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Triple coalescence singularity in a dynamical atomic process

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We show that the high energy limit for amplitude of the double electron capture to the bound state of the Coulomb field of a nucleus with emission of a single photon is determined by behavior of the wave function in the vicinity of the singular triple coalescence point.

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It is well known that the solution $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ of the Schrödinger equation for a two-electron system in the Coulomb field of infinitely heavy point nucleus is singular at the triple coalescence point $\mathbf{r}_1 = \mathbf{r}_2 = 0$ [1–4]. The wave function can be presented as a generalized power series containing logarithmic terms. The behavior of $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ near this point is not very important in calculations of the binding energy since the corresponding phase volume is small. On the contrary it becomes crucial for calculation of the local energy $E(\mathbf{r}_1, \mathbf{r}_2) = H\Psi(\mathbf{r}_1, \mathbf{r}_2)/\Psi(\mathbf{r}_1, \mathbf{r}_2)$ [4]. However the triple coalescence point did not manifest itself in a dynamical process until now.

In this letter we present for the first time an observable effect in which the interesting behavior of the two electron wave function $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ near the point $\mathbf{r}_1 = \mathbf{r}_2 = 0$ (as well as that near the double coalescence points $\mathbf{r}_1 = 0$ and $\mathbf{r}_2 = 0$) plays an important role. For that we consider the double electron capture followed by the emission of a single photon in the high energy limit. Since the first attempts to detect this process in collisions of a light atom with a heavy nucleus [5] a number of experimental [6, 7] and theoretical [8–10] papers were devoted to this reaction.

Neglecting the internal motion of the electrons in the light atom we consider the capture of two continuum electrons with equal linear momenta $\mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p}$ [8]. The process is characterized by the kinetic energy per nucleon E_N (MeV/u). The corresponding electron kinetic energies are $\varepsilon = E_N m/m_N$ where m/m_N is the ratio of the electron mass to the nucleon mass. We consider the case corresponding to nonrelativistic continuum electrons $\varepsilon \ll m$, i.e. $E_N \ll m_N$ (in the system of units with $\hbar = c = 1$), thus we put $p = (2m\varepsilon)^{1/2}$. We assume the charge Z of the heavy nucleus to be much larger than that of the light atom Z_1, i.e. $Z \gg Z_1$. On the other hand we assume Z to be small enough for the description of the bound state by the Schrödinger equation, i.e. $(\alpha Z)^2 \ll 1$, with $\alpha = 1/137$ the fine structure constant.

The energy of the emitted photon is $\omega = 2\varepsilon + I$ with $I > 0$ standing for the binding energy of the two electrons in the ground state of the heavy nucleus (we consider this very case). The momentum $\mathbf{q} = 2\mathbf{p} - \mathbf{k}$ with $\mathbf{k}$ standing for the photon momentum is transferred to the nucleus. We consider the high-energy limit of the chosen process

$$\varepsilon \gg I_1, \tag{1}$$

with I_1 standing for the single-electron binding energy. Since $Z \gg 1$ we can put $I_1 = \eta^2/2m$ with $\eta = m\alpha Z$ being the characteristic momentum of the bound $1s$ state. Thus condition (1) is equivalent to $\xi^2 \ll 1$ for

$$\xi = m\alpha Z/p. \tag{2}$$

The parameter ξ describes also the interaction between the incoming electrons and the nucleus. For $\xi^2 \ll 1$ this interaction can be treated perturbatively. Thus the electronic wave function of the initial state can be obtained by an iteration of the Lippmann–Schwinger equation

$$\Phi = \Phi_0 + GV\Phi, \tag{3}$$

with $V = V_{eN} + V_{ee}$, while V_{eN} and V_{ee} stand for the interactions between an electron and the nucleus and between the electrons correspondingly, G is the Green function of two free noninteracting electrons, while Φ_0 is the product of plane waves.

Due to conditions (1) the electrons transfer the large momentum $q \gg \eta$ to the nucleus. This can take place

in the initial or final states. The two mechanisms provide contributions of the same order of magnitude to the amplitude

$$F = \langle \Psi | \gamma | \Phi \rangle, \tag{4}$$

where γ is the operator of the interaction between the electrons and the photon, for which we assume the gradient form. Each act of exchange by the large momentum $q \gg \eta$ between the continuum electrons and the nucleus provides a small factor η^4/q^4 [11] since each of the functions G and V on the right-hand side of Eq. (3) drops as $1/q^2$. (For the Coulomb case this can be shown explicitly since the Fourier transform of the wave function drops as q^{-4}). Thus to obtain the lowest order of expansion of the amplitude (4) in powers of ξ we must include the two lowest terms of iteration of Eq. (3) putting

$$\begin{gathered} \Phi = \Phi_0 + \Phi_1; \quad \Phi_1 = \Phi_{1N} + \Phi_{1e}; \\ \Phi_{1N} = GV_{eN}\Phi_0; \quad \Phi_{1e} = GV_{ee}\Phi_0. \end{gathered} \tag{5}$$

Using Eq. (5) we can write

$$\begin{gathered} F = F_0 + F_1; \quad F_1 = F_{1N} + F_{1e}; \quad F_0 = \langle \Psi | \gamma | \Phi_0 \rangle; \\ F_{1N} = \langle \Psi | \gamma | \Phi_{1N} \rangle; \quad F_{1e} = \langle \Psi | \gamma | \Phi_{1e} \rangle, \end{gathered} \tag{6}$$

where we expect F_0 and F_1 to provide contributions of the same order.

