-mechanical initial fluctuations of the electron beam.

As the free-electron-laser (FEL) physics matures to the point where it is possible to reliably model the growth of the radiation field, it becomes appropriate to seek a more complete description of this field in terms of its density matrix. Even though few measurements have been reported to date,[1] such a description gives an experimentally verifiable characterization of FEL light. For example, the measurements of photon statistics or coherence properties of FEL radiation would probe the density matrix.

While a quantum-mechanical description of the FEL is not necessary to compute the density matrix of the radiation field, it provides the most natural setting to do that. Furthermore, several recent proposals[2,3] envision a FEL operating in the 1-Å regime where the purely quantum effects may be detectable. Finally, the quantum-mechanical calculations presented for the FEL may be directly applicable to processes which are intrinsically nonclassical (channeling,[4] for example).

The calculation presented below for the density matrix of the radiation field generalizes on several previous attempts.[5-10] We obtain the full density matrix, rather than, for example, calculating only the second moment of the number operator, we take into account realistic initial conditions for the electron beam, and our model includes the exponential growth regime of the FEL radiation.

In what follows we consider the single-pass model, which is the relevant setup at short wavelengths, and we build on the quantum mechanical description of the FEL developed in Ref. 11. For the linearized one-dimensional single-mode problem with a circularly polarized wiggler, the solution for the annihilation operator of the radiation field in the Heisenberg picture is given by

$$a(\tau)=f_1(\tau)x(0)+f_2(\tau)y(0)+f_3(\tau)a(0)\,, \tag{1}$$

where

$$f_1(\tau)=\exp\left[-i\frac{\omega_0}{2\omega_w\rho}\left(\frac{\gamma_0}{\gamma_R}\right)^2\tau\right]e^{-i\delta\tau}\sum_{i=1}^{3}\frac{\sqrt{\rho}[(\lambda_j+\lambda_k)-\delta]}{(\lambda_i-\lambda_j)(\lambda_i-\lambda_k)}e^{i\lambda_i\tau}\,, \tag{2a}$$

$$f_2(\tau)=\exp\left[-i\frac{\omega_0}{2\omega_w\rho}\left(\frac{\gamma_0}{\gamma_R}\right)^2\tau\right]e^{-i\delta\tau}\sum_{i=1}^{3}\frac{i\sqrt{\rho}[\delta-(\lambda_j+\lambda_k)+\rho^{-1}]}{(\lambda_i-\lambda_j)(\lambda_i-\lambda_k)}e^{i\lambda_i\tau}\,, \tag{2b}$$

$$f_3(\tau)=\exp\left[-i\frac{\omega_0}{2\omega_w\rho}\left(\frac{\gamma_0}{\gamma_R}\right)^2\tau\right]\sum_{i=1}^{3}\frac{\lambda_j\lambda_k-\delta(\lambda_j+\lambda_k)-2\rho+\delta^2}{(\lambda_i-\lambda_j)(\lambda_i-\lambda_k)}e^{i\lambda_i\tau}\,. \tag{2c}$$

[As the modes decouple in linear theory, the solution given by Eqs. (1) and (2), with a different interpretation of the parameter δ, is also applicable in the many-mode case.] In Eqs. (2a)–(2c), the indices i,j,k are not the same and λ_i's are solutions to the eigenvalue equation $\lambda^3-\delta\lambda^2+2\rho\lambda+1=0$. Without the corrections of $O(\rho)$, Eqs. (2a)–(2c) have been given in Ref. 5. $x(0)$ and $y(0)$ are the initial values of non-Hermitian operators for the electron collective variables

$$x=\left[\frac{(p_R^2+M^2)}{(k_0+k_w)Np_R}\right]^{1/2}\sum_{j=1}^{N}\delta\phi_j e^{-i\phi_{0j}}\,, \tag{3a}$$

$$y=\left[\frac{(p_R^2+M^2)}{(k_0+k_w)Np_R}\right]^{1/2}\sum_{j=1}^{N}\delta p_j e^{-i\phi_{0j}}\,, \tag{3b}$$

