Interpretation of a Schrödinger-like equation derived from a non-Markovian process

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Hydrodynamical equations for the probability density ρ and the local velocity $\mathbf{v}$ of a non-Markovian stochastic process have been recently obtained. The corresponding complex equation in terms of the wave function ψ coincides with the Schrödinger equation if the first-order terms only are retained. The second-order terms vanish and the third-order terms could be considered as QED-type corrections. To obtain the coefficient D_4 of the third-order term the probability density ρ for a free particle is obtained by stochastic electrodynamics. This solution is substituted in the new complex equation, thus obtaining D_4. By this coefficient the calculation of the Lyman-α wavelength is in agreement with the best direct measurements for the transition $2P \rightarrow 1S$. The $1S$ displacement is 1% of the QED value for the Lamb shift. It is suggested how the new negative contribution could be the difference between the $(1+0.01)$ QED value for the $3S$ state and the corresponding experimental value, which is 20% less than that given by QED.

I. INTRODUCTION

In a recent paper[1] the density-gradient expansion has been rigorously proved, and the conditions (or limitations) under which the expansion is valid have been given. The validity of the density-gradient expansion has been extended to non-Markovian stochastic processes and, as an application, new hydrodynamical equations for the probability density ρ and the local average velocity $\langle \mathbf{v} \rangle$ have been derived. In a motion with inertia and without friction it holds $\langle \mathbf{v} \rangle = \nabla\varphi$ where φ is the velocity potential and the derived hydrodynamical equations are[1]

$$\partial_t \rho + \nabla\cdot(\rho\nabla\varphi) = 0 \ , \tag{1}$$

$$\partial_t \varphi + \tfrac{1}{2}(\nabla\varphi)^2 + V + \tfrac{1}{4}D_2^2\left[\frac{1}{2}\left[\frac{\nabla\rho}{\rho}\right]^2 - \frac{\nabla^2\rho}{\rho}\right] - \frac{D_2 D_4}{4\rho}\left[\frac{1}{\rho}\nabla^2\nabla^2\rho + \nabla^2\left[\frac{1}{\rho}\nabla^2\rho - \frac{1}{\rho^2}(\nabla\rho)^2\right]\right] , \tag{2}$$

where we have neglected the terms in D_4^2 because, *a posteriori,* they give negligible corrections and

$$D_2 = \tfrac{1}{3}\lambda c, \quad D_4 = \tfrac{1}{30}\lambda^3 c \ , \tag{3}$$

λ being the mean free path (or extintion length for the memory of diffusion) of the random-walk equivalent to the considered stochastic process and V the external potential per unit mass.

To derive Eqs. (1)–(3) use has been made of the Taylor expansion of the probability density ρ

$$\rho(\mathbf{r}-\boldsymbol{\lambda}) = \rho(\mathbf{r}) - \boldsymbol{\lambda}\cdot\nabla\rho + \tfrac{1}{2}\boldsymbol{\lambda}\boldsymbol{\lambda}:\nabla\nabla\rho - \tfrac{1}{6}\boldsymbol{\lambda}\boldsymbol{\lambda}\boldsymbol{\lambda}\vdots\nabla\nabla\nabla\rho + \cdots \ . \tag{4}$$

The first two terms of Eq. (4) lead to Eqs. (1) and (2) without the terms in the large square brackets. These two real equations are equivalent to a single Schrödinger-like, complex equation

$$iD_2\partial_t\psi = -\tfrac{1}{2}D_2^2\nabla^2\psi + \frac{V}{m}\psi \ , \tag{5}$$

as can be shown by the position

$$\psi = \rho^{1/2}\exp(i\varphi/D_2) \ . \tag{6}$$

Full agreement with the Schrödinger equation is obtained if

$$\lambda = \frac{3\hbar}{mc} \ , \quad \text{hence} \ , \quad D_2 = \frac{\hbar}{m} \ . \tag{7}$$

Let us retain four terms of the expansion as explicity written in Eq. (4). The contributions coming from the third term of Eq. (4) vanish and those coming from the fourth term are contained in the second set of large square brackets of Eq. (2).