Let us start with the calculation of the amplitude F_0. Denote $\varphi_0(i, \mathbf{p}_i) = e^{i(\mathbf{p}_i \mathbf{r}_i)}$, then $\Phi_0 = \varphi_0(1, \mathbf{p}_1)\varphi_0(2, \mathbf{p}_2)$ (recall that in our case $\mathbf{p}_1 = \mathbf{p}_2$). Below we assume that the electron which emits the photon is labelled by "1". Thus

$$F_0 = 2 \int d^3 r_1 d^3 r_2 \Psi(\mathbf{r}_1, \mathbf{r}_2) \gamma_1 \varphi_0(1, \mathbf{p}) \varphi_0(2, \mathbf{p}) \tag{7}$$

with the operator γ_1 acting on $\mathbf{r}_1$. Since $p \gg \eta$, the integral (7) over r_2 is saturated by $r_2 \sim 1/p \ll 1/\eta$, while $1/\eta$ is the characteristic scale of the bound state wave function Ψ. Keeping r_1 to be finite we can expand the function $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ near the point $r_2 = 0$. Limiting ourselves to the linear terms of the expansion we can write

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \left(1 + r_2 \frac{\partial}{\partial r_2} - \frac{(\mathbf{r}_1 \mathbf{r}_2)}{r_1} \frac{\partial}{\partial \rho}\right) \tilde{\Psi}(r_1, r_2, \rho) \Big|_{r_2 = 0}, \tag{8}$$

with $\tilde{\Psi}(r_1, r_2, \rho) = \Psi(\mathbf{r}_1, \mathbf{r}_2)$, $\rho = |\mathbf{r}_1 - \mathbf{r}_2|$. Following [11] we can present

$$\tilde{\Psi}(r_1, 0, r_1) = \lim_{\lambda \to 0} \tilde{\Psi}(r_1, 0, r_1) e^{-\lambda r_2}$$

and obtain for the corresponding contribution $F_{0\mathrm{lin}}$ to F_0 (lower index "lin" corresponds to the terms linear in r_2 in (8))

$$F_{0\mathrm{lin}} = -\frac{16\pi(\mathbf{ep})}{p^4} J_0; \quad J_0 = \int d^3 r_1 \tilde{\Psi}'_{r_2}(r_1, 0, r_1) e^{i(\mathbf{p}\mathbf{r}_1)}, \tag{9}$$

with $\mathbf{e}$ the vector of the photon polarization, $\tilde{\Psi}'_{r_2}$ denotes the partial derivative of the function $\tilde{\Psi}$ with respect to r_2 at $r_2 = 0$.

The contribution F_{1N} to the amplitude is composed by the lowest order Coulomb corrections to the plane waves, describing continuum wave functions in the amplitude F_0. Due to the operator γ the correction to the wave function of the electron "1" contains a small factor of the order ξ. Thus the amplitude F_{1N} can be presented as

$$F_{1N} = 2 \int \frac{d^3 p'}{(2\pi)^3} \times \frac{\langle \Psi | \gamma_1 | \varphi_0(1, \mathbf{p}) \varphi_0(2, \mathbf{p}') \rangle \langle \varphi_0(2, \mathbf{p}') | V_{eN}(2) | \varphi_0(2, \mathbf{p}) \rangle}{\varepsilon - p'^2/2m} \tag{10}$$

with $V_{eN}(2)$ standing for the interaction between the electron "2" and the nucleus. Straightforward calculation provides

$$F_{1N} = -\frac{16\pi\eta(\mathbf{e} \cdot \mathbf{p})}{p^4} J_1; \quad J_1 = \int d^3 r_1 \tilde{\Psi}(r_1, 0, r_1) e^{i(\mathbf{p} \cdot \mathbf{r}_1)}. \tag{11}$$

Thus

$$F_{0lin} + F_{1N} = -\frac{16\pi(\mathbf{e} \cdot \mathbf{p})}{p^4} (J_0 + \eta J_1) = 0. \tag{12}$$

Now, the last equation is due to the Kato cusp condition $\tilde{\Psi}'_{r_2}(r_1, 0, r_1) = -\eta \tilde{\Psi}(r_1, 0, r_1)$ [12] which can be viewed as the result of cancellation of the terms $1/r_2$ in the Schrödinger equation.

