Regularized analytic evaluation of vacuum polarization in a Coulomb field

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(Received 9 February 1990)

We have calculated analytically by a new Mellin transform method the vacuum-polarization contribution to the energy shift in a Coulomb field. Our method gives a *finite* answer which to lowest order in $(Z\alpha)$ for S states is $\Delta E^{\mathrm{VP}} = -(4\alpha/3\pi)[(Z\alpha)^4/N^3]\frac{29}{144}$. The method further allows a high-Z approximation. A magnetic contribution to the vacuum polarization is also indicated.

Vacuum polarization is an important effect in quantum electrodynamics (QED), both in practice (Coulomb energy shifts, heavy ions, mesic atoms, . . .) and conceptually, because it represents the most divergent term in perturbation theory and enters significantly in renormalization methods and in the idea of a "running coupling" constant. In a Coulomb field one first calculates the modification of the potential due to the charge density of the vacuum polarization (Uehling potential) and then evaluates its expectation value to obtain the energy shifts due to vacuum polarization. Calculations with relativistic Coulomb wave functions were first carried out in a classic paper by Wichmann and Kroll.[1] They were further studied by a number of authors,[2-5] also numerically,[6-8] with a view of extending the result to high-Z values and to include the charge distribution of the nucleus.[9]

We present here an entirely new analytical calculation of the vacuum-polarization energy shifts in a Coulomb field. We calculate directly the energy shifts. A method based on Mellin transformations and specifying the poles in the inverse transform provides automatically a finite regularized result.

Vacuum polarization is a part of the general energy shift ΔE_n of a level n of a quantum system due to radiative self-energy effects which is given by[10] (in units $c=\hbar=1$)

$$\Delta E_n = \frac{e^2}{2}\int d\mathbf{x}\,\bar{\psi}_n(\mathbf{x})\gamma_\mu\psi_n(\mathbf{x})P\int\frac{d\mathbf{k}}{(2\pi)^3}\int d\mathbf{y}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k^2}\sum\!\!\!\!\!\!\int_s\bar{\psi}_s(\mathbf{y})\gamma^\mu\psi_s(\mathbf{y})$$
$$-\frac{e^2}{2}\sum\!\!\!\!\!\!\int_s d\mathbf{x}\,d\mathbf{y}\,\bar{\psi}_n(\mathbf{x})\gamma_\mu\psi_s(\mathbf{x})\int\frac{d\mathbf{k}}{(2\pi)^3}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\bar{\psi}_s(\mathbf{y})\gamma^\mu\psi_n(\mathbf{y})\left[\frac{1}{E_s-E_n-k}-\frac{1}{E_s-E_n+k}\right]$$
$$-\frac{e^2}{2}\sum\!\!\!\!\!\!\int_{\substack{s\\(s<n)}}\int d\mathbf{x}\,d\mathbf{y}\,\bar{\psi}_n(\mathbf{x})\gamma_\mu\psi_s(\mathbf{x})\int\frac{d\mathbf{k}}{(2\pi)^3}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\bar{\psi}_s(\mathbf{y})\gamma^\mu\psi_n(\mathbf{y})\frac{i\pi}{2k}\delta(E_s-E_n-k)\ . \tag{1}$$

Here ψ_n is a fixed level and we sum on the right-hand side over all levels ψ_s, discrete and continuous. The first term is the contribution of the vacuum polarization, the second that of self-energy (or Lamb shift proper), and the third term is the spontaneous emission. The third term has been exactly and analytically evaluated recently for relativistic Coulomb wave functions.[11] Here we shall evaluate the first term

$$\Delta E_n^{\mathrm{VP}} = \frac{e^2}{2}\int d\mathbf{x}\,d\mathbf{y}\,\bar{\psi}_n(\mathbf{x})\gamma_\mu\psi_n(\mathbf{x})\bar{\psi}_s(\mathbf{y})\gamma^\mu\psi_s(\mathbf{y})P\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k^2}\ . \tag{2}$$

We summarize first the spin algebra and angular integrations.

