Corrections to the energy levels of a spin-zero particle bound in a strong field

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Formulas for the corrections to the energy levels and wave functions of a spin-zero particle bound in a strong field are derived. The general case of the sum of a Lorentz-scalar potential and zero component of a Lorentz-vector potential is considered. The forms of the corrections differ essentially from those for spin-$\frac{1}{2}$ particles. As an example of application of our results, we evaluated the electric polarizability of a ground state of a spin-zero particle bound in a strong Coulomb field.

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I. INTRODUCTION

As known, in many cases the perturbation theory (PT) is a very fruitful method to obtain analytic results for various corrections. The formulas of PT for the Dirac equation are similar to that for the Schrödinger equation and have simple forms (see, e.g., [1,2]). However, it is essentially more complicated to derive the formulas of PT for the Klein-Gordon-Fock equation because this equation contains a second derivative over time. In the present paper, we derive the first- and second-order corrections to the energy levels, and the first-order correction to the wave function of a spin-zero particle bound in a strong field. We consider a general case of a sum of the Lorentz-scalar and the Lorentz-vector potentials. This may be useful at the consideration of the effects of the strong interaction in pionic atoms. Using our formula for the correction to the energy level, we evaluate the electric polarizability of a ground state of a spin-zero particle bound in a strong Coulomb field.

II. PERTURBATION THEORY

The relativistic equation for the wave function of a spin-zero particle (Klein-Gordon-Fock equation) bound in the external time-independent field has the form

$$\left[\left(i\frac{\partial}{\partial x^{\mu}} - eA_{\mu}(\mathbf{r})\right)^2 - m^2 - 2mV(\mathbf{r})\right]\Psi(\mathbf{r},\mathbf{t}) = 0, \qquad (1)$$

where $V(\mathbf{r})$ is the Lorentz-scalar potential, $A_{\mu}(\mathbf{r})$ is the Lorentz-vector potential, e and m are the charge and mass of the particle, respectively; we set $\hbar = c = 1$. The corresponding current, which obeys the continuity equation, reads

$$J_{\mu} = \Psi^*(\mathbf{r},\mathbf{t}) i \frac{\overleftrightarrow{\partial}}{\partial x^{\mu}} \Psi(\mathbf{r},\mathbf{t}) - 2eA_{\mu}(\mathbf{r})|\Psi(\mathbf{r},\mathbf{t})|^2. \qquad (2)$$

For $\boldsymbol{A}=0$, the solution with the fixed energy E_n, $\Psi(\mathbf{r},\mathbf{t}) = \exp(-iE_n t)\Phi_n(\mathbf{r})$, obeys the equation

$$\{[E_n - U(\mathbf{r})]^2 - \mathbf{p}^2 - m^2 - 2mV(\mathbf{r})\}\Phi_n(\mathbf{r}) = 0, \qquad (3)$$

where $U(\mathbf{r}) = eA_0(\mathbf{r})$. The nonrelativistic approximation of this equation is the Schrödinger equation with the potential $U_{\mathrm{nr}}(\mathbf{r}) = U(\mathbf{r}) + V(\mathbf{r})$. From Eq. (2), we find the normalization of the wave function

$$2\int d\mathbf{r}[E_n - U(\mathbf{r})]|\Phi_n(\mathbf{r})|^2 = 1. \qquad (4)$$

Then we multiply both sides of Eq. (3) by $\Phi_k(\mathbf{r})$ with $E_k \neq E_n$ and take the integral over $\mathbf{r}$. Integrating by parts the term with $\mathbf{p}^2$ and using the equation for $\Phi_k(\mathbf{r})$, Eq. (3) with n replaced by k, we obtain

$$\int d\mathbf{r}[E_k + E_n - 2U(\mathbf{r})]\Phi_k^*(\mathbf{r})\Phi_n(\mathbf{r}) = 0. \qquad (5)$$

Then we represent the potentials in the form $V(\mathbf{r}) = V_0(\mathbf{r}) + \delta V(\mathbf{r})$ and $U(\mathbf{r}) = U_0(\mathbf{r}) + \delta U(\mathbf{r})$. Let $\phi_n(\mathbf{r})$ be the solution of the Klein-Gordon-Fock equation in the potentials $V_0(\mathbf{r})$, $U_0(\mathbf{r})$ with the corresponding energy ε_n. Let us write

$$\Phi_n(\mathbf{r}) = \phi_n(\mathbf{r}) + \delta\phi_n(\mathbf{r}), \quad E_n = \varepsilon_n + \delta\varepsilon_n.$$