To solve Eqs. (1) and (2) it is convenient to eliminate φ and the following equation has been derived[1] by the position (6):

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + m\psi V - \tfrac{1}{4}\hbar D_4\left[\frac{1}{\rho}\nabla^2\nabla^2\rho + \nabla^2\left[\frac{1}{\rho}\nabla^2\rho - \frac{1}{\rho 2}(\nabla\rho)^2\right]\right]\psi \ . \tag{8}$$

By assuming the same extintion length $\lambda_2=\lambda_4=\lambda$ for both D_2 and D_4, the following expression for D_4 has been obtained in Ref. 1 by Eqs. (3) and (7):

$$D_4=\frac{9}{10}\frac{\hbar^3}{m^3c^2} . \tag{9}$$

As a remark, we observe that, even by a position more general than (6), it is not possible to obtain an equation in ψ only (i.e., without ρ), for instance, of the kind[2]

$$iD_2\partial_t\psi=-\tfrac{1}{2}D_2^2\nabla^2\psi+V\psi-\tfrac{1}{2}D_2D_4\nabla^2\nabla^2\psi , \tag{10}$$

which is the equation which generates hydrodynamical equations most similar (but not just equal) to Eqs. (1) and (2).

In fact, Eqs. (1) and (2) together with the general position

$$\psi=\rho^{1/2}\exp[iF(\varphi)] ,$$

where $F(\varphi)$ is an *a priori* arbitrary function of φ, imply an equation containing terms such as $\nabla^2\psi$, $\nabla^2\nabla^2\psi$, $\nabla^2(1/\rho)(\nabla\rho)^2$, $\nabla^2[(1/\rho)\nabla^2\rho]$ and a combination of $\partial_t\psi$ and $V\psi$ whose coefficient's ratio is $-im/F'$. The condition that this ratio be as in the Schrödinger equation implies $F=\varphi m/\hbar$, i.e., position (6) with D_2 as in (7). As a consequence no additional terms arise from the general position to eliminate the explicit ρ dependence and one is left with just Eq. (8) once the terms in D_4^2 have been neglected.

By the same argument, the further generalized position

$$\varphi=\rho^{1/2}\exp[iF(\rho,\varphi)]$$

implies $F=(m/\hbar)\varphi+A(\rho)$, $A(\rho)$ being an arbitrary function of ρ. The condition of the existence of just the term $-\hbar^2\nabla^2\psi/2m$ implies $A=0$.

II. PERTURBATIVE CALCULATIONS FOR THE HYDROGEN ATOM

Equation (8) can be formally treated as a Schrödinger equation with perturbation $H_1(\rho)$ given by

$$H_1(\rho)\psi=-\frac{9\hbar^4}{40m^3c^2}\psi\left[\frac{1}{\rho}\nabla^2\nabla^2\rho+\nabla^2\left[\frac{1}{\rho}\nabla^2\rho-\frac{1}{\rho^2}(\nabla\rho)^2\right]\right] \tag{11}$$

with $\rho=\psi\psi^*$.

To evaluate the contribution of this term to the energy levels of the hydrogen atom, standard nondegenerate perturbation theory can be applied once $H_1(\rho)$ shows invariance under rotations and the divergences [*a priori* present in Eq. (11)] are integrable. This is certainly true for the energy levels w_1 and w_2 relative to the states u_{2lm} by using the averaged expression

$$\rho_{2l}=\int|u_{2lm}|^2d\Omega/4\pi .$$

In these cases the corrections to the energy levels are given by

$$\delta w_n=\int d^3\mathbf{x}\,u^*_{nlm}(x)H_1(\rho_{nlm})u_{nlm}(x) . \tag{12}$$

The other cases could be treated by using nonvanishing superposition of pure states u_{nlm} with u_{100} and then by taking ρ averaged over its angular part.