The relativistic Coulomb functions are written as

$$\psi_n(\mathbf{r}) = \begin{vmatrix} f_n & \Omega_n \\ ig_n & \Omega_n' \end{vmatrix},\quad n\equiv(j_n,l_n,m_n),\quad n'\equiv(j_n,l_n',m_n);\quad l_n'=l_n\pm1\ ,$$

where f_n are the "large" and g_n the "small" components. The product of the two currents in (2) is

$$\bar{\psi}_n(\mathbf{r})\gamma^\mu\psi_n(\mathbf{r})\bar{\psi}_s(\mathbf{r}')\gamma_\mu\psi_s(\mathbf{r}') = \psi_n^\dagger(\mathbf{r})\psi_n(\mathbf{r})\psi_s^\dagger(\mathbf{r}')\psi_s(\mathbf{r}') - \psi_n^\dagger(\mathbf{r})\boldsymbol{\alpha}\psi_n(\mathbf{r})\psi_s^\dagger(\mathbf{r}')\boldsymbol{\alpha}\psi_s(\mathbf{r}')\ . \tag{3}$$

We shall refer to the first term as the "electric" part, and the second as the "magnetic" part. We next use the expansion into spherical harmonics

$$\int d\mathbf{k}\,e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = (4\pi^2)\sum_{l,m}j_l(kr)j_l(kr')Y_{lm}(\hat{r})Y_{lm}(\hat{r}') \tag{4}$$

to perform the angular integrations

$$\int d\hat{r}\psi_n^\dagger(\mathbf{r})\psi_n(\mathbf{r})=\frac{2j_n+1}{\sqrt{4\pi}}[|f_{+\kappa_n}(r)|^2+|g_{+\kappa_n}(r)|^2+|f_{-\kappa_n}(r)|^2+|g_{-\kappa_n}(r)|^2]W_{nn}^{lm} , \quad (5)$$

where $\kappa_n=|j_n+\frac{1}{2}|$, and

$$W_{nn}^{lm}=(-1)^{1/2-m_n}[1+(-1)^l]\sqrt{2l+1}\begin{pmatrix} j_n & j_n & l \\ -\frac{1}{2} & \frac{1}{2} & 0\end{pmatrix}\begin{pmatrix} j_n & j_n & l \\ -m_n & -m_n' & m\end{pmatrix} , \quad (6)$$

and similarly for the integral $\int d\hat{r}\,'$. The magnetic part gives

$$\int d\hat{r}\psi_n^\dagger(\mathbf{r})\alpha\psi_n(\mathbf{r})=\frac{2j_n+1}{\sqrt{4\pi}}[f_n^\dagger(r)\mathbf{K}_{nn}^{lm}g(r)+\text{H.c.}] . \quad (7)$$

The expression for $\mathbf{K}$ is long and is given elsewhere;[11] we shall not need it in this paper. In W_{nn}^{lm} and $\mathbf{K}_{nn}^{lm}$ we can read off the selection rules. For $j_n=\frac{1}{2}$, for example, only the $l=0$ term in W_{nn}^{lm}, and only the $l=1$ term in $\mathbf{K}_{nn}^{lm}$ contribute—hence the names "electric" and "magnetic."

For small $Z\alpha$, because g_n are $Z\alpha$ times smaller than f_n, the electric part of the vacuum polarization involving $|f_n|^2$ is $Z\alpha$ times larger than the magnetic part involving $(f_n^\dagger\mathbf{K}g_n)$. Wichmann and Kroll[1] and others have only calculated the electric part. For comparison we also discuss this term here:

$$\Delta E_n^{\text{VP}}=-\frac{e^2}{4\pi}(2J_n+1)\sum_{lm}\sum\!\!\!\!\!\!\int_s(2J_s+1)\int dr\,dr'V_l(r,r')\{W_{nn}^{lm}W_{ss}^{lm}(|f_n|^2+|g_n|^2)(|f_s|^2+|g_s|^2)$$
$$-[f_n^\dagger(r)\mathbf{K}_{nn}^{lm}g_n(r)+\text{H.c.}][f_n^\dagger(r')\mathbf{K}_{ss}^{lm}g_s(r')+\text{H.c.}]\} , \quad (8)$$

where we have introduced a potential $V_l(r,r')$ by

$$V_l(r,r')\equiv\frac{2}{\pi}r^2r'^2\int_0^\infty j_l(kr)j_l(kr')dk=\frac{r^2r'^2}{2l+1}\frac{r_<^l}{r_>^{l+1}} . \quad (9)$$

We shall evaluate the sum over discrete and continuous states.