The first-order correction to the wave function, $\delta\phi_n^{(1)}(\mathbf{r})$, with respect to perturbations $\delta V(\mathbf{r})$ and $\delta U(\mathbf{r})$ obeys the equation

$$\begin{aligned}\{[\varepsilon_n - U_0(\mathbf{r})]^2 - \mathbf{p}^2 - m^2 - 2mV_0(\mathbf{r})\}\delta\phi_n^{(1)}(\mathbf{r}) \\ = \{2m\delta V(\mathbf{r}) - 2[\varepsilon_n - U_0(\mathbf{r})][\delta\varepsilon_n^{(1)} - \delta U(\mathbf{r})]\}\phi_n(\mathbf{r}).\end{aligned} \qquad (6)$$

Multiplying both sides of Eq. (6) by $\phi_n^*(\mathbf{r})$, taking the integral over $\mathbf{r}$, and using normalization condition (5), we obtain

$$\delta\varepsilon_n^{(1)} = \int d\mathbf{r}\{2m\delta V(\mathbf{r}) + 2\delta U(\mathbf{r})[\varepsilon_n - U_0(\mathbf{r})]\}|\phi_n(\mathbf{r})|^2. \qquad (7)$$

Then we multiply Eq. (3) by $\phi_n^*(\mathbf{r})$, take the integral over $\mathbf{r}$, and collect the terms of the second order in $\delta V(\mathbf{r})$ and $\delta U(\mathbf{r})$. We have

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$$\delta\varepsilon_n^{(2)} = \int d\mathbf{r}\{2m\delta V(\mathbf{r}) - 2[\delta\varepsilon_n^{(1)} - \delta U(\mathbf{r})][\varepsilon_n - U_0(\mathbf{r})]\}\phi_n^*(\mathbf{r})\delta\phi_n^{(1)}(\mathbf{r}) - \int d\mathbf{r}[\delta\varepsilon_n^{(1)} - \delta U(\mathbf{r})]^2|\phi_n(\mathbf{r})|^2. \quad (8)$$

Let us introduce the Green's function $\mathcal{D}_n(\boldsymbol{r},\boldsymbol{r}')$, which obeys the equation

$$\{[\varepsilon_n - U_0(\mathbf{r})]^2 - \mathbf{p}^2 - m^2 - 2mV_0(\mathbf{r})\}\mathcal{D}_n(\boldsymbol{r},\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}') - \frac{1}{N_n}\phi_n(\mathbf{r})\phi_n^*(\mathbf{r}'),$$

$$N_n = \int d\mathbf{r}|\phi_n(\mathbf{r})|^2, \quad (9)$$

and the conditions

$$\int d\mathbf{r}'\mathcal{D}_n(\boldsymbol{r},\boldsymbol{r}')\phi_n(\mathbf{r}') = 0, \qquad \int d\mathbf{r}\phi_n^*(\mathbf{r})\mathcal{D}_n(\boldsymbol{r},\boldsymbol{r}') = 0. \quad (10)$$

It is obvious that $\mathcal{D}_n(\boldsymbol{r},\boldsymbol{r}')$ is nothing but the reduced Green's function of the Schrödinger equation, divided by $2m$, with the effective energy $\tilde{E}_n=(\varepsilon_n^2-m^2)/2m$, and the effective potential $\tilde{V}(\boldsymbol{r})=V_0(\boldsymbol{r})+(\varepsilon_n/m)U_0(\boldsymbol{r})-U_0^2(\boldsymbol{r})/2m$. We assume that Eq. (9) can be solved. For instance, the solution is well known for the pure Coulomb field, $U_0(\boldsymbol{r})=-Ze^2/r$, $V_0(\boldsymbol{r})=0$, where Z is an atomic charge number and e is the electron charge.