However, it is not necessary to exploit these cases since the first two mentioned cases give results which are not in agreement with experiments. In fact, Eq. (12) applied to the ground state of a hydrogen atom gives

$$\delta w_1=\tfrac{36}{5}\alpha^2w_1 \tag{13}$$

and applied to the first excited l state gives

$$\delta w_2=\tfrac{3}{40}\alpha^2w_1 , \tag{14}$$

$\alpha=e^2/\hbar c$ being the fine-structure constant and $w_1=-Rhc$ the ground energy level of the hydrogen atom (R is the Rydberg constant). We notice that the result (13) is quite different from the fine-structure result $\delta w_{1D}=\frac{1}{4}\alpha^2w_1$ derived from the Dirac equation.[3]

If one considers the wavelength relative to the transition $2P\rightarrow 1S$

$$\Delta w=w_2+\delta w_2-w_1-\delta w_1=Rhc(0.75+\tfrac{57}{8}\alpha^2) , \tag{15}$$

with $R=R_\infty m_p/(m_e+m_p)$, one finds the value 1215.0(7) Å by using the recent values[4] of R_∞, while the generally admitted experimental value[3,5] is 1215.6(8) Å. The fifth significant figure is different and this is sufficient to rule out the validity of the correction terms. The explanation of this disagreement lies in the doubt already expressed after Eq. (38) of Ref. 1, i.e., that the number of adjacent cells (across which the diffusion is considered) is not well specified. In other words, what is unknown is the distance λ (called mean free path) at which there is extintion of the diffusion memory. In terms of the equivalent random walk, λ corresponds to a deviation of the initial velocity by an angle $\pi/2$. This uncertainty is already contained in the first coefficient D_2 and that is why, in preceding works[6] D_2 has been left unknown and determined experimentally (i.e., to be equal to that contained in the Schrödinger equation). Now the point is that the extintion length λ_2 for the first coefficient D_2 may be different from λ_4 relevant to D_4. To have an indication of the D_4 value we find, in the next section, the correct solution of the free particle in stochastic electrodynamics (SED). This solution has its own validity since we have never seen it published in international journals.

III. THE PROPAGATOR OF A FREE PARTICLE IN STOCHASTIC ELECTRODYNAMICS

The free diffusion in SED has been studied by Pesquera and Santos[7] as the limit of a harmonically bound electron when its characteristic frequency goes to zero. However, this is not correct because the stochastic process for both velocity and position is stationary in a bound state but not for a free particle. The propagator for a free particle has also been given by one of us[8] well aware of this fact [see what is said between Eqs. (9) and (10) of Ref. 8]. The stochastic process for the velocity was related in Ref. 8 to that of the acceleration whose process is stationary. Consequently, the solution for the velocity was correct. But then, also because the same formal connection appeared between position and velocity, the inverse Wiener-

Khintchin relation was applied to connect the dispersion in position to the velocity correlation. But the latter is not correct and the leading term proportional to t^2 was missing. Fortunately, although what was called the "elementary" propagator was wrong, what was called the "effective" propagator was correct because the initial distribution of the velocities and the main motion with inertia implied the missing term proportional to t^2.

A correct procedure to obtain the propagator has been given by de la Peña in a preprint[9] never published. However, de la Peña ascribed the difficulties of SED to the use of the Abraham-Lorentz equation and used, instead, an integral equation with consequent mass renormalization and Yukawa distribution for probability density of the electron charge. All this is useless. What is important is the truncation of the zero-point-field (ZPF) spectral probability density which has to occur in correspondence of the spin frequency $\omega_c = mc^2/\hbar$ because this is the maximum frequency radiated by the electron if it has a realistic version of Dirac's Zitterbewegung. The ZPF spectrum could also be increasing after ω_c because of the radiation of the quark's Zitterbewegung, but the effect of this additional radiation is negligible in correspondence of the atomic frequencies. The effect of the truncation at ω_c has already been studied and a new effect has been foreseen.[10] Vice versa, the simple assumption of a truncation at ω_c eliminates any divergence and leads to what is called the Zitterbewegung assumption because the consequent mean-square value of the speed is so high that it is practically not influenced by the nucleus and the other electrons in an atom. Once assumed the truncation at ω_c the use of either the Abraham-Lorentz equation or of an integral equation (as used in Refs. 9 and 10) only gives negligible corrections compared with the results obtainable from Newton's law we might adopt in the following:

$$\mathbf{a}(t) = e\mathbf{E}(t)/m \ , \tag{16}$$

where $\mathbf{a}$, e, m are the acceleration, the charge, and the mass, respectively, of an electron in the stochastic field $\mathbf{E}$. The time integrations over t give

$$\mathbf{v}(t) = \mathbf{v}(0) + \frac{e}{m}\int_0^t dt' \mathbf{E}(t') \ , \tag{17}$$

$$\mathbf{r}(t) = \mathbf{r}(0) + \mathbf{v}(0)t + \frac{e}{m}\int_0^t dt' \int_0^{t'} dt'' \mathbf{E}(t'') \ . \tag{18}$$