The discrete radial functions are

$$\begin{bmatrix} f_n(r) \\ g_n(r)\end{bmatrix}=U_n(r)\begin{bmatrix}\sqrt{1+\epsilon_n}[F_n(r)+G_n(r)] \\ \sqrt{1-\epsilon_n}[F_n(r)-G_n(r)]\end{bmatrix} , \quad (10)$$

where

$$U_n(r)=\left[\frac{\Gamma(2\gamma_n+n_r+1)}{4N_n(N_n-\kappa_n)n_r!}\right]^{1/2}\frac{(2p_N)^{3/2}(2p_Nr)^{\gamma_n-1}e^{-p_Nr}}{\Gamma(2\gamma_n+1)} ,$$

$$F_n(r)=n_r\phi(1-n_r,2\gamma_n+1;2p_Nr) ,$$

$$G_n(r)=(N_n-\kappa_n)\phi(-n_r,2\gamma_n+1;2p_Nr) ,$$

with

$$p_N=\frac{Z\alpha}{N_n},\quad \epsilon_n=\frac{E_n}{m}=(1+p_N^2)^{1/2},\quad N=[n^2-2n_r(|\kappa_n|-\gamma_n)]^{1/2} ,$$

$$n_r=n-|\kappa_n|,\quad \kappa_n=\pm(j_n+\tfrac{1}{2}),\quad \gamma_n=[\kappa_n^2-(Z\alpha)^2]^{1/2}$$

We expand the confluent hypergeometric functions ϕ into power series

$$F_n(r)=\sum_{n_1}A_{n_1}(2p_Nr)^{n_1},\quad G_n(r)=\sum_{n_1}B_{n_1}(2p_Nr)^{n_1} ,$$

where

$$\begin{bmatrix} A_{n_1} \\ B_{n_1}\end{bmatrix}=\frac{1}{(2\gamma_n+1)_{n_1}n_1!}\begin{bmatrix} n_r(1-n_r)n_1 \\ (N_n-\kappa_n)(-n_r)_{n_1}\end{bmatrix} .$$

Thus

$$|f_n|^2+|g_n|^2=\sum_{n_1 n_2} a_{n_1 n_2}\lambda_{n_1}(p_N r)\lambda_{n_2}(p_N r)\ , \tag{11}$$

where

$$a_{n_1 n_2}=\left[\frac{\Gamma(2\gamma_n+n_r+1}{4N_n(N_n-\kappa_n)n_r!\Gamma^2(2\gamma_n+1)}\right](A_{n_1}A_{n_2}+B_{n_1}B_{n_2}-2\epsilon_n A_{n_1}B_{n_2})$$

and

$$\lambda_{n_i}(p_N r)=(2p_N)^{3/2}(2p_N r)^{\gamma_n+n_i-1}e^{-p_N r},\quad i=1,2\ .$$

Now we come to the evaluation of the sum $e\sum_s[|f_s(r')|^2+|g_s(r')|^2]W_{ss}$ over both discrete and continuum positive-energy states, which is the most difficult part of the calculation. The calculation of the sum becomes simpler if we use the technique of the Green's function of Coulomb wave functions initiated by Wichmann and Kroll.[1] Because of completeness relations the Green's functions necessarily involve both positive- and negative-energy solutions. But the negative-energy solutions are equivalent to positive-energy solutions with the sign of the charge reversed.[10] Consequently, we can extend our sum over states s to negative energy (with $e\to -e$) and take half of it. Thus,

$$e\sum_s(|f_s|^2+|g_s|^2)=\frac{e}{2}\sum_{E_s>0}(|f_s|^2+|g_s|^2)-\frac{e}{2}\sum_{E_s<0}(|f_s|^2+|g_s|^2)\ . \tag{12}$$

This sum can now be written as a contour integral in terms of the Green's function $K(r_i,r_2,z)$ of the radial Coulomb problem:

$$\frac{1}{2}\left[\sum\!\!\!\!\!\!\int_{E_s>0}-\sum\!\!\!\!\!\!\int_{E_s<0}\right](|f_s|^2+|g_s|^2)=\frac{1}{2\pi i}\left[\int_{C+}+\int_{C-}\right]dz\,\mathrm{tr}K(r;r';z)\ . \tag{13}$$

The contours $C_\pm(z)$ are shown in Fig. 1, together with the modified contours $(C_1C_2C_3C_4I)$:

$$K(r,r';z)=\frac{1}{k(z)}\begin{bmatrix}W_1^{(2)}(r_>,z)\\ W_2^{(2)}(r_>,z)\end{bmatrix}(W_1^{(1)}(r_<,z),W_2^{(1)}(r_<,z))\ , \tag{14}$$

$$\begin{aligned}W_{\substack{1\\2}}^{(1)}(r_<,z)=[2r_<(z^2-1)^{1/2}]^{\gamma}e^{ir_<(z^2-1)^{1/2}}\Bigg[&\left[\kappa-\frac{iZ\alpha}{(z^2-1)^{1/2}}\right]\begin{bmatrix}i\sqrt{z+1}\\ \sqrt{z-1}\end{bmatrix}\\ &\times\phi(\gamma-i\nu,2\gamma+1,-2i(z^2-1)^{1/2}r<)\\ &+\begin{bmatrix}i\sqrt{z+1}\\ \sqrt{z-1}\end{bmatrix}(\gamma-i\nu)\phi(\gamma+1-i\nu,2\gamma+1,-2i(z^2-1)^{1/2}r_<)\Bigg]\ ,\end{aligned} \tag{15}$$

