1G16 水素原子の Dirac 方程式を Foldy-Wouthuysen 変換を用いて解く試みにおいて陽子由来の Vector Potential を考慮するとき現れる発散積分についての考察

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Divergent integral arising in solving the hydrogen-atom Dirac-equation with including the vector potential of the proton source by using the Foldy-Wouthuysen transformation

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INTRODUCTION: Recently, Sun et al. [1] pointed out that the Dirac equation for the hydrogen atom is gauge invariant if the vector potential of the proton source is included. Thus the Dirac equation should be read as

$$(c\vec{\alpha}\bullet\vec{\pi}+\beta mc^2-eV)\Psi=E\Psi \qquad (1\text{-}1)$$

where $\vec{\pi}=\vec{p}+e\vec{A}$, $\vec{A}=\frac{1}{c^2}\vec{\mu}\times\frac{\vec{r}}{r^3}$, $\vec{\mu}$ is the magnetic momentum of the proton and $-eV$ is the scalar potential by the proton. However, the gauge invariant Dirac equation has not been rigorously solved yet. Recently, Fukui et al. [2] tried that to solve the gauge invariant Dirac equation with using the Foldy-Wouthuysen transformation. However, it appears a divergent integral in their article, although they calculate it by the integration by part. However, mathematically speaking, their integration by part is not valid. The obtained value by them is just the finite part of the divergent integral. They calculated the shielding constant of the NMR spectroscopy with no singular results. So which may we use the finite part of the divergent integral or not? Such is the motivation of the present research.

DIVERGENT INTEGRAL: Fukui et al. [2] calculate the divergent integral by doing the integration by part, as given by

$$\int d\vec{r}\exp(-\alpha_1 r^2)\frac{\partial}{\partial x}\frac{1}{r}\frac{\mu_x y-\mu_y x}{r^3}\exp(-\alpha_2 r^2) \qquad (2\text{-}1)$$

$$=-\int d\vec{r}\left[\frac{\partial}{\partial x}\exp(-\alpha_1 r^2)\right]\frac{1}{r}\frac{\mu_x y-\mu_y x}{r^3}\exp(-\alpha_2 r^2) \qquad (2\text{-}2)$$

Mathematically speaking, the integral (2-1) is divergent in the meaning of the Riemann integral, but integral (2-2) is convergent in the same meaning so that the above derivation is not valid.

FOLDY-WOUTHUYSEN TRANSFORMATION: Applying the Foldy-Wouthuysen

transformation to the Dirac equation, we have the Hamiltonian h_+ which is too much complicated to write down here, so we show only one term among the total Hamiltonian (given by Fukui et al. [2]), which is given by

$$\vec{\sigma}\bullet\vec{\pi}V\vec{\sigma}\bullet\vec{\pi}=\vec{\sigma}\bullet(\vec{p}+e\vec{A})\,V\,\vec{\sigma}\bullet(\vec{p}+e\vec{A}) \qquad (3\text{-}1)$$

where $\vec{\sigma}$ is the Pauli spin matrix and the momentum $\vec{p}=\frac{\hbar}{i}\nabla$. Applying the usual formula for the Pauli spin matrix to (3-1), we have the term given by

$$i\vec{\sigma}\bullet(-i\nabla\times Ve\vec{A}) \qquad (3\text{-}2)$$

Thus we need the matrix element of $\nabla\times V\vec{A}$, which is divergent, as shown previously.

Of course, such is convergent for each of the finite nucleus models.

RESULTS: We calculate each matrix element over the 1s Slater-type orbital (STO) and over the 1s Non-integer n STO (NInSTO) of the hydrogen atom for the point charge nucleus and for several finite nucleus models (Spherical shell charge density distribution (CDD), Homogeneous CDD, and Gaussian CDD).

TABLE I. The comparison of the value of the matrix element, $<1s|(\nabla\times V\vec{A})_z|1s>$, over the 1s STO with that over the 1s NInSTO for several finite nucleus models. The value is except for $\mu_Z/c^2=0.8099702(-7)\,\sigma_{PZ}/2$, where σ_{PZ} is the Pauli spin matrix of the proton.

Finite nucleus model	1s STO	1s NInSTO
Point charge	∞	50077.64
Spherical Shell CDD (SSCDD)	100335.48	100389.12
Homogeneous CDD (HCDD)	-24.80.	-26.88
Gaussian CDD (GCDD)	-25.53	-31.40

1s STO $=\frac{\zeta^{3/2}}{\pi}\exp(-\zeta r)$; 1s NInSTO $=\sqrt{\frac{(2\zeta)^{2\nu+1}}{4\pi\Gamma(2\nu+1)}}\,r^{\nu-1}\exp(-\zeta r)$; $\zeta=1$;

$\nu=\sqrt{1-(1/c^2)}=0.99997337$; $c=137.035999139$

The other results, all discussions, and the conclusion as the use of the Gaussian-type orbital is doubtful in the relativistic calculations will be shown at September.

[1] W-M Sun, X-S Chen, X-F Lu, and F Wang, Phys. Rev. A82, 012107 (2010)

[2] H. Fukui, et al. Mol. Phys. 102, 641-648 (2004)