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On the dissociation (fragmentation) of atoms, molecules, atomic clusters and atomic nuclei in strong laser fields

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Abstract

The relativistic, classical motion of free charges in strong laser fields is briefly reviewed. It is shown that, under certain conditions, strong laser fields in bound quantum assemblies of particles like atoms, molecules, atomic clusters and atomic nuclei may govern a non-relativistic motion of the electric charges which preserves the quantum structure of the energy levels while shifting them by the time-dependent interaction energy. The effect of this interaction is a fine splitting of the quantum energy levels, which look like a dense distribution of classical energy continuum; it is the dressed states of the coherent-state formulation of the quasi-classical approximation. Consequently, fragmentation may occur of such bound assemblies of particles in strong radiation fields. The fragmentation probability is estimated, as well as the lifetime of the bound states of quantum particles in strong laser fields.

With the advent of high-power lasers strong electromagnetic fields became available for investigating atomic, molecular and nuclear dynamics. A laser beam with intensity $10^{20}w/cm^2$generates in its focus an electric field $E \simeq 10^9 statvolt/cm$ ($3 \times 10^{12}V/m$, and a similar magnetic field $10^5 Ts$); this is three orders of magnitude higher than the atomic electric fields. The motion of the electric charges under the action of such fields is relativistic, (quasi-) classsical and (quasi-) free.

Indeed, a classical charge q with mass m, initially at rest, subjected to the action of a radiation field with the vector potential $A_0 \cos(\omega t - kx)$ oriented along the z-axis, performs oscillations $z = -2\eta\lambda \sin(\omega t - kx)$ and acquires a drift

$$x = \frac{\eta^2}{1+\eta^2}\left[ct + \frac{\lambda}{2}\sin 2(\omega t - kx)\right] \tag{1}$$

along the x-axis, where $\eta = qA_0/2mc^2$, $\lambda = c/\omega$ being the wavelength of the radiation; its energy is $\mathcal{E} = mc^2[1 + 2\eta^2\cos^2(\omega t - kx)]$. A similar characterization holds for quantum Volkov wavepackets (see also **Annex**).[1] As we can see, the coupling of the electrical charges to the radiation field is governed by the parameter $\eta = qA_0/2mc^2$; for an electronic charge in an optical radiation field with frequency $\omega = 2\pi \cdot 10^{15}s$ and an electric field with the amplitude $E_0 = 10^9 statvolt/cm$ this parameter acquires the value $\eta = qA_0/2mc^2 = qE_0/2mc\omega \simeq 1$. In molecules and atomic clusters (as well as in atoms) such high-intensity radiation fields are more than sufficient to expel electrons and to lead to dissociation (fragmentation). Weaker radiation fields generate more interesting effects in these atomic systems; a non-relativistic approximation is valid in this case. For instance, a laser beam with intensity $10^{18} - 10^{19}w/cm^2$, generates an electric field $E \simeq$

$10^8 statvolt/cm$ and a magnetic field $10^4 Ts$, which correspond to $\eta = 0.1$ and to a non-relativistic approximation. In atomic nuclei, a laser beam intensity $10^{20} w/cm^2$ or more (electric field higher than $E = 10^9 statvolt/cm$) leads to a value of the parameter η much smaller than unity and a proton coupling ($\geq 1MeV$) comparable to the cohesion energy per nucleon ($8 - 10MeV$); it follows that the disrupting effects of a radiation field together with the binding nuclear forces may be treated in the atomic nuclei in the non-relativistic approximation too. Henceforth, we assume electrical charges moving in molecules, atomic clusters and atomic nuclei in the non-relativistic limit.

It is worth noting that, while the motion along the z-axis is performed under the action of the electric field, with an average velocity $qE_0/m\omega = c\eta$ (which agrees with the exact solution $z = -2\eta\lambda \sin(\omega t - kx)$ given above[1]), the motion along the x-axis is due to a combined effect of the electric and magnetic field; in the non-relativistic limit the drift along the x-axis is vanishing ($c \to \infty$, $\eta \to 0$), while the motion along the z-axis (along the electric field) is preserved; indeed, the effect of the magnetic field is diminished by the factor v/c in the non-relativistic limit of the Lorentz force.