It is easy to check that the solution of Eq. (6) has the form

$$\delta\phi_n^{(1)}(\boldsymbol{r}) = \int d\mathbf{r}'\mathcal{D}_n(\boldsymbol{r},\boldsymbol{r}')\{2m\delta V(\mathbf{r}') - 2[\delta\varepsilon_n^{(1)} - \delta U(\mathbf{r}')][\varepsilon_n - U_0(\mathbf{r}')]\}\phi_n(\mathbf{r}') + \beta\phi_n(\mathbf{r}), \quad (11)$$

where the constant β is fixed by the normalization condition (4). We have

$$\beta = -2\int\int d\mathbf{r}d\mathbf{r}'\phi_n^*(\mathbf{r})[\varepsilon_n - U_0(\mathbf{r})]\mathcal{D}_n(\mathbf{r},\mathbf{r}') \times\{2m\delta V(\mathbf{r}') - 2[\delta\varepsilon_n^{(1)} - \delta U(\mathbf{r}')][\varepsilon_n - U_0(\mathbf{r}')]\}\phi_n(\mathbf{r}') - \int d\mathbf{r}[\delta\varepsilon_n^{(1)} - \delta U(\mathbf{r})]|\phi_n(\mathbf{r})|^2. \quad (12)$$

Substituting Eq. (11) into Eq. (8), we finally obtain

$$\delta\varepsilon_n^{(2)} = \int\int d\mathbf{r}d\mathbf{r}'\phi_n^*(\mathbf{r})\{2m\delta V(\mathbf{r}) - 2[\delta\varepsilon_n^{(1)} - \delta U(\mathbf{r})][\varepsilon_n - U_0(\mathbf{r})]\}\mathcal{D}_n(\mathbf{r},\mathbf{r}')\{2m\delta V(\mathbf{r}') - 2[\delta\varepsilon_n^{(1)} - \delta U(\mathbf{r}')][\varepsilon_n - U_0(\mathbf{r}')]\}\phi_n(\mathbf{r}') - \int d\mathbf{r}[\delta\varepsilon_n^{(1)} - \delta U(\mathbf{r})]^2|\phi_n(\mathbf{r})|^2. \quad (13)$$

Note that the term $\beta\phi_n(\mathbf{r})$ in Eq. (11) does not contribute to Eq. (13) because of Eq. (7).

III. ELECTRIC POLARIZABILITY

As an application of our results, let us consider the electric polarizability α_{1s} of a ground state of a spin-zero particle bound in a strong Coulomb field. For spin-$\frac{1}{2}$ particle the polarizability was obtained in Ref. [3,4].

For the perturbation $\delta U(\mathbf{r})=-e\mathcal{E}\cdot\boldsymbol{r}$, we have $\delta\varepsilon^{(1)}=0$, and $\delta\varepsilon^{(2)}$ can be written in the form

$$\delta\varepsilon^{(2)} = -\tfrac{1}{2}\alpha_{1s}\mathcal{E}^2. \quad (14)$$

From Eq. (13), we find

$$\alpha_{1s} = \frac{2}{3}\alpha\left\{\int d\mathbf{r}r^2\phi_{1s}^2(r) - 4\int\int d\mathbf{r}d\mathbf{r}'\phi_{1s}(r)\left(\varepsilon_{1s} + \frac{Ze^2}{r}\right)\mathcal{D}_{1s}(\mathbf{r},\mathbf{r}')\left(\varepsilon_{1s} + \frac{Ze^2}{r'}\right)\phi_{1s}(r')(\boldsymbol{r}\cdot\boldsymbol{r}')\right\}, \quad (15)$$

where $\alpha=e^2=\frac{1}{137}$ is the fine structure constant. The wave function and the energy of the ground state has the form (see, e.g., [5])

$$\phi_{1s}(r) = \sqrt{A}(2\varkappa r)^{\gamma-1/2}\exp(-\varkappa r), \quad \varepsilon_{1s} = m\sqrt{\frac{1}{2}+\gamma},$$

$$\gamma = \sqrt{\frac{1}{4}-(Z\alpha)^2}, \quad \varkappa = m\sqrt{\frac{1}{2}-\gamma}, \quad A = \frac{Z\alpha\varkappa^2}{\pi\Gamma(2\gamma+2)}, \quad (16)$$

