Bohr's correspondence principle and x-ray generation by laser-stimulated electron-ion recombination

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Considering Bohr's correspondence principle and energy conservation laws, we derive by means of some elementary classical considerations of electron motion in a laser field an expression for the width of the laser-stimulated x-ray spectrum in electron-ion recombination and we find a classical expression for the power distribution of x-ray radiation, both of which agree surprisingly well with the results of the corresponding quantum-mechanical calculations presented earlier.

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According to Bohr's correspondence principle, classical physics should be considered as a limiting case of quantum physics. More precisely, whenever quantum theory is used to describe the behavior of systems that can also be treated successfully by classical theory, the corresponding predictions of both should agree. The correspondence principle played a very important role in the beginning stages of the development of quantum mechanics. Bohr's original model of the hydrogen atom was based partly on the views of this principle by adapting classical mechanics with his quantization postulates. In Bohr's formula for the frequencies $\nu_q = \nu_{n,l}$, emitted or absorbed by the hydrogen atom between the energy levels n and l, there is no direct relation to the classical radiation frequency ν_c emitted by the electron accelerating on the orbit of radius a_n about the proton. If, however, $l=n-1$ and n becomes very large, then we find that $\nu_q \to \nu_c = (m\alpha^2 Z^2/2\pi)/n^3$ (α denoting the fine-structure constant and $\hbar=c=1$) for the electron moving at a large distance from the proton, thus behaving like a classical charge, emitting light with the same frequency as its circular frequency when it orbits the proton [1,2]. It is now rather commonly accepted that the predictions of classical and quantum-mechanical theories should agree for large quantum numbers. A historically important example for the validity of the correspondence principle is the agreement between the formulas of radiation power emitted by a classical dipole oscillator and the corresponding atomic quantum oscillator, if the classical dipole moment is replaced (up to a factor of 2) by the quantum-mechanical dipole matrix element [1]. In general, it is believed that in the limit of soft photons, or for a large number of photons in the light beam, the predictions of quantum electrodynamics should agree with the corresponding results of classical electrodynamics. As a remarkable example of the validity of this conclusion, we may consider Compton scattering. Here the Klein-Nishina formula, with all radiative corrections included, agrees in the soft-photon limit with the classical Thomson scattering formula [4].

It is worth mentioning, however, that such conclusions are not valid in general. For instance, Gao [3], studying recently the rotational-vibrational states of diatomic molecules close to the dissociation threshold, made the surprising discovery that the semiclassical predictions of dissociation became less accurate for higher quantum numbers. The problem is that a state with a large quantum number is not necessarily "more classical." On the contrary, we can obtain the correct classical limit for such states for which the quantum-mechanical wave function of a particle has a shorter wavelength. It appears that ultracold atoms can have wave functions of extremely long wavelength, such that even if a pair of them attracts each other at a large distance, corresponding to a system equivalent to a molecule in a highly excited vibrational state, the semiclassical theory might not apply.

Our above discussion and examples show that it should be worthwhile to look for possible other manifestations of the validity of the correspondence principle. Therefore, it will be the main objective of our present work to discuss in the context of the correspondence principle certain features of the power spectrum of x rays that are emitted during the recombination of electrons with ions in the presence of a strong laser field. Such a possibility of x-ray generation was discussed recently by the present authors [5] and by Kuchiev and Ostrovsky [6]. In particular, we have shown that this power spectrum has the shape of a plateau of the width $4\sqrt{2U_p E_{\mathbf{p}}}$, where U_p is the ponderomotive energy of the electron in the laser field and $E_{\mathbf{p}}$ is the initial kinetic energy of the electron. Within the framework of our approximate quantum-mechanical analysis, presented in [5] and essentially based (though with different initial conditions) on the inverse form of the *Keldysh-Faisal-Reiss* model (see the comprehensive review by Reiss [7]), we were able to estimate that the maximum energy of emitted x-ray quanta is $\omega_{\max}=E_{\mathbf{p}}+U_p+|E_B|+2\sqrt{2U_p E_{\mathbf{p}}}$, where E_B denotes the binding energy of the electron in the atom. We shall show in our present investigation that similar results can be obtained by analyzing a classical model for x-ray generation, to be outlined below. An interesting feature of this model turns out to be that it describes the shape of the power spectrum as well as the positions of its maxima more correctly than the approximate quantum formula derived in [5].