With an average (non-relativistic) velocity $v = qE_0/m\omega$ the charge goes over a distance $d = v/\omega = qE_0/m\omega^2 = 2\eta\lambda$ in a period ω^{-1}, where $\lambda = c/\omega$ is the radiation wavelength; for moderate fields $E \simeq 10^8 statvolt/cm$ the parameter η acquires the value $\eta = 0.1$ (for electron), which gives $d = 0.2\lambda$; for optical radiation ($\lambda = c/\omega = 5 \times 10^{-6} cm$) this distance is much larger than the atomic and molecular (or nuclear) dimension; for an ionic charge d is of the order $10^{-8} cm$, which is comparable to atomic and molecular dimensions; a similar situation occurs in atomic nuclei. It follows that in one radiation period the charge covers many times the atomic or molecular (or nuclear) linear dimensions; under these circumstances, the energy of the charge in the radiation field $qA_0 \cos(\omega t - kx)$ is added to the (preserved) quantum energy levels E_n, *i.e.* we may write

$$W_n = E_n + qA_0 \cos(\omega t - kx) \ ; \tag{2}$$

moreover, for relevant distances much shorter than the radiation wavelength (dipolar approximation) we may write also

$$W_n = E_n + qA_0 \cos \omega t \ ; \tag{3}$$

the corresponding wavefunctions read

$$\psi_n = e^{-\frac{i}{\hbar}(E_n t + \frac{qA_0}{\omega} \sin \omega t)} \varphi_n(\mathbf{r}_1, \mathbf{r}_2, ...) \ , \tag{4}$$

where φ_n are the time-independent wavefunctions (spins included).

The wavefunction given by equation (4) can be represented as a series of Bessel functions,

$$\psi_n = \sum_{m=-\infty}^{+\infty} J_{-m}\left(\frac{qA_0}{\hbar\omega}\right) e^{-\frac{i}{\hbar}(E_n - m\hbar\omega)t} \varphi_n(\mathbf{r}_1, \mathbf{r}_{2,}...) \ ; \tag{5}$$

in the presence of the radiation field, the wavefunctions become superpositions of wavefunctions with energies $E_n - m\hbar\omega$; these superpositions are very dense, because, usually $|E_n| \gg \hbar\omega$; we can see that each energy level E_n is splitted in an infinite number of densely-distributed energy levels $m\hbar\omega$, consisting of an undetermined number m of (optical) photons $\hbar\omega$; the external radiation field both increases and decreases the original energy levels ($-\infty < m < +\infty$).

[1]For $z = f(t, x)$ the velocity is calculated by $v_z = \frac{dz}{dt} = \frac{\partial z}{\partial t} + v_x \frac{\partial f}{\partial x}$, and similarly for v_x for a function $x = g(t, x)$.

The original energy levels are negative, $E_n < 0$, as for any bound assembly of particles. Among the new energy levels $E_n - m\hbar\omega$ there exist energies $E_{nf} + Q_{nf}$, where $E_{nf} < 0$ is the binding energy of free fragments and $Q_{nf} > 0$ is the released energy, such as

$$E_n - m\hbar\omega = E_{nf} + Q_{nf} \ , \tag{6}$$

or

$$m = -\frac{E_{nf} - E_n + Q_{nf}}{\hbar\omega} \ ; \tag{7}$$

we note that this m depends on the original state n. Usually, $E_{nf} \geq E_n$, so that $m < 0$. We assume that the energy levels E_n and the wavefunctions $\varphi_n(\mathbf{r}_1, \mathbf{r}_{2,}, ...)$ correspond to N nucleons for atomic nuclei, or to N atoms in atomic clusters, or to N electrons for molecules or atoms; we assume further that an atomic nuclei with N nucleons may fission in a number of fragments with N_1, N_2, ... nucleons, $N = N_1 + N_2 + ...$, with wavefunctions $\varphi_1(\mathbf{r}_1, \mathbf{r_2}, ...\mathbf{r}_{N_1})$, $\varphi_2(\mathbf{r}_{N_1+1}, \mathbf{r}_{N_1+2}, ...\mathbf{r}_{N_1+N_2})$, and so on; a similar partition may exist for molecules, where, in general, we may include the nuclei coordinates; for atoms there exist only two such wavefunctions, one corresponding to a number of released electrons, the other corresponding to the resulting ion. For identical fragments the corresponding wavefunctions are properly symmetrized. Under these circumstances, the amplitude of fragmentation is given by