where $\delta\phi_j=\phi_j-\phi_{0j}$, $\delta p_j=p_j-p_R$, and p_R and ϕ_{0j} are the equilibrium expectation values of the electron momentum (resonant momentum) and the phase relative to the radiation field, respectively; $\phi_j=(k_0+k_w)z_j-\omega_0 t-\psi_0 t$, $\psi_0=\omega_0(1-\gamma_R^2/\gamma_0^2)$; $m^2\gamma_R^2=p_R^2+M^2$ and analogously for γ_0 (p_0 is the expectation value of the average initial electron momentum); M^2 is the effective mass, $M^2=m^2+e^2A_w^2$, A_w is the strength of the wiggler vector potential, and a_w is the dimensionless quantity $a_w=eA_w/m$; δ is the detuning,

$$\delta=\frac{1}{2\rho\gamma_R^2}(\gamma_0^2-\gamma_R^2)\,;$$

ρ is Pierce's parameter,

$$\rho=\left[\tfrac{1}{4}a_w\left(\frac{\gamma_0}{\gamma_R}\right)^2\frac{\Omega_p}{\omega_w}\right]^{2/3},$$

with $\Omega_p=(4\pi n_0 e^2/m\gamma_0^3)^{1/2}$ (Ref. 12); τ is the dimensionless time, $\tau=2\omega_w\rho(\gamma_R/\gamma_0)^2 t$; k_0 and k_w are the wave numbers of the radiation and wiggler field, respectively, $\omega_0=k_0$, $\omega_w=k_w$; N is the total number of electrons, and V the quantization volume. By the linearization assumption ϕ_{0j} satisfies $\sum_{j=1}^{N} e^{in\phi_{0j}}=0$ for $n=\pm 1, \pm 2, \ldots$. (We note that linearization is performed about the equilibrium which corresponds to the absence of the radiation field, monoenergetic electron beam of momentum p_R, and a uniform distribution of electrons in phase satisfying $\sum_{j=1}^{N} e^{\pm i\phi_{0j}}=0$. For $|n|\geq 2$ the linearization assumption is the usual approximation[12] which holds for a large number of electrons.) We have set $\hbar=c=1$, but we will recover the powers of $\hbar$ and c in the final result in order to manifestly separate classical from quantum-mechanical effects. x, y, and a evaluated at the same time satisfy the following commutation relations: $[a,a^\dagger]=1$, $[x,y^\dagger]=[x^\dagger,y]=i$, and all of the other commutators vanish. The commutator between $a(\tau)$ and $a^\dagger(\tau)$ implies $i[f_1(\tau)f_2^*(\tau)-f_1^*(\tau)f_2(\tau)]+|f_3(\tau)|^2=1$, which can be directly verified. It can now be seen that in terms of dimensional variables the first factor in equations (2a)-(2c) is $e^{-i\omega_0 t}$, i.e., the free-field time evolution of a.

To examine the photon statistics of FEL radiation we use the formalism of expanding the density matrix in terms of coherent states,[6,13] and we pass to the Schrödinger picture in which the density matrix is a function of time. We begin by computing the normal ordered characteristic function,[13] $\chi_N(\lambda)=\langle\exp[\lambda a^\dagger(\tau)]\exp[-\lambda^* a(\tau)]\rangle$, where the angular brackets stand for the expectation value. It is assumed that initially the density matrix is a product of the density matrix describing the field and the one describing the electrons. The initial state of the field is taken to be a coherent state with amplitude α_0. (There is no essential limitation in this choice for the initial state of the field, as the ensuing calculations can easily be repeated for another, for example, thermal, initial distribution of photons.) Then

$$\chi_N(\lambda)=e^{\lambda f_3^*\alpha_0^*-\lambda^* f_3\alpha_0}\chi^{\rm el}\,, \tag{4}$$

where $\chi^{\rm el}$ is the electron part of χ_N. Using the fact that for any two operators A and B which both commute with $[A,B]$, $e^A e^B=e^{A+B}e^{[A,B]/2}$, and employing the commutators for x, $x^\dagger$, y, and $y^\dagger$,

$$\chi^{\rm el}=e^{-|\lambda|^2{\rm Im}(f_1 f_2^*)}\langle\exp[\lambda(f_1^* x^\dagger+f_2^* y^\dagger)-\lambda^*(f_1 x+f_2 y)]\rangle\,. \tag{5}$$