If we consider a classical electron moving in a laser field, described by a vector potential $\mathbf{A}_L(t)$, then its time-dependent energy is equal to

$$E(t) = \frac{1}{2m}[\mathbf{p} - e\mathbf{A}_L(t)]^2, \tag{1}$$

where we assume the vector potential of the laser field in the dipole approximation to be given by $\mathbf{A}_L(t)=\mathbf{A}_0\cos\omega_L t$. Choosing the laser field to be adiabatically turned off at $t\to-\infty$, $\mathbf{p}$ will be the initial kinetic momentum of the electron and $E(t)$ in Eq. (1) is then its classical laser-dressed energy at time t. If at a certain instant of time t the electron gets captured by an ion in the presence of the laser field, then the energy of the emitted x-ray photon will be equal to $\omega_X(t)=|E_B|+E(t)$. Here we assumed for a moment that the total laser-dressed energy of the electron gets converted into the energy of the x-ray photon and that processes in which, apart from this x-ray photon, also some laser photons are emitted to, or absorbed from, the laser field are much less probable. In addition, we shall assume that the intensity of the emitted x-ray radiation, having energy in the interval $[\omega_X,\omega_X+d\omega_X]$, is proportional to the time during which the ''classically laser-dressed'' electron possesses energy lying within the interval $[E(t),E(t)+d\omega_X]$. This means that the power spectrum of x-ray radiation, $S(\omega_X,\mathbf{n},\mathbf{p})$, derived in our previous work [5], is proportional to the probability density of finding the electron with an instant energy given by $E(t)=\omega_X(t)-|E_B|$. Hence, this classical probability density can be evaluated and is equal to

$$\rho_c(\omega_X)=\frac{\omega_L}{\pi}\frac{1}{|\omega_X'(t(\omega_X))|}, \tag{2}$$

where the prime denotes the derivative with respect to the time and $t(\omega_X)$ is the solution of the equation

$$\omega_X=|E_B|+\frac{1}{2m}(\mathbf{p}-e\mathbf{A}_0\cos\omega_L t)^2. \tag{3}$$

The above probability density $\rho_c(\omega_X)$ has been normalized to 1, viz.,

$$\int_{\omega_{\min}}^{\omega_{\max}}\rho_c(\omega_X)d\omega_X=1, \tag{4}$$

where $\omega_{\min}$ and $\omega_{\max}$ are the classical minimum and maximum values of the generated x-ray frequencies. In order to derive the solution for $t(\omega_X)$, we have to choose a time interval of one-half of a laser cycle, i.e., $[t_0,t_0+\pi/\omega_L]$, in which Eq. (3) has a unique solution $t(\omega_X)$ and we have to make use of the following sequence of equations:

$$1=\frac{\omega_L}{\pi}\int_{t_0}^{t_0+\pi/\omega_L}dt=\frac{\omega_L}{\pi}\int_{\omega_{\min}}^{\omega_{\max}}\frac{d\omega_X}{|\omega_X'(t(\omega_X))|}. \tag{5}$$

Moreover, we can show that

$$|\omega_X'(t(\omega_X))|=2\omega_L\{(\omega_X-|E_B|)\times[2U_p-(\sqrt{\omega_X-|E_B|}-\sqrt{E_{\mathbf{p}}})^2]\}^{1/2}. \tag{6}$$