Taking the ensemble averages of Eqs. (17) and (18) gives

$$\langle \mathbf{v}(t) \rangle = \mathbf{v}(0) \ , \tag{19}$$

$$\langle \mathbf{r}(t) \rangle = \langle \mathbf{r}(0) \rangle + \langle \mathbf{v}(0) \rangle t = \mathbf{r}_0 + \mathbf{v}_0 t \ , \tag{20}$$

because $\langle \mathbf{E}(t) \rangle = 0$.

We now consider the component along the x axis of Eq. (18) and calculate the mean-square deviation

$$\Delta^2 x = \langle x^2(t) \rangle - \langle x(t) \rangle^2$$
$$= \left\langle x^2(0) + 2x(0)v(0)t + v^2(0)t^2 \right\rangle + \frac{e^2}{m^2}\int_0^t dt' \int_0^{t'} dt'' \int_0^t dt''' \int_0^{t'''} dt'''' \left\langle E_x(t'') E_x(t'''') \right\rangle - x_0^2 - 2x_0 v_0 t - v_0^2 t^2 \ . \tag{21}$$

We now exploit the power spectral density of the ZPF and its consequent correlation with the assumed cutoff

$$\langle E_x(t'') E_x(t'''') \rangle = \int_0^{\omega_c} d\omega \frac{2\hbar}{3\pi c^3} \omega^3 \cos[\omega(t'' - t'''')] \ . \tag{22}$$

Substituting Eq. (22) in Eq. (21) and performing the easy integrations over t gives

$$\Delta x_t^2 = \Delta x_0^2 + 2\Delta(x_0, v_0)t + \Delta v_{x0}^2 t^2 + \frac{e^2}{m^2}\int_0^{\omega_c} d\omega \frac{2\hbar}{3\pi c^3} \left[\frac{2}{\omega}[1 - \cos(\omega t)] - 2t \sin(\omega t) + \omega t^2 \right] , \tag{23}$$

where $\Delta(x_0, v_0) = \langle x(0)v(0) \rangle - \langle x(0) \rangle \langle v(0) \rangle$ is usually small. Neglecting it and integrating over ω gives

$$\Delta x_t^2 = \Delta x_0^2 + \Delta v_{x0}^2 t^2 + \frac{2e^2\hbar}{3\pi m^2 c^3}\{2\gamma + 2\ln(\omega_c t) - 2\,\mathrm{Ci}(\omega_c t) + 2[\cos(\omega_c t) - 1] + \tfrac{1}{2}\omega_c^2 t^2\} \ , \tag{24}$$

where Ci is the cosine integral and $\gamma = 0.5772$ is the Euler constant.

$$\Delta x_t^2 \simeq \Delta x_0^2 + t^2\left(\Delta v_{x0}^2 + \frac{1}{3\pi}\alpha c^2\right) \ , \quad \omega_c t \gg 1 \ . \tag{25}$$

For $\omega_c t \ll 1$ it is more convenient to start from Eq. (23) in which we expand $1 - \cos(\omega t)$ and $t \sin(\omega t)$ to the fourth order in t. The easy integration gives

$$\Delta x_t^2 = \Delta x_0^2 + \Delta v_{x0}^2 t^2 + \frac{\alpha}{6\pi} c^2 \omega_c^2 t^4 \ , \quad \omega_c t \ll 1 \ . \tag{26}$$

IV. EVALUATION OF THE COEFFICIENT D_4

Our claim is that Eq. (8) is more refined than Schrödinger's and that the small corrective terms have to be added to all the others found in quantum mechanics. What was wrong in Ref. 1 was the assumption that the extinction length for λ_2 in $D_2=\frac{1}{3}\lambda_2 c$ was equal to the λ_4 in $D_4=\frac{1}{30}\lambda_4^3 c$. We have found in Sec. III an explicit solution for the free particle in the context of the same stochastic process with inertia by which Eq. (8) has been derived. We therefore exploit this solution to evaluate the unknown coefficient D_4.