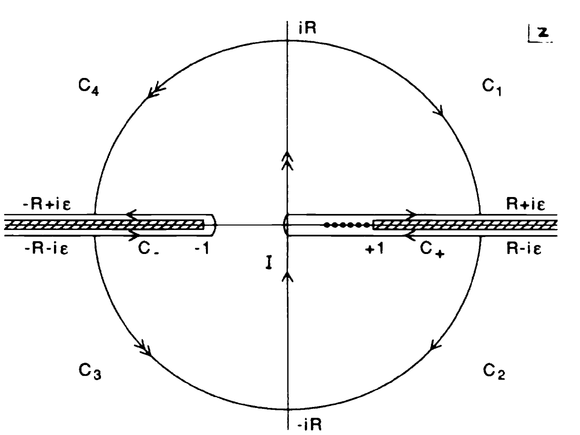

FIG. 1. Contours of z integrations $C_\pm$ and deformed contours C_i, I.

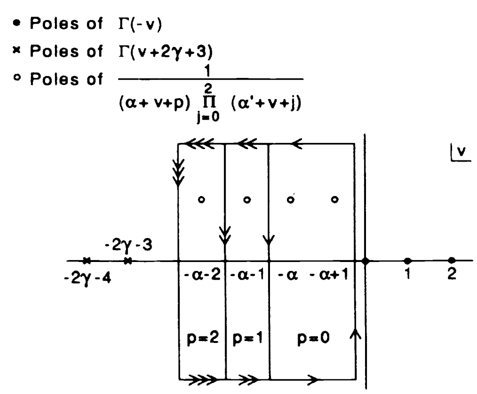

FIG. 2. Contours of v integrations.

$$W^{(2)}_{\substack{1\\2}}(r_>,z)=\begin{bmatrix} i\sqrt{z+1}\\ \sqrt{z-1}\end{bmatrix}[2r_>(z^2-1)^{1/2}]^\gamma e^{ir_>(z^2-1)^{1/2}}\left[\left[\kappa-\frac{iZ\alpha}{(z^2-1)^{1/2}}\right]\chi(\gamma-i\nu,2\gamma+1,-2ir_>(z^2-1)^{1/2}) + \begin{bmatrix}1\\-1\end{bmatrix}(\gamma-i\nu)\chi(\gamma+1-i\nu,2\gamma+1,-2ir_>(z^2-1)^{1/2})\right],$$

$$k(z)=-2(z^2-1)^{1/2}\left[\kappa-\frac{iZ\alpha}{(z^2-1)^{1/2}}\right]\frac{\Gamma(-\gamma-i\nu)\Gamma(2\gamma+1)}{\Gamma(-2\gamma)\Gamma(\gamma-i\nu)}\exp\left[\frac{i\pi}{2}(2\gamma+1)\right], \tag{16}$$

$$\begin{aligned}\phi(\alpha,\gamma;z)&=\frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma-\alpha)}\int_0^1 dt\, e^{zt}t^{\alpha-1}(1-t)^{\gamma-\alpha-1},\\ \chi(\alpha,\gamma;z)&=\frac{\Gamma(\alpha+1-\gamma)}{\Gamma(\alpha)\Gamma(1-\gamma)}\int_0^\infty dt\, e^{-zt}t^{\alpha-1}(1+t)^{\gamma-\alpha-1}.\end{aligned} \tag{17}$$

Evaluating $K(r,r';z)$, and inserting everything into (8) we obtain (with $e^2/4\pi=\alpha$)

$$\begin{aligned}\Delta E_n^{\rm VP}=&\alpha(2J_n+1)\sum_{lm}W^{lm}_{nn}\sum_{\kappa=1}^{\infty}2\kappa W^{lm}_{ss}\\ &\times\sum_{n_1n_2}a_{n_1n_2}\left[\int_{C+}+\int_{C-}\right]\frac{dz}{2\pi i}\frac{2i}{(z^2-1)^{1/2}}T_{\alpha,\alpha'}\int_0^1 dt\, t^{\alpha-1}(1-t)^{2\gamma-\alpha}\int_0^\infty dt\, t'^{\alpha'-1}(1+t')^{2\gamma\alpha'}\\ &\times\int_0^\infty r^2dr\int_0^\infty r'^2dr'\lambda_{n_1}(p_Nr)\lambda_{n_2}(p_Nr)[-2i(z^2-1)^{1/2}r']^{2\gamma}e^{+2i(z^2-1)^{1/2}(1-t+t')r'}\frac{r^l_<}{(2l+1)r_>^{l+1}},\end{aligned} \tag{18}$$