$$A_{nf} = J_{-m}\left(\frac{qA_0}{\hbar\omega}\right) e^{-\frac{i}{\hbar}(E_n - E_{nf} - Q_{nf} - m\hbar\omega)t} F_{nf} = J_{-m}\left(\frac{qA_0}{\hbar\omega}\right) F_{nf} \ , \tag{8}$$

where

$$F_{nf} = \int d\mathbf{r}_1 d\mathbf{r}_2 ... d\mathbf{r}_N \varphi_1^*(\mathbf{r}_1, \mathbf{r_2}, ...\mathbf{r}_{N_1}) \varphi_2^*(\mathbf{r}_{N_1+1}, \mathbf{r}_{N_1+2}, ...\mathbf{r}_{N_1+N_2}) ... \varphi_n(\mathbf{r}_1, \mathbf{r}_{2,}...) \tag{9}$$

is the fragmentation matrix element. Since, usually, $qA_0 \gg \hbar\omega$ we can use the asymptotic expression for the Bessel function, and get

$$A_{nf} = \sqrt{\frac{2\hbar\omega}{\pi q A_0}} \cos\left(\frac{qA_0}{\hbar\omega} - \frac{\pi}{2}m - \frac{\pi}{4}\right) F_{nf} \ ; \tag{10}$$

we may take $E_{nf} = E_n$ and the fragmentation amplitude becomes

$$A_{nf} = \sqrt{\frac{2\hbar\omega}{\pi q A_0}} \cos\left(\frac{qA_0 + \frac{\pi}{2}Q_{nf}}{\hbar\omega} - \frac{\pi}{4}\right) F_{nf} \ . \tag{11}$$

A qualitative estimation shows that the fragmentation matrix element F_{nf} (which gives the momentum conservation) is approximately equal to unity in absolute value. The fragmentation probability is given by

$$|A_{nf}|^2 = \frac{2\hbar\omega}{\pi q A_0} \cos^2\left(\frac{qA_0 + \frac{\pi}{2}Q_{nf}}{\hbar\omega} - \frac{\pi}{4}\right) |F_{nf}|^2 \ . \tag{12}$$

For small values of the released energy Q_{nf} and $|F_{nf}| = 1$, the fragmenation probability reads

$$|A_{nf}|^2 = \frac{2\hbar\omega}{\pi q A_0} \cos^2\left(\frac{qA_0}{\hbar\omega} - \frac{\pi}{4}\right) = \frac{\hbar\omega}{\pi q A_0}\left[1 + \frac{1}{2}\cos\frac{2qA_0}{\hbar\omega}\right] \ ; \tag{13}$$

we can see that the fragmentation probability in strong radiation fields depends slightly on the nature and structure of the quantum assemblies; it is almost a universal quantity, which depends only on the radiation field, as expected.

It is interesting to estimate the total probability of fragmentation; for this, we should sum over all possible fragmentation configurations in equation (12). The interaction is introduced and removed in time $T = 1/\alpha$ (and a factor $e^{\alpha|t|}$ should be inserted in the fragmentation amplitude); it produces an uncertainty $\hbar\alpha$ in the released energy and a number $\hbar\alpha/\hbar\omega$ of fragmentation states; the result of summing up over all these fragmentation configurations is the multiplication by α/ω in the constant contribution to equation (12) (the oscilalting contribution vanishes by summation); we get

$$\sum |A_{nf}|^2 = \frac{\hbar\alpha}{\pi q A_0} \; ; \tag{14}$$

and the lifetime of any assembly of bound quantum particles is $\tau = \pi q A_0/\hbar\alpha^2$. We can see that a sudden interaction ($\alpha \gg 1$) causes a very short lifetime, as expected, while an adiabatic interaction ($\alpha \to 0$) may leave the assembly unafected. In a radiation field which lasts a very long time ($\alpha \to 0$), the fragmentation probability is very small.