Since $x(t)$ and $v_x(t)$ in Sec. III are both linear functionals of $E_x(t)$ [see Eqs. (17) and (18)] and $E_x(t)$ is Gaussian, all the moments of x and v_x are related by the laws that correspond to a bivariate Gaussian distribution. We are interested here in the marginal probability density of x only, given by

$$\rho(x,t)=\frac{1}{(2\pi)^{1/2}\Delta x_t}\exp\left[-\frac{x^2}{2\Delta x_t^2}\right], \tag{27}$$

where Δx_t is given by Eq. (24) and we have chosen, for simplicity, $x_0=v_0=0$. For long times Δx_t is given by Eq. (25) which is just equal to the solution of the only leading part of Eq. (8), i.e., of the Schrödinger equation. The corresponding solution for ψ is

$$\psi(x,t)=\left[(2\pi)^{1/2}\Delta x_0\left[1+\frac{2i}{m\hbar}(\Delta p^*)^2 t\right]\right]^{-1/2} \times\exp\left[-\frac{x^2}{4\Delta x_0^2}[1+2i(\Delta p^*)^2 t/m\hbar]^{-1}\right], \tag{28}$$

where

$$(\Delta p^*)^2=\Delta p_0^2+\frac{\alpha}{3\pi}m^2c^2 . \tag{29}$$

The above solution is obtainable from the Schrödinger equation and initial conditions characterized by a dispersion $\Delta x(0)$ in position and a dispersion Δp^* in momemtum related by

$$\Delta x_0\Delta p^*=\hbar/2 . \tag{30}$$

The correction terms due to D_4 in the complete Eq. (8) reduce appreciably the diffusion for short times but they are negligible for long times as appears from the comparison of Eq. (24) with Eq. (25). For short times we have still the solution (28) but with [see Eq. (26)]

$$(\Delta p^*_{t\to 0})^2=(\Delta p_0)^2+\frac{\alpha}{6\pi}m^2c^2\omega_c^2 t^2 . \tag{31}$$

Substituting Eq, (28) with Eqs. (29) and (31) in Eq. (8) gives, for $x\to 0$ and in the limit for short t values,

$$(\Delta p_0)^2/\hbar m=2\Delta x_0^2(\hbar/m)-3D_4/\Delta x_0^4 . \tag{32}$$

By Eqs. (29) and (30) we get Δp_0 so that Eq. (32) gives

$$D_4=\frac{4\alpha}{9\pi}\frac{mc^2}{\hbar}\Delta x_0^4 . \tag{33}$$

Since the solution obtained corresponds to the wave packet having the minimum initial indetermination, the Δx_0 has to be equal to the Compton radius R_c because all of our procedure is based on the realistic interpretation of the Dirac's Zitterbewegung. The Compton radius R_c can be related to the spin radius $R_s=\hbar/mc$ by assuming a uniform distribution of the spin axes between $\theta=0$ and $\pi/2$

$$R_c=\int_0^{\pi/2}d\theta\sin\theta R_s\cos\theta=\tfrac{1}{2}R_s=\frac{\hbar}{2mc} . \tag{34}$$

Taking $\Delta x_0=R_c$, Eq. (33) gives

$$D_4=\frac{\alpha}{36\pi}\frac{\hbar^3}{m^3c^2} , \tag{35}$$

which is $\alpha/(32.4\pi)$ times the preceding value used in Ref. 1. The corresponding increase of the $1S$ state is given by Eq. (13) multiplied by $\alpha/(32.4\pi)$. The result in frequency is

$$\nu=h^{-1}\delta w_1=\frac{1}{12\pi}\alpha^3 Rc=90.3875\ \text{MHz} , \tag{36}$$

which is 1% of the Lamb shift for the $1S$ state.[11]

At this small level the wavelength corresponding to the $2P\to 1S$ transition is in agreement with the *direct* measurement.[5] We now have to compare our results with the Lamb shift values.