where we have set

$$T_{\alpha\alpha'}=\left[\frac{iZ\alpha}{(z^2-1)^{1/2}}\left[\frac{\delta_{\alpha,\gamma-i\nu}\delta_{\alpha',\gamma-i\nu}+\delta_{\alpha,\gamma+1-i\nu}\delta_{\alpha',\gamma+1-i\nu}}{\Gamma(\alpha)\Gamma(2\gamma+1-\alpha')}\right]-z\left[\frac{\delta_{\alpha,\gamma-i\nu}\delta_{\alpha',\gamma+1-i\nu}}{\Gamma(\alpha)\Gamma(2\gamma+1-\alpha')}-\frac{\delta_{\alpha,\gamma+1-i\nu}\delta_{\alpha',\gamma-i\nu}}{\Gamma(\alpha')\Gamma(2\gamma+1-\alpha)}\right]\right]. \tag{19}$$

Here we have used the symmetry of $|f_s|^2+|g_s|^2$ with respect to the sign $\pm\kappa_s$ of the quantum number κ_s over which we sum. The variable ν for continuum states is $\nu=(\alpha z)E/p$, z is the energy variable measured in units of the electron mass. The Kroenecker δ's just tell the values of α and α'.

The radial integrations can be performed exactly:

$$\begin{aligned}R&=\int_0^\infty r^2dr\int_0^\infty r'^2dr'\frac{r^l_<}{(2l+1)r_>^{l+1}}(2p_N)^3[-2i(z^2-1)^{1/2}r']^{2\gamma}(2p_Nr)^{2\gamma_n+n_1+n_2-2}e^{-2p_N+2i(z^2-1)^{1/2}(1-t+t')r'}\\ &=\frac{1}{2l+1}\frac{\Gamma(b)(-iy)^{2\gamma}}{(1+ay)^b}\{c_1^{-1}{}_2F_1[1,b;c_1+1;(1+ay)^{-1}]+c_2^{-1}{}_2F_1[1,b;c_2+1;ay(1+ay)^{-1}]\},\end{aligned} \tag{20}$$

where

$$b=2\gamma+2\gamma_n+n_1+n_2+1,\quad c_1=2\gamma_n+n_1+n_2+l+1,\quad c_2=2\gamma+l+1, \tag{21}$$

$$y=(z^2-1)^{1/2}/p_N,\quad a=-i(1-t+t'). \tag{22}$$

We still have to perform the integrations over dt and dt' and the contour integration over dz in Eq. (16). Functions of the type R in (17) are properly defined by specifying their contours in the Mellin transform plane (they are of the class of Fox functions[12]). The Mellin transform $M[R]$ of R in the energy variable y,

$$\mathcal{F}(w)=M[f]\equiv\int_0^\infty dx\, x^{w-1}f(x), \tag{23}$$

turns out to be rather simple:

$$\mathcal{R}(w)=a^{-2(\gamma+w)}\frac{\Gamma(2\gamma+w)\Gamma(b-2\gamma-w)}{(l+w)(l+1-w)}, \tag{24}$$

where we have dropped here the subscript s on γ. In order to obtain (24) we have used a series representation of ${}_2F_1$, transformed the series term by term and then resumed it. Thus R is well defined as an inverse transform of (24) when a contour is specified. Now Eq. (18) becomes

$$\Delta E_n^{\mathrm{VP}}=\gamma(2J_n+1)\sum_{lm} W_{nn}^{lm}\sum_{\kappa=1}^{\infty}2\kappa W_{ss}^{lm}\sum_{n_1n_2}a_{n_1n_2}\left[\int_{C+}+\int_{C-}\right]\frac{dz}{2\pi i}$$
$$\times\frac{2i}{(z^2-1)^{1/2}}\int_{C_w-i\infty}^{C_w+i\infty}\frac{dw}{2\pi i}\frac{\Gamma(2\gamma+w)\Gamma(b-2\gamma-w)y^{-w}}{(l+w)(l+1-w)(-i)^{2\gamma+w}}J_{\alpha\alpha'}(w)T_{\alpha\alpha'}\ , \tag{25}$$