(We suppress the arguments of $f_{1,2,3}$ which are understood to be τ and of x, y, and a which are evaluated at $\tau=0$.) Written in terms of single electron momentum and position operators, the argument of the second exponential in Eq. (5) is

$$\sum_j [\delta z_j(\xi_j-\xi_j^*)+\delta p_j(\nu_j-\nu_j^*)]\,,$$

where $\xi_j=\frac{1}{2}\lambda f_1^* e^{-i\phi_{0j}}K'$, $\nu_j=\frac{1}{2}\lambda f_2^* e^{-i\phi_{0j}}K$, and K and K' are constants given by

$$K=2\left[\frac{p_R}{(p_R^2+M^2)N(k_0+k_w)}\right]^{1/2},$$

$$K'=2\left[\frac{(p_R^2+M^2)(k_0+k_w)}{p_R N}\right]^{1/2}.$$

To proceed further we invoke the assumption of the initial statistical independence of the electrons[14] and write the initial electron density matrix as a product of density matrices for single electrons. In addition, we impose the equality of the density matrices for single electrons. Hence it is needed to compute (with the index j temporarily suppressed),

$$\bar\chi^{\rm el}\equiv\langle\exp[\delta z(\xi-\xi^*)+\delta p(\nu-\nu^*)]\rangle$$

$$=\exp(-2i\,{\rm Im}\xi\,{\rm Im}\nu)\langle\exp(2i\delta p\,{\rm Im}\nu)\exp(2i\delta z\,{\rm Im}\xi)\rangle\,.$$

The relation with $\chi^{\rm el}$ is

$$\chi^{\rm el}=\exp[-|\lambda|^2{\rm Im}(f_1 f_2^*)]\prod_{j=1}^{N}\bar\chi_j^{\rm el}\,.$$

We model the initial electron state as follows: a statistical mixture over $\delta\bar p$ and $\delta\bar z$ of wave packets centered in momentum at $\delta\bar p$ and in position at $\delta\bar z$. For the electron wave functions we take the minimum uncertainty wave packet with the width Δ in momentum,

$$\psi_{\delta\bar p\delta\bar z}(\delta p)=\frac{1}{(2\pi\Delta^2)^{1/4}}\exp(-i\delta p\delta\bar z)\times\exp\left[-\frac{(\delta p-\delta\bar p)^2}{4\Delta^2}\right]. \tag{6}$$

The density matrix is

$$\rho=\int d(\delta\bar z)d(\delta\bar p)|\delta\bar p,\delta\bar z\rangle R(\delta\bar p,\delta\bar z)\langle\delta\bar p,\delta\bar z|\,,$$

where $\langle\delta p|\delta\bar p,\delta\bar z\rangle=\psi_{\delta\bar p,\delta\bar z}(\delta p)$. Using

$$\bar\chi^{\rm el}=\exp(-2i\,{\rm Im}\xi\,{\rm Im}\nu)\times{\rm Tr}[\rho\exp(2i\delta p\,{\rm Im}\nu)\exp(2i\delta z\,{\rm Im}\xi)]\,,$$

an integration in the momentum representation yields

$$\bar\chi^{\rm el}=\exp[-2\Delta^2({\rm Im}\nu)^2]\exp\left[\frac{-1}{2\Delta^2}({\rm Im}\xi)^2\right]\int d(\delta\bar z)d(\delta\bar p)R(\delta\bar p,\delta\bar z)\exp(2i\delta\bar z\,{\rm Im}\xi)\exp(2i\delta\bar p\,{\rm Im}\nu)\,. \tag{7}$$

Next, we write $R(\delta\bar p,\delta\bar z)=P(\delta\bar p)Z(\delta\bar z)$, i.e., the distributions in $\delta\bar p$ and $\delta\bar z$ are independent (which can be expected to hold for the range of z over which ψ changes by 2π).