References

[1] M. Apostol, "Motion of an electric charge under the action of laser fields", J. Theor. Phys. **233** (2015).

Annex

The equation of motion of a charge q with mass m under the action of an electromagnetic field reads

$$\frac{d}{dt}\frac{m\mathbf{v}}{\sqrt{1-\frac{v^2}{c^2}}} = q\mathbf{E} + \frac{q}{c}\mathbf{v}\times\mathbf{H} \;, \tag{15}$$

where $\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{A}}{\partial tt}$ is the electric field, $\mathbf{H} = curl\mathbf{A}$ is the magnetic field and $\mathbf{A}$ is the vector potential (and c denotes the speed of light). Since

$$\frac{d\mathbf{A}}{dt} = \frac{\partial\mathbf{A}}{\partial t} + (\mathbf{v}grad)\mathbf{A} \tag{16}$$

and $(\mathbf{v}grad)\mathbf{A} + \mathbf{v}\times curl\mathbf{A} = grad(\mathbf{vA})$, equation () can be recast as

$$\frac{d}{dt}\left(\frac{m\mathbf{v}}{\sqrt{1-\frac{v^2}{c^2}}} + \frac{q}{c}\mathbf{A}\right) = \frac{q}{c}grad(\mathbf{vA}) \; ; \tag{17}$$

on the other hand, multiplying equation () by $\mathbf{v}$ we get the energy equation

$$\frac{d}{dt}\frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}} = q\mathbf{vE} \; . \tag{18}$$

For a vector potential $\mathbf{A}=(0,0,A_0\cos(\omega t-kx))$, an electric field $\mathbf{E}=-(1/c)\partial\mathbf{A}/\partial t=(0,0,A_0k\sin(\omega t-kx))$ and a magnetic field $\mathbf{H}=curl\mathbf{A}=(0,-A_0k\sin(\omega t-kx))$ we get from equation ()

$$\frac{d}{dt}\frac{mv_x}{\sqrt{1-\frac{v^2}{c^2}}}=\frac{q}{c}kA_0v_z\sin(\omega t-kx)\ ,$$

$$\frac{d}{dt}\frac{mv_y}{\sqrt{1-\frac{v^2}{c^2}}}=0\ , \tag{19}$$

$$\frac{d}{dt}\left(\frac{mv_z}{\sqrt{1-\frac{v^2}{c^2}}}+\frac{q}{c}A_0\cos(\omega t-kx)\right)=0\ ;$$

we may take $v_y=0$ and

$$\frac{\beta_z}{\sqrt{1-\beta^2}}=-2\eta\cos(\omega t-kx)\ \ , \tag{20}$$

or

$$\beta_z=\frac{2\eta\cos(\omega t-kx)}{\sqrt{1+4\eta^2\cos^2(\omega t-kx)}}\sqrt{1-\beta_x^2}\ \ , \tag{21}$$

where $\beta_{x,z}=v_{x,z}/c$ and $\eta=qA_0/2mc^2$. The first equation () can be written as

$$\frac{d}{dt}\frac{\beta_x}{\sqrt{1-\beta^2}}=2\eta\omega\beta_z\sin(\omega t-kx)=\frac{2\eta^2\omega\sin 2(\omega t-kx)}{\sqrt{1+4\eta^2\cos^2(\omega t-kx)}}\sqrt{1-\beta_x^2}\ ; \tag{22}$$

according to this equation β_x has a constant component beside oscillating contributions; it goes like η^2 for $\eta\rightarrow 0$ and goes to unity for $\eta\rightarrow\infty$; it follows that the constant component of the β_x is $\beta_x=\eta^2/(1+\eta^2)$, *i.e.* the drift velocity along the wave propagation direction.