The value of J_1 can be obtained by integrating (11) three times in parts. This provides $J_1 = -(8\pi/p^2)\varphi'_{r_1}(r_1 = 0)$ with $\varphi(r_1) = \tilde{\Psi}(r_1, 0, r_1)$. Using the expansion

$$\tilde{\Psi}(r_1, r_2, \rho) = \left(1 - \eta r_1 - \eta r_2 + \frac{m\alpha}{2} \rho + \ldots\right) \tilde{\Psi}(0, 0, 0) \tag{13}$$

at $r_1, r_2 \to 0$ (the dots stand for nonlinear terms) [2–4] we find $J_1 = 8\pi\alpha Z N^2/p^4$, with $N^2 = \tilde{\Psi}(0, 0, 0)$ as the value of the wave function at the origin. Thus the Z dependence of the amplitudes F_{0lin} and F_{1N} is expressed by the factor $Z^2 N^2 \sim Z^5$. Both amplitudes F_{0lin} and

F_{1N} describe the contributions in which each of the electrons transfers momentum of the order $p \gg \eta$ to the nucleus, providing a factor $\sim \alpha Z$ to the total amplitude. According to (12) such contributions cancel.

However there is another contribution to the amplitude F_{eN} in which one of the captured electrons looses its large momentum p by transferring it to the second electron. The latter transfers the momentum $2\mathbf{p}$ to the nucleus. Such contribution has the same energy dependence as the amplitude, depending on Z as Z^4, since the electron interaction with the nucleus, proportional to αZ is replaced by the electron–electron interaction which is proportional to α. This contribution is described by the nonlinear terms of expansion (13) for the wave function denoted by dots on the right-hand side. However due to the singularity at the point $r_1 = r_2 = \rho = 0$ the expansion (13) beyond the linear terms is not the Taylor series and the coefficients cannot be presented in terms of partial derivatives. The leading nonlinear terms are obtained in [2–4].

The contribution F_{1e} can be calculated in similar way. It also behaves as Z^4, e.g.

$$F_{1e} = -16\pi^2 \alpha \eta N^2 (\mathbf{e} \cdot \mathbf{p})/p^7. \qquad (14)$$

Finally, the high energy limit of the amplitude is

$$F = 2\Big(\int d^3r_1 d^3r_2 \Psi(\mathbf{r}_1, \mathbf{r}_2) \times$$

$$\times \gamma_1 e^{i(\mathbf{p}_1\mathbf{r}_1)+i(\mathbf{p}_2\mathbf{r}_2)} - 16Z\Lambda - 2\Lambda \Big), \qquad (15)$$

with $\mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p}$, $\Lambda = 4\pi^2 \alpha \eta N^2 (\mathbf{e} \cdot \mathbf{p})/p^8$. The three terms in brackets correspond to the contributions F_0, F_{1N} and F_{1e}. Since the integral is determined by $r_1 \sim r_2 \sim p^{-1} \to 0$, one should use generalized power series found in [2–4] for calculations.

Equation (15) is true for $\omega \ll \eta$. At larger values of photon energies there are some additional terms corresponding to the two-step mechanism [13] in which the process can be viewed as the eN scattering followed by quasifree emission of the photon. The effects of internal motion of the target electrons [10] (in experiments the light atom is the target) provide the contributions of the order $m\alpha Z_1/p$ being thus beyond the high energy limit. These effects can be incorporated into Eq. (15).

In conclusion we recognize that the amplitude F in Eq. (15) depends sensitively on behavior the two electron wave function at the points $\mathbf{r}_1 = 0$, $\mathbf{r}_2 = 0$ and $\mathbf{r}_1 = \mathbf{r}_2 = 0$. So the measurement of the cross sections for double electron capture with emission of a single photon in the high energy limit gives information on the wave function at the double and triple coalescence points. Such a possible experimental access to the triple coalescence point was not yet proposed in literature. In the experiments [5–7] the projectiles which captured two electrons were registered in coincidence with the photon. This enables to distinguish the process among the other capture processes in spite of its small cross section. Detection of the process at small values of ξ would be a bright manifestation of the three particle singularity in a dynamical process.

Of course, Eq. (4) describes also the amplitude of double photoionization with momenta of the outgoing electrons $\mathbf{p}_1 = \mathbf{p}_2$, $|\mathbf{p}_i| \gg \eta$. It determines the double differential cross section $d\sigma/d\varepsilon d\tau$ at $\varepsilon_1 = \varepsilon_2$, $\tau = (\mathbf{p}_1\mathbf{p}_2)/p_1p_2 = 1$, which thus depends on the wave function behavior at the triple coalescence point. However this region provides a minor contribution to the differential cross section $d\sigma/d\varepsilon$, which runs beyond the high energy limit. The contribution to the double photoionization cross section is still smaller. On the contrary, in the double electron capture with single photon emission the triple coalescence singularity determines the high energy limit of the cross section.

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