To find $Z(\delta\bar z)$, we proceed as follows: We want the distribution for the average of N random variables $\delta\bar z_j$, each one of which has a distribution $D_z(\delta\bar z_j)$, centered at 0. Further, using the estimate for the random electron distribution in phase from Ref. 11, we write the second moment of $Z(\delta\bar z)$ as $1/k_0^2$. Then the central limit theorem gives

$$Z(\delta\bar z)=\frac{k_0}{\sqrt{2\pi}}\exp\left[\frac{-(\delta\bar z)^2k_0^2}{2}\right].$$

For $P(\delta\bar{p})$ we proceed in an analogous manner, but with the center of each $D_p(\delta\bar{p}_j)$, and hence of $P(\delta\bar{p})$ at δp_0 (so that δp_0+p_R is the average initial electron momentum). The width of $P(\delta\bar{p})$ is the thermal spread, denoted by Δp. Thus,

$$P(\delta\bar{p})=\frac{1}{\sqrt{2\pi}(\Delta p)}\exp\left[-\frac{(\delta\bar{p}-\delta p_0)^2}{2(\Delta p)^2}\right].$$

Substituting now the expressions for $Z(\delta\bar{z})$ and $P(\delta\bar{p})$ into Eq. (7) yields

$$\bar{\chi}_j^{\rm el}=\exp(2i\delta p_0 \mathrm{Im}\,v_j)\exp\{-2(\mathrm{Im}\,v_j)^2[(\Delta p)^2+\Delta^2]\}\times\exp\left[-2(\mathrm{Im}\,\xi_j)^2\left(\frac{1}{4\Delta^2}+\frac{1}{k_0^2}\right)\right]. \quad (8)$$

Into this equation we insert the definitions of v_j and ξ_j. Then, summing the argument of the exponential over j, using the linearization assumption $\sum_{j=1}^{N}e^{\pm 2i\phi_{0j}}=0$, and approximating to $O(1/\gamma^2)$ $\frac{1}{4}K'^2N$ by $p_R k_0$, and $\frac{1}{4}K^2N$ by $1/(k_0 p_R)$, yields

$$\chi_N(\lambda)=\exp(\lambda f_3^* \alpha_0^* -\lambda^* f_3\alpha_0)\exp(-|\lambda|^2\langle n\rangle_{\rm th}). \quad (9)$$

Here, with powers of $\hbar$ included,

$$\langle n\rangle_{\rm th}=\mathrm{Im}(f_1 f_2^*)+|f_2|^2\left(\frac{(\Delta p)^2}{p_R\hbar k_0}+\frac{\Delta^2}{p_R\hbar k_0}\right)+|f_1|^2\left(\frac{p_R}{\hbar k_0}+\frac{p_R\hbar k_0}{4\Delta^2}\right). \quad (10)$$

We now obtain the effective density operator for the radiation field at time τ. As Eq. (9) is the expression for

$$\mathrm{Tr}[\rho_{\rm el}(0)\rho_{\rm rad}(0)U(\tau)e^{\lambda a^\dagger(0)}e^{-\lambda^* a(0)}U^\dagger(\tau)],$$

where $U(\tau)$ and $U^\dagger(\tau)$ are the usual time-evolution operators, we trace out the electron variables to get

$$\chi_N(\tau)=\mathrm{Tr}[\rho_{\rm rad,eff}(\tau)e^{\lambda a^\dagger(0)}e^{-\lambda^* a(0)}]. \quad (11)$$