where we have introduced the symbol

$$J_{\alpha\alpha'}(w)=\int_0^1 dt\int_0^{\infty}dt'\,t^{\alpha-1}(1-t)^{2\gamma-\alpha}t'^{\alpha'-1}(1+t')^{2\gamma-\alpha'}(1-t+t')^{-(2\gamma+w)}\ , \tag{26}$$

which after t' integration is

$$J_{\alpha\alpha'}(w)=\int_0^1 dt\, t^{\alpha-1}(1-t)^{2\gamma-\alpha}B(w,\alpha')(1-t)^{-2\gamma-w}{}_2F_1\left[2\gamma+w,\alpha';\alpha'+w;\frac{t}{t-1}\right]\ , \tag{27}$$

$$J_{\alpha\alpha'}(w)=\Gamma(w)\int\frac{dv}{2\pi i}\Gamma(-v)\frac{\Gamma(a+v)\Gamma(\alpha'+v)\Gamma(2\gamma+w+v)(-1)^{\gamma+v}}{\Gamma(\alpha+v+w)\Gamma(\alpha'+w+v)\Gamma(2\gamma+w)}\ ,$$

or (28)

$$J_{\alpha\alpha'}(w)=\Gamma(w)\int\frac{dv}{2\pi i}\Gamma(-v)\frac{\Gamma(\alpha'+v)\Gamma(2\gamma+w+v)(-1)^{\alpha+v}}{\Gamma(\alpha'+v+w)\Gamma(2\gamma+w)(\alpha+v)}{}_2F_1(1-w,\alpha+v;\alpha+v+1;1)\ ,$$

where the hypergeometric function ${}_2F_1$ is convergent for positive values of $\mathrm{Re}(w)$. In the w plane we have the poles at $w=b-2\gamma+r$ with $r=0,1,2,\ldots$ and this gives a $(Z\alpha)$ expansion of ΔE_n^{VP}. The first pole is at

$$w_0=b-2\gamma=2\gamma_n+n_1+n_2+1\cong 3\ . \tag{29}$$

It is obtained for $n_1=n_2=0$ and $\gamma_n\cong 1$ which corresponds to $j_n=\frac{1}{2}$. Thus the coefficient of the lowest-order vacuum polarization is proportional to $\alpha(Z\alpha)^4$. Here we calculate $J_{\alpha\alpha'}(w)$ only for $j_n=\frac{1}{2}$ and $l_n=0$ or S waves. In this case l is zero or one.

In W_{nn}^{lm} ($\mathbf{K}_{nn}^{lm}$) it is zero (one) and

$$W_{nn}^{00}=W_{ss}^{00}=1\ . \tag{30}$$

Then $J_{\alpha\alpha'}(w_0)$ is

$$J_{\alpha\alpha'}(w_0\approx 3)=\Gamma(3)\int\frac{dv}{2\pi i}\Gamma(-v)\frac{\Gamma(2\gamma+3+v)}{\Gamma(2\gamma+3)}\sum_{p=0}^{2}\frac{(-1)^{\alpha+v+p}\Gamma(3)}{\Gamma(3-p)p!(\alpha'+v)(\alpha'+v+1)(\alpha'+v+2)(\alpha+v+p)}\ . \tag{31}$$

In the v integration we choose the contour such that the power of (-1), or $a+v+p$ will be non-negative. The poles and the integration contours are shown in Fig. 2.

The results of the v integrations are

$$J_{\alpha\alpha'}(w_0\approx 3)=\frac{\Gamma(3)}{\Gamma(2\gamma+3)}\left\{\frac{\Gamma(\alpha)\Gamma(2\gamma+3-\alpha)}{2}[-\psi(\alpha)+\psi(2\gamma+3-\alpha)-3+\ln(-1)]\right.$$
$$+2\Gamma(\alpha+1)\Gamma(2\gamma+2-\alpha)[\psi(\alpha+1)-\psi(2\gamma+2-\alpha)+\tfrac{1}{2}-\ln(-1)]$$
$$\left.+\frac{\Gamma(\alpha+2)\Gamma(2\gamma+1-\alpha)}{2}[-\psi(\alpha+2)+\psi(2\gamma+1-\alpha)+\tfrac{3}{2}+\ln(-1)]\right\}\ ,$$

$$J_{\alpha,\alpha+1}(w_0\approx 3)=\frac{\Gamma(3)}{\Gamma(2\gamma+3)}\left\{\frac{\Gamma(\alpha)\Gamma(2\gamma+3-\alpha)}{3!}\right.$$
$$+\Gamma(\alpha+1)\Gamma(2\gamma+2-\alpha)[-\psi(\alpha+1)+\psi(2\gamma+2-\alpha)-2+\ln(-1)]$$
$$\left.-\Gamma(\alpha+2)\Gamma(2\gamma+1-\alpha)[-\psi(\alpha+2)+\psi(2\gamma+1-\alpha)+\ln(-1)]\right\}\ , \tag{32}$$