For the derivation of this equation, we assumed that the initial electron momentum points parallel to the polarization vector of the laser field, viz., $\mathbf{p}||\mathbf{A}_0$. This choice turned out to be the most favorable geometry for the generation of x-rays in the recombination process, as we discussed in [5]. For this geometry, the possible energies ω_X of x ray photons lie within the range $[\omega_{\min},\omega_{\max}]$, where the minimum and maximum frequencies are correspondingly defined by the expressions

$$\omega_{\min}=|E_B|+2U_p+E_{\mathbf{p}}-2\sqrt{2U_pE_{\mathbf{p}}}, \tag{7}$$

$$\omega_{\max}=|E_B|+2U_p+E_{\mathbf{p}}+2\sqrt{2U_pE_{\mathbf{p}}}. \tag{8}$$

The classical model presented above predicts that for a given value of the initial electron momentum, the power spectrum of x-ray radiation is limited to the range $[\omega_{\min},\omega_{\max}]$. It might seem that the drawback of this model is that the probability density $\rho_c(\omega_X)$ is infinite at the end points of the interval $[\omega_{\min},\omega_{\max}]$. In a realistic experiment, however, we measure the intensity of x-ray radiation within a certain interval near a given frequency ω_X, due to the finite resolution of the measuring apparatus. Therefore, the above classical probability density $\rho_c(\omega_X)$ should be averaged in addition over a certain frequency range in the vicinity of ω_X. Then we obtain a finite and continuous classical probability density for the generation of high-energy photons ω_X. For simplicity, we assume that the experimental apparatus counts all photons in the interval $[\omega_X-\delta,\omega_X+\delta]$, such that its resolution is equal to 2δ. In this case, the averaged probability density is equal to

$$\overline{\rho_c}(\omega_X)=\frac{1}{2\delta}\int_{\omega_X-\delta}^{\omega_X+\delta}d\omega\rho_c(\omega). \tag{9}$$

The integral can be evaluated and yields $\overline{\rho_c}(\omega_X)$ in the following form

$$\overline{\rho_c}(\omega_X)=\frac{1}{2\delta}\begin{cases}0 & ;\ \omega_X<\omega_{\min}-\delta\\ f(\omega_X+\delta)-f(\omega_{\min}) & ;\ \omega_{\min}-\delta<\omega_X<\omega_{\min}+\delta\\ f(\omega_X+\delta)-f(\omega_X-\delta) & ;\ \omega_{\min}+\delta<\omega_X<\omega_{\max}-\delta\\ f(\omega_{\max})-f(\omega_X-\delta) & ;\ \omega_{\max}-\delta<\omega_X<\omega_{\max}+\delta\\ 0 & ;\ \omega_X>\omega_{\max}+\delta\end{cases}, \tag{10}$$

where the function $f(\omega)$ is equal to

$$f(\omega)=\frac{1}{\pi}\arcsin\left(\frac{2\sqrt{\omega-|E_B|}-\sqrt{\omega_{\max}-|E_B|}-\sqrt{\omega_{\min}-|E_B|}}{\sqrt{\omega_{\max}-|E_B|}-\sqrt{\omega_{\min}-|E_B|}}\right). \tag{11}$$