Let us introduce the function $\mathbf{F}(\mathbf{r})$

$$\mathbf{F}(\mathbf{r}) = \int d\mathbf{r}'\mathcal{D}_{1s}(\mathbf{r},\mathbf{r}')\left(\varepsilon_{1s} + \frac{Ze^2}{r'}\right)\boldsymbol{r}'\phi_{1s}(r'). \quad (17)$$

It is convenient to represent it in the form

$$\mathbf{F}(\mathbf{r}) = \frac{2\sqrt{A}\varepsilon_{1s}}{\varkappa^2}(2\varkappa r)^{\gamma-3/2}\exp(-\varkappa r)g(2\varkappa r)\boldsymbol{r}, \quad (18)$$

where the function $g(x)$ satisfies the equation, following from Eq. (9):

$$g''(x) + \left(\frac{2\gamma+1}{x} - 1\right)g'(x) - \frac{2}{x^2}g(x) = \frac{x+1-2\gamma}{8}. \quad (19)$$

Substituting Eqs. (17) and (18) into Eq. (15), we obtain

$$\alpha_{1s} = \frac{\alpha\varepsilon_{1s}}{3\varkappa^4}\left\{\left(\frac{1}{2}-\gamma\right)\left(\gamma+\frac{3}{2}\right)(\gamma+1) - \frac{1}{\Gamma(2\gamma+1)}\int_0^\infty dx(x+1-2\gamma)x^{2\gamma+1}\exp(-x)g(x)\right\}. \quad (20)$$

The general solution of Eq. (19) has the form

$$g(x) = -\frac{x}{4} - \frac{x^2}{16} + \frac{x}{4}{}_2F_2\left[\begin{array}{c}1,\ 1\\ \gamma+2+\nu,\ \gamma+2-\nu\end{array}\middle| x\right] + ax^{-\gamma+\nu}{}_1F_1\left[\begin{array}{c}-\gamma+\nu\\ 1+2\nu\end{array}\middle| x\right] + bx^{-\gamma-\nu}{}_1F_1\left[\begin{array}{c}-\gamma-\nu\\ 1-2\nu\end{array}\middle| x\right], \tag{21}$$

where ${}_pF_q$ is the hypergeometric function, $\nu=\sqrt{\gamma^2+2}$, and a and b are some constants to be determined from the boundary conditions at $x=0$ and $x=\infty$. The condition at $x=0$ gives $b=0$. The constant a should be chosen to provide the cancellation of the exponentially large terms of $g(x)$ at $x\to\infty$. The large-x asymptotics of the hypergeometric functions in Eq. (21) can be calculated from their integral representations, see [6]. The asymptotics have the form

$$\begin{aligned}&{}_2F_2\left[\begin{array}{c}1,\ 1\\ \gamma+2+\nu,\ \gamma+2-\nu\end{array}\middle| x\right]\\ &\sim \Gamma[2+\gamma+\nu,2+\gamma-\nu]\frac{\exp(x)}{x^{2\gamma+2}}\sum_n \times\frac{(1+\gamma+\nu)_n(1+\gamma-\nu)_n}{x^n n!}x^{-\gamma\pm\nu}{}_1F_1\left[\begin{array}{c}-\gamma\pm\nu\\ 1\pm2\nu\end{array}\middle| x\right]\\ &\sim \frac{\Gamma[1\pm2\nu]}{\Gamma[\pm\nu-\gamma]}\frac{\exp(x)}{x^{2\gamma+1}}\sum_n\frac{(1+\gamma+\nu)_n(1+\gamma-\nu)_n}{x^n n!}.\end{aligned} \tag{22}$$

Thus, we obtain

$$g(x) = -\frac{x}{4} - \frac{x^2}{16} + \frac{x}{4}{}_2F_2\left[\begin{array}{c}1,\ 1\\ \gamma+2+\nu,\ \gamma+2-\nu\end{array}\middle| x\right] - \frac{\Gamma[2+\gamma+\nu,2+\gamma-\nu,\nu-\gamma]}{4\Gamma[1+2\nu]}x^{-\gamma+\nu}{}_1F_1\left[\begin{array}{c}-\gamma+\nu\\ 1+2\nu\end{array}\middle| x\right], \tag{23}$$