The remaining trace runs only over the radiation field (hence the subscript eff for effective). Next, we assume that $\rho_{\rm rad,eff}(\tau)$ has a diagonal representation in terms of coherent states,[13] $\rho_{\rm rad,eff}=\int d^2\alpha|\alpha\rangle P(\alpha)\langle\alpha|$, where $d^2\alpha\equiv d(\mathrm{Re}\alpha)d(\mathrm{Im}\alpha)$, and we use[13]

$$P(\alpha)=\frac{1}{\pi^2}\int \exp(\alpha\lambda^*-\alpha^*\lambda)\chi_N(\lambda)d^2\lambda.$$

A straightforward calculation then yields

$$P(\alpha)=\frac{1}{\pi\langle n\rangle_{\rm th}}\exp\left[-\frac{|\alpha-f_3\alpha_0|^2}{\langle n\rangle_{\rm th}}\right]. \quad (12)$$

This is an eminently reasonable result. The field produced by a FEL is a superposition[13] of a coherent state of amplitude $f_3\alpha_0$, and of a chaotic state (pure noise), with the expectation value for the number operator given by $\langle n\rangle_{\rm th}$. The intensity of FEL radiation, on the other hand, is $\langle a^\dagger a\rangle(\tau)=|f_3|^2|\alpha_0|^2+\langle n\rangle_{\rm th}$, as can be easily shown by using the expression above. We also note that as $\tau\to 0$, $f_1,f_2\to 0$, and $f_3\to 1$, which produces $P(\alpha)=\delta^2(\alpha-\alpha_0)$, in agreement with the assumption that the radiation field is initially in a coherent state of amplitude α_0.

The coherent part of the field is due to the amplification of the initial coherent signal. The sources of the noisy part can be identified term by term in Eq. (10): (i) noncommutativity of δp_j and δz_j (quantum effect); (ii) thermal spread of initial electron momentum distribution (classical effect); (iii) width of electron wave packet in momentum (quantum effect); (iv) random distributions of electrons in phase-shot noise (classical effect); and (v) width of electron wave packet in position (quantum effect). [The classical sources of noise carry a factor of $1/\hbar$ due to the definition of $f_{1,2}$, Eqs. (2a) and (2b) and of the electron collective variables, Eqs. (3a) and (3b).] For most FEL's of current experimental interest the classical sources of fluctuations can be expected to be dominant over the other terms.[11] The product of the third and the fifth terms of Eq. (10), on the other hand, gives the lower limit of quantum fluctuations discussed in Ref. 11, in agreement with our choice of the minimum uncertainty wave packet.

In the results presented so far we have not specified the value of Δ. While we do not invoke physical arguments to do that, we notice which value minimizes $\langle n\rangle_{\rm th}$ (minimum of quantum effects in $\langle n\rangle_{\rm th}$). As $|f_1(\tau)|^2\simeq\rho^2|f_2(\tau)|^2$ for $\rho\ll 1$, the minimum of Eq. (10) is reached at $\Delta=(\frac{1}{2}p_R\hbar k_0\rho)^{1/2}$. For typical experimental values for FEL parameters, for this value of Δ, $\Delta\ll\Delta p$. For example, $p_R c=100$ MeV, $\lambda_w=1$ cm, $\rho=1\times10^{-2}$, $a_w=3.0$, $\Delta p/p_R=0.05\%$ gives $\Delta/\Delta p\simeq 0.01$, which is probably too small to be detected [both Δ and Δp enter squared in Eq. (10)]. This ratio can be, however, significantly altered for more unusual FEL designs. For the 1-Å FEL we take[3] $p_R c=1.6$ GeV, $\lambda_w=0.1$ cm, $\rho=1.3\times10^{-3}$, $a_w=1.0$, and $\Delta p/p_R=0.1\%$. This yields $\Delta/\Delta p\simeq 0.1$, with experimentally measurable consequences, such as the start-up time from noise.