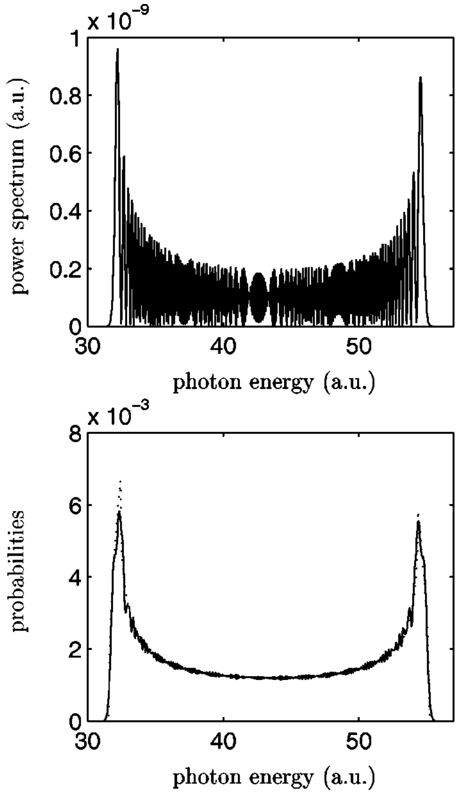

FIG. 1. The upper frame presents the differential power spectrum calculated with our Coulomb-Volkov scattering state for the geometry in which the laser beam and the x-ray photon propagate in the x direction while the polarization vectors are parallel to the z direction, whereas the electron momentum $\mathbf{p}$ points antiparallel to the z direction. The laser photon energy and intensity are equal to $\omega_L = 1.17$ eV and $I = 10^{14}$ W cm^{-2}, respectively. The initial electron kinetic energy is $E_{\mathbf{p}} = 42.5$ (a.u.) $= 1156$ eV. The lower frame shows a comparison of the quantum-mechanical probability distribution $\overline{p}_q(\omega_X)$ (continuous line) with the classical one $\overline{p}_c(\omega_X)$ (dotted line). We observe a very good agreement as a manifestation of Bohr's correspondence principle applied here to laser-assisted electron-ion recombination.

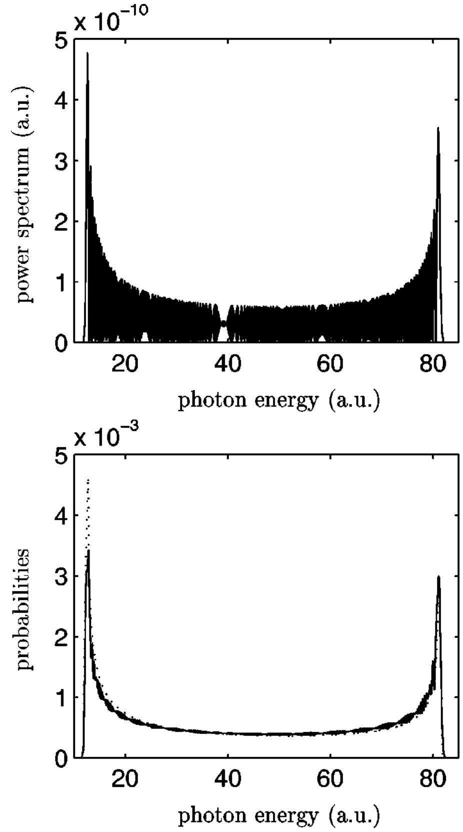

FIG. 2. The same as in Fig. 1 but for the higher laser field intensity $I = 10^{15}$ W cm^{-2}. We observe larger discrepancies between the data for small x-ray photon energies from within the plateau. These differences originate from the fact that for such low energies, the recombining electrons cannot be considered as classical particles interacting with a laser field alone, because now the interaction with the ionic potential becomes important.

The averaged classical probability density $\overline{\rho}_c(\omega_X)$ is a continuous function of ω_X, while quantum theory predicts that the x-ray frequencies can differ only by multiples of the laser frequency ω_L. Therefore, in order to be able to compare the predictions of the classical and quantum-mechanical models, we have to also discretize the classical probability density. From our point of view, the most natural discretization prescription for the present problem is the following:

$$\overline{p}_c(\omega_X) = \int_{\omega_X - (1/2)\omega_L}^{\omega_X + (1/2)\omega_L} d\omega \overline{\rho}_c(\omega) \approx \omega_L \overline{\rho}_c(\omega_X), \tag{12}$$