$$J_{\alpha,\alpha-1}(w_0\approx 3)=\frac{\Gamma(3)}{\Gamma(2\gamma+3)}\left\{-\frac{\Gamma(\alpha-1)\Gamma(2\gamma+4-\alpha)}{3!}\right.$$
$$+\Gamma(\alpha)\Gamma(2\gamma+3-\alpha)[\psi(\alpha)-\psi(2\gamma+3-\alpha)-\tfrac{3}{2}-\ln(-1)]$$
$$+\Gamma(\alpha+1)\Gamma(2\gamma+2-\alpha)[-\psi(\alpha+1)+\psi(2\gamma+2-\alpha)+1+\ln(-1)]$$
$$\left.-\Gamma(\alpha+2)\Gamma(2\gamma+1-\alpha)/3!\right\} .$$

Here $\psi(z)$ is the logarithmic derivative of the Γ function and comes from the Cauchy formula for second-order poles. Then we substitute $J_{\gamma-i\nu,\gamma-i\nu}J_{\gamma+1-i\nu,\gamma+1-i\nu}$, $J_{\gamma-i\nu,\gamma+1-i\nu}$, and $J_{\gamma+1-i\nu,\gamma-i\nu}$ into Eq. (25). The result is

$$\Delta E_n^{\mathrm{VP}}=-\alpha\sum_{\kappa=1}^{\infty}2\kappa\left[\int_{C+}+\int_{C-}\right]\frac{dz}{2\pi i}\frac{4i(-i)^{-2\gamma-3}}{6(z^2-1)^2}\left[\frac{Z\alpha}{N_n}\right]^3 .$$
$$\times\left[\frac{iZ\alpha}{\sqrt{z^2-1}}\left\{\frac{\Gamma(\gamma+3+i\nu)}{\Gamma(\gamma+1+i\nu)}[-\psi(\gamma-i\nu)+\psi(\gamma+3+i\nu)-3+\ln(-1)]\right.\right.$$
$$+\frac{2\Gamma(\gamma+1-i\nu)\Gamma(\gamma+2+i\nu)}{\Gamma(\gamma-i\nu)\Gamma(\gamma+1+i\nu)}[-\psi(\gamma+2+i\nu)+\psi(\gamma+1-i\nu)+\tfrac{1}{2}-\ln(-1)]$$
$$+\frac{\Gamma(\gamma+2-i\nu)}{2\Gamma(\gamma-i\nu)}[\psi(\gamma+1+i\nu)-\psi(\gamma+2-i\nu)+\tfrac{3}{2}+\ln(-1)]$$
$$+\frac{\Gamma(\gamma+2+i\nu)}{\Gamma(\gamma+i\nu)}[\psi(\gamma+2+i\nu)-\psi(\gamma+1-i\nu)-3+\ln(-1)]$$
$$+\frac{2\Gamma(\gamma+2-i\nu)\Gamma(\gamma+1+i\nu)}{\Gamma(\gamma+1-i\nu)\Gamma(\gamma+i\nu)}[\psi(\gamma+2-i\nu)-\psi(\gamma+1+i\nu)+\tfrac{1}{2}-\ln(-1)]$$
$$\left.+\frac{\Gamma(\gamma+3-i\nu)}{2\Gamma(\gamma+1-i\nu)}[-\psi(\gamma+3-i\nu)+\psi(\gamma+i\nu)+\tfrac{3}{2}+\ln(-1)]\right\}$$
$$-z\left\{-\frac{\Gamma(\gamma+3+i\nu)}{3!\Gamma(\gamma+i\nu)}+\frac{\Gamma(\gamma+1-i\nu)\Gamma(\gamma+2+i\nu)}{|\Gamma(\gamma-i\nu)|^2}\right.$$
$$\times[-\psi(\gamma+1-i\nu)+\psi(\gamma+2+i\nu)-2+\ln(-1)]-\frac{\Gamma(\gamma+2-i\nu)\Gamma(\gamma+1+i\nu)}{|\Gamma(\gamma-i\nu)|^2}$$
$$\times[-\psi(\gamma+2-i\nu)+\Gamma(\gamma+1+i\nu)+\ln(-1)]+\frac{\Gamma(\gamma+3+i\nu)}{3!}$$
$$-\frac{\Gamma(\gamma+1-i\nu)\Gamma(\gamma+2+i\nu)}{|\Gamma(\gamma-i\nu)|^2}[\psi(\gamma+1-i\nu)-\psi(\gamma+2+i\nu)+\tfrac{3}{2}-\ln(-1)]$$
$$\left.\left.+\frac{\Gamma(\gamma+3-i\nu)}{3!\Gamma(\gamma-i\nu)}-\frac{\Gamma(\gamma+2-i\nu)\Gamma(\gamma+1+i\nu)}{|\Gamma(\gamma-i\nu)|^2}\;[-\psi(\gamma+2-i\nu)+\psi(\gamma+1+i\nu)+1+\ln(-1)]\right\}\right] \tag{33}$$