Equation (12) can be used to predict the coherence properties of radiation produced by FEL's. Regarding spatial coherence, the field is only first-order coherent (as we treat a single-mode problem). Defining the degree of nth-order coherence[15] as

$$g^{(n,n)}(z_1,\ldots,z_{2n})=\frac{\Gamma^{(n,n)}(z_1,\ldots,z_{2n})}{\left[\prod_{j=1}^{2n}\Gamma^{(1,1)}(z_j,z_j)\right]^{1/2}},$$

where $\Gamma^{(n,n)}(z_1,\ldots,z_{2n})$ is the nth order correlation function

$$\Gamma^{(n,n)}(z_1,\ldots,z_{2n})=\mathrm{Tr}[\rho(0)A_s^{(-)}(t,z_1)\ldots A_s^{(-)}(t,z_n)A_s^{(+)}(t,z_{n+1})\ldots A_s^{(+)}(t,z_{2n})],$$

and $(+)$ and $(-)$ denote positive and negative frequency parts of the vector potential $\mathbf{A}_s$, gives[16] for FEL radiation

$$|g^{(n,n)}(z_1,\ldots,z_{2n})|=\frac{n!L_n(-|f_3\alpha_0|^2/\langle n_{\rm th}\rangle)}{(1+|f_3\alpha_0|^2/\langle n_{\rm th}\rangle)^n}.$$

Here $L_n(x)$ is the Laguerre polynomial. It is now clear that in the limit $|f_3\alpha_0|^2 \gg \langle n_{\rm th}\rangle$, $|g^{(n,n)}| \simeq 1$, which is fully coherent, whereas in the limit $|f_3\alpha_0|^2 \ll \langle n_{\rm th}\rangle$, $|g^{(n,n)}| \simeq n!$, which is thermal. Temporal coherence is a more delicate question since $P(\alpha)$ is explicitly a function of time. For two arbitrary points in time the field does not possess first-order coherence, $|g^{(1,1)}(t_1,t_2)| \neq 1$ [the step leading to Eq. (11) does not go through]. A calculation of this quantity is given in Ref. 17. For $t_1 - t_2 \ll 1/(2\rho\omega_w|\mathrm{Im}\lambda|)$, however, i.e., for time separations which are much smaller than the characteristic evolution time of the density marix, the radiation field is first-order coherent. As in the case of spatial coherence, in this limit, Eq. (12) predicts that none of the higher-order correlation functions will factor out, i.e., the FEL radiation possesses only first-order temporal coherence. Finally, we mention that Eq. (12) confirms the finding of Ref. 14 that for reasonable initial conditions for the electron beam, FEL's cannot produce radiation in a squeezed state. In such a state $\chi_N(\lambda) = \exp(\lambda\mu - \lambda^*\mu^* + |\lambda|^2 g)$ for some μ and some real positive g.[18] Consequently, $P(\alpha)$ is not defined.

We remark on the results announced by other authors. In Refs. 7 and 8 perturbation theory in $p_j - p_0$ is applied to first order. (The limitation of this method is that it generates secularities in time, and hence is valid only for very short times; in particular exponential growth is not captured.) $\langle n|\rho|n\rangle$ is computed for the initial electron beam where all electrons are in momentum eigenstates, and where the radiation field is initially the vacuum. For the coherent initial state of the field the photon number variance, $\langle n^2\rangle - \langle n\rangle^2$, is computed. Thermal distribution is found for $\langle n|\rho|n\rangle$, and a nonpreservation of the initial coherent state. This is in agreement with Eq. (12); our result, however, describes, in addition, the amplification of the spontaneous emission, as well as other higher-order effects that also have a thermal distribution. Reference 9 also claims a thermal distribution of photons during FEL start-up. There the radiation field equation is solved assuming a given motion of the electrons. The result of Ref. 5, on the other hand, is the limiting case of our result when $\Delta p = 0$, the shot noise is neglected, and Δ is taken to be $(\frac{1}{2}\hbar k_0 p_R)^{1/2}$. Finally, Ref. 10 studies the start-up of an oscillator by applying fourth-order perturbation theory in $e^2 A_w/(p_R^2 + M^2)^{1/2}(\pi/V\omega_0)^{1/2}$ (again secular in t). Thermal statistics is found for $\langle n|\rho|n\rangle$.

This work was supported by the U. S. Department of Energy, Grants No. DE-FG02-86ER53222 and No. DE-AS05-80ER10666.

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