which leads to the probability that in the process of recombination a photon of energy from the interval $[\omega_X - \frac{1}{2}\omega_L, \omega_X + \frac{1}{2}\omega_L]$ gets emitted. This classical result should then be compared with the corresponding quantum-mechanical probability $\overline{p}_q(\omega_X)$, which is proportional to the power spectrum $S(\omega_X, \mathbf{n}, \mathbf{p})$ of x-ray radiation that we have calculated quantum mechanically in [5] and which we have normalized such that the total probability of emission of any x-ray photon is equal to 1. Here too we have to account for the finite resolution of the experimental apparatus. Hence $\overline{p}_q(\omega_X)$ is proportional to the power spectrum, averaged in a similar way as was done for the classical probability distribution, namely

$$\overline{p}_q(\omega_X) = N \sum_{\omega_X - \delta \leqslant \omega \leqslant \omega_X + \delta} S(\omega, \mathbf{n}, \mathbf{p}), \tag{13}$$

where N is the normalization factor to be determined from the normalization condition

$$\sum_{\omega_X} \overline{p}_q(\omega_X) = 1. \tag{14}$$

For our numerical examples, illustrating the validity of the correspondence principle in the present problem, we considered a Nd:YAG laser of frequency $\omega_L = 1.17$ eV, and took a rather high initial energy of the ingoing electron of $E_{\mathbf{p}} = 1156$ eV. We assumed that the resolution of the experimental apparatus, measuring the energy of the x-ray photons, is $2\delta=20\omega_L$, which is a reasonable value for the energetic x-ray radiation considered here. In Figs. 1 and 2, we compare the classical and quantum-mechanical probabilities $\overline{p_c}(\omega_X)$ and $\overline{p_q}(\omega_X)$, respectively, for the two laser field intensities $I=10^{14}$ W cm^{-2} and $I=10^{15}$ W cm^{-2}. We also present the quantum-mechanical differential power spectra $S(\omega_X,\mathbf{n},\mathbf{p})$ evaluated for these two intensities by means of our inverse KFR model, derived in our foregoing work [5]. It should be noted that in this model the ingoing laser-dressed electron is described by a generalized Coulomb-Volkov wave, which turns out to be more precise than the one originally proposed by Jain and Tzoar [8] (see the critical analysis in [9]) and which has been derived independently by several authors [10–12] (see also our review [13]). As expected, the exact results of our quantum-mechanical model are smoothed out by the averaging procedure, but the most important finding is that the shapes of the classical and quantum-mechanical probability distributions are almost identical. We may expect that for smaller laser frequencies, the agreement should be even better, since in that case the application of the correspondence principle should become more adequate. Because of numerical difficulties we cannot present such a comparison for a CO_2 laser and for the same initial electron kinetic energy. It appears that the minimum and maximum x-ray energies of the frequency plateau, determined by Eqs. (7) and (8), agree better with the exact values than the approximate ones, estimated by us in our quantum-mechanical work [5]. The discrepancy between the classical and quantum-mechanical probability distributions is particularly striking for small x-ray energies from within the plateau region. This has its origin in the fact that for such small energies, the electron cannot be treated as a classical particle interacting with the laser field only but not with the ionic potential.

Though the classical model presented here reproduces the shape of the power spectrum and determines the energy boundaries of the plateau remarkably well, we have to emphasize that it does not, however, enable us to estimate the absolute values of the power spectrum, for which a quantum-mechanical calculation is required. Moreover, our model can also not predict the rapid oscillations of the data of the power spectrum in the inner part of the frequency plateau, since these oscillations are due to quantum-mechanical interference effects that result from the summation of probability amplitudes corresponding to different quantum paths, but which lead to the same final state. For example, quantum mechanically the electron can virtually absorb a number of laser photons and, after having been captured by the ion, can again virtually emit the same number of laser photons. On the other hand, the very good agreement between the classical and quantum-mechanical probability distributions near the maximum x-ray photon energy of the plateau suggests that in this region there is only one dominant quantum-mechanical ionization path, namely the direct emission of an x-ray photon during the recombination process, as we have initially assumed for our classical model. Finally, our surprisingly successful application of the correspondence principle to the present problem is in accord with the successful application of similar classical considerations to above-threshold ionization and harmonic generation [14,15].

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