In Eq. (33) we have only a z integration and a κ summation. All Γ and ψ functions are analytic functions of $i\nu$. So the integrand is analytic except the branch cuts at $|z|\geq 1$. We deform the contour of z integration as in Fig. 1. Then

$$\left[\int_{C+}+\int_{C-}\right]\frac{dz}{2\pi i}I(z)=\left[\int_{C_1}+\int_{C_2}+\int_{C_3}+\int_{C_4}+2\int_I\right]\frac{dz}{2\pi i}I(z) , \tag{34}$$

where C_1, C_2, C_3, and C_4 are segments of the circle with the radius R and I is from $-iR$ to $+iR$. When R goes to infinity the contribution of C_1, C_2, C_3, and C_4 to the integral is zero and I gives a finite contribution.

To do the z integration and κ summation we assume $Z\alpha$ to be small. Then we expand all the Γ and ψ functions into the series of $Z\alpha$ or ν and take only the terms up to $Z\alpha$ in the large square brackets of Eq. (33). We also approximate γ to $|\kappa|$. Then we get the lowest-order contribution in $(Z\alpha)$ to the vacuum polarization of the S waves. It is

$$\Delta E_n^{\mathrm{VP}}=4\alpha(Z\alpha)\left[\frac{Z\alpha}{N_n}\right]^3\sum_{\kappa=1}^{\infty}(-1)^{\kappa}\kappa\int_{-i\infty}^{-i\infty}\frac{dz}{2\pi i(z^2-1)^{5/2}}$$
$$\times(\{-\tfrac{1}{4}(\kappa+1)[3(\kappa+2)-5\kappa]\}-z^2\{\tfrac{1}{6}[\kappa(\kappa+1)+\kappa(\kappa+2)+(\kappa+1)(\kappa+2)]-\tfrac{5}{2}\kappa^2\}+O(Z\alpha)) . \tag{35}$$

The κ summation and z integration are done as follows:

$$\sum_{k=1}^{\infty}(-1)^k k(k+1)(k+2)=-\tfrac{3}{8}\ ,$$
$$\sum_{k=1}^{\infty}(-1)^k k^2(k+1)=\sum_{k=1}^{\infty}(-1)^k k^2(k+2)=\sum_{k=1}^{\infty}(-1)^k k^3=\tfrac{1}{8}\ , \tag{36}$$

$$\int_{-i\infty}^{i\infty}\frac{dz}{2\pi i(z^2-1)^{5/2}}=\frac{2i}{3\pi}\ ,$$
$$\int_{-i\infty}^{i\infty}\frac{dz}{2\pi i}\frac{z^2}{(z^2-1)^{3/2}}=-\frac{i}{3\pi}\ . \tag{37}$$

Then we substitute all these values into Eq. (35). It gives

$$\Delta E_n^{\mathrm{VP}}=-\frac{4\alpha}{3\pi}\frac{29}{144}(Z\alpha)\left[\frac{Z\alpha}{N_n}\right]^3 \quad \text{for the } S \text{ states}\ . \tag{38}$$

In the standard QED, the energy shift is calculated as the expectation value of the Uehling potential between the S states[7] and it is given by

$$\Delta E_n^{\mathrm{VP}}=-\frac{4\alpha}{3\pi}\frac{29}{145}(Z\alpha)\cdot\left[\frac{Z\alpha}{n}\right]^3 \quad \text{for the } S \text{ states}\ . \tag{39}$$

The difference between these two results $\frac{29}{144}$ vs $\frac{29}{145}=\frac{1}{5}$ is of order $\alpha(Z\alpha)^5$. To this order there are many other contributions which we have listed during various steps in the calculation. Our method now allows, in principle, to calculate in the same way all the next-order terms, including the magnetic term proportional to $\bar{K}$, Eq. (7), which has never been calculated before. The Mellin transform method has another advantage: namely, to study the vacuum polarization in the important high-Z region by taking the poles in the right-hand w plane.

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