Our contribution is additional to all known contributions, as the Darwin term, the spin-orbit coupling, the relativistic corrections, the Lamb shift. The first mentioned contribution also came from a first-order expansion of a stochastic process and we trust them. The Lamb shift should be calculated in the same framework of a stochastic process. If we consider as exact the QED calculations of the Lamb shift, the agreement between the experimental and QED values for the $1S$ state is such that our additional contribution should be ruled out. However, it is known that the Lamb shift for the $3S$ state calculated by QED is 20% higher than the experimental value.[12] Our negative result (reduced for the $3S$ state) is such that a better agreement between theory and experiment should be found for the $3S$ state. It is therefore reasonable to raise the doubt on the Lamb shift calculations. It would be a sufficient increase of 1% to have agreement with the experimental value for the $1S$ state if we include our negative contribution. A rough estimation for $2S$ and $3S$ states gives a positive answer. To calculate our contribution for these states in a reliable value we are developing a new perturbative method because the standard procedure cannot be applied to the "mixed" Eq. (8), partially in ψ and partially in ρ.

V. CONCLUSIONS

The high value for D_4 found in Ref. 1 is due to the assumption of a mean free path (or extinction length for the memory) λ_4 equal to λ_2 (where $D_2=\frac{1}{3}\lambda_2 c$). This high value can be excluded by the calculation of the wavelength associated to the transition $2P-1S$ which is in disagreement with the direct experimental value for this transition, as shown in Sec. II. The mean-square dispersion Δx_t^2 for a free particle in the environment of stochas-

tic electrodynamics has been calculated in Sec. III. This has its own interest because there was not a correct treatment in the international literature.

The result of Sec. III has been used in Sec. IV to evaluate the coefficient D_4 on the basis that Eq. (8) has been obtained by the same stochastic process that leads to the solution (27) for the probability density ρ of a free particle. For both $\omega_c t \gg 1$ and $\omega_c t \ll 1$ (where ω_c is the spin frequency $mc^2/\hbar$), our solution (27) for ρ is approximately equal to that of a free particle obtained by the "pure" Schrödinger equation [given by the leading part of our Eq. (8)]. The correction due to D_4 vanishes for $\omega_c t \gg 1$ while it is important, and negative, for $\omega_c t \ll 1$. We therefore took the uncertainty principle to connect the dispersions Δx_0 and Δp^* in correspondence of the solution for $\omega_c t \gg 1$. Then we substituted the solution for $\omega_c t \ll 1$ in Eq. (8) and we got Eq. (33) and finally Eq. (35) by choosing $\Delta x_0 = R_c$ where R_c is the Compton radius. By this value Eq. (8) becomes

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + m\psi V - \frac{\alpha}{144\pi}\frac{\hbar}{m^3c^2}\left[\frac{1}{\rho}\nabla^2\nabla^2\rho + \nabla^2\left[\frac{1}{\rho}\nabla^2\rho - \frac{1}{\rho^2}(\nabla^2\rho)^2\right]\right]\psi \,. \tag{37}$$

We claim that this should be a quantum equation more refined than Schrödinger's. Obviously the electron has a polarizable spin, then the relativistic corrections should be taken into account so that a better, and we consider exhaustive, *first-order* quantum equation is that of Dirac. Since the correction terms due to Eq. (37) are very small, they can simply be added to those given by the Dirac equation. Then there are the radiative QED corrections due to the vacuum fluctuations. In order to be coherent with the stochastic approach, the radiactive corrections should be calculated by the zero-point field acting on an electron moving along a circle with the light speed, in agreement with the Zitterbewegung obtained from the Dirac equation.[13] If we consider the QED calculations for the Lamb's shift, there is agreement between QED and experiments for the $1S$ and $2S$ states but the QED value is 20% higher than the experimental value for the $3S$ state. We suggest that another increase of 1% plus our negative contribution can give agreement with all the states. To have a sure answer we are developing a new perturbative method because the standard one is not applicable to Eq. (37), in which ρ appears in the denominator, for the $2S$ and $3S$ states.

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