Using the integral representation of ${}_pF_q$, see [6], we obtain the following identity

$$\begin{aligned}&{}_2F_2\left[\begin{array}{c}1,\ 1\\ \gamma+2+\nu,\ \gamma+2-\nu\end{array}\middle| x\right] - \frac{\Gamma[2+\gamma+\nu,2+\gamma-\nu,\nu-\gamma]}{\Gamma[1+2\nu]x^{1+\gamma-\nu}}{}_1F_1\left[\begin{array}{c}-\gamma+\nu\\ 1+2\nu\end{array}\middle| x\right]\\ &= \int_0^1 dz(1-z)^{\gamma+\nu}\int_0^1 dt t^{\nu-\gamma-2}\exp[zx(1-1/t)].\end{aligned} \tag{24}$$

Substituting Eqs. (24) and (23) into Eq. (20) and integrating over x, z, and t, we come to the final result for the polarizability α_{1s}

$$\begin{aligned}\alpha_{1s} = \frac{\alpha(\gamma+1)\sqrt{\gamma+1/2}}{3m^3(1-2\gamma)}\Bigg\{&\frac{12\gamma^2+64\gamma+37}{2(1-2\gamma)}\\ &- \frac{2(2\gamma+1)}{\gamma+\nu+1}\Bigg(\frac{1-2\gamma}{\gamma+\nu+2}{}_3F_2\left[\begin{array}{cc}1,\ 2\gamma+3, & \gamma+\nu+1\\ \gamma+\nu+2, & \gamma+\nu+3\end{array}\middle| 1\right]\\ &+ \frac{(2\gamma+3)}{\gamma+\nu+3}{}_3F_2\left[\begin{array}{cc}1,\ 2\gamma+4, & \gamma+\nu+1\\ \gamma+\nu+2, & \gamma+\nu+4\end{array}\middle| 1\right]\Bigg)\Bigg\}.\end{aligned} \tag{25}$$

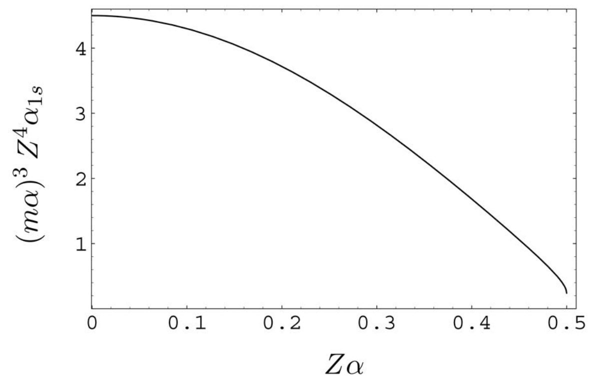

FIG. 1. Polarizability in units $(m\alpha)^{-3}Z^{-4}$ as a function of $Z\alpha$.

The polarizability for arbitrary state can be obtained similarly. Figure 1 shows the polarizability α_{1s} in units $(m\alpha)^{-3}Z^{-4}$ as a function of $Z\alpha$.

At $Z\alpha\ll 1$, we have

$$\alpha_{1s} = \frac{9}{2(m\alpha)^3Z^4}\left[1 - \frac{121}{27}(Z\alpha)^2 + \left(\frac{229}{72}+\frac{4\pi^2}{81}\right)(Z\alpha)^4 + \cdots\right]. \tag{26}$$

At $Z\alpha\to 1/2$, the polarizability has finite value $\sim 3.84\alpha/m^3$. Our formula for polarizability cannot be applied for $Z\alpha>\frac{1}{2}$ because we did not take into account the effect of finite nuclear size. Besides, in a pionic atom it is necessary to account for the effects of the strong interaction that become dominant for the ground state at large Z. It is interesting to compare the polarizabilities of a ground state, calculated for spin-0 particle and spin-$\frac{1}{2}$ particle. It turns out that the functions $f(Z)=Z^4\alpha_{1s}$ obey the relation $f(Z)_{S=0}\approx f(2Z)_{S=1/2}$ with accuracy of a few percent.

In summary, we have derived the formulas for the corrections to the energy levels and wave functions of a spin-zero particle bound in a strong field. These formulas may be useful at the consideration of various effects in pionic atoms. As an example, we evaluated the electric polarizability of a ground state of a spin-zero particle bound in a strong Coulomb field.

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