Momentum representation of Dirac relativistic wave functions

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A momentum representation of the Dirac relativistic wave functions for a hydrogenlike atom is obtained in a simple form by means of Fourier transformation. The expressions given are convenient for analytic as well as numerical applications.

The electronic momentum distributions in atomic systems are needed in the calculations of inner-shell ionization cross sections in a binary-encounter approximation, the problems related to Compton profiles, and many others. The Fourier transforms of nonrelativistic hydrogen functions and Slater type orbitals are well known.[1–3] However, in many of the applications the relativistic effects are seen to be important, for example, in low-energy inner-shell ionization. Therefore, it is of interest to have the momentum representation of Dirac relativistic wave functions convenient for analytic work or numerical applications wherein self-consistency effects are not included. The momentum representation of the Dirac relativistic wave functions has been considered earlier by Rubinowitz,[4] who utilized the direct Fourier transformation from configuration space and also by Levy,[5] who obtained the same results by solving directly the Dirac equation in the momentum representation. However, the final results were obtained by a complex form inconvenient for numerical as well as analytic applications. Recently, Komarov and Nankov[6] obtained the wave functions convenient for numerical applications by means of Fourier transformation. On the other hand, Lombardi[7] has obtained wave functions in a representation using variables p_r, p_θ, p_ϕ which have been chosen properly conjugate to the appropriate position variables. Following Weniger and Steinborn[3] or Komarov and Nanikov,[6] one can easily get the momentum representation of the Dirac relativistic wave functions. However, Dirac wave functions have spin-angle functions $\chi^{\mu}_{\kappa}(\hat{r})$ or $\chi^{\mu}_{\kappa}(\hat{p})$ instead of simple spherical harmonic functions $y_l^m(\hat{r})$ or $y_l^m(\hat{p})$ as compared to nonrelativistic or Slater wave functions. This is to say that orbital angular momentum $l(\kappa)$ which is integral goes over to nonintegral $l(\gamma)$ in the radial equation of relativistic mechanics,[8] where $\gamma=[\kappa^2-(\alpha Z)^2]^{1/2}$. This results in an expression which is not in the form of terminating series unlike the nonrelativistic expression. In this work we show that the resulting expression can still be a terminating series if the expressions are transformed appropriately. The final expressions obtained are simple and convenient for analytic applications. The Dirac wave functions for hydrogenlike atoms are given by[9,10]

$$\psi^{\mu}_{\kappa}(\vec{r})=\begin{pmatrix} g(r)\chi^{\mu}_{\kappa}(\hat{r}) \\ if(r)\chi^{\mu}_{-\chi}(\hat{r})\end{pmatrix} , \tag{1}$$

where $g(r)$ and $f(r)$ are upper and lower component radial wave functions, respectively. χ^{μ}_{κ} are the usual spin-angle functions.[9] The corresponding wave functions in the momentum representation are given by

$$\phi^{\mu}_{\kappa}(\vec{p})=(2\pi)^{-3/2}\int e^{i\vec{p}\cdot\vec{r}}\psi^{\mu}_{\kappa}(\vec{r})\,d\vec{r} = \begin{pmatrix} G(p)\chi^{\mu}_{\kappa}(\hat{p}) \\ iF(p)\chi^{\mu}_{-\kappa}(\hat{p})\end{pmatrix} , \tag{2}$$

where

$$G(p)=i^{l}\left(\frac{2}{\pi}\right)^{1/2}\int_0^\infty j_l(pr)g(r)r^2dr , \tag{3}$$

$$F(p)=i^{\bar{l}}\left(\frac{2}{\pi}\right)^{1/2}\int_0^\infty j_{\bar{l}}(pr)f(r)r^2dr . \tag{4}$$

Here $\bar{l}=l(-\kappa)=l-\kappa/|\kappa|$ and $|\kappa|=j+\frac{1}{2}$.

Following Weniger and Steinborn,[3] we get

$$\begin{aligned} K(l,n)&=\int_0^\infty r^{\gamma+1/2}e^{-p_0r}J_{l+1/2}(pr)\,{}_1F_1(-n,2\gamma+1,2p_0r)\,dr \\ &=\frac{\Gamma(n+1)\Gamma(2\gamma+1)}{\Gamma(l+\frac{3}{2})}2^{-l-1/2}p^{l+1/2}\sum_{m=0}^{n}\frac{(-2p_0)^m\Gamma(l+m+\gamma+2)}{\Gamma(m+1)\Gamma(n-m+1)\Gamma(2\gamma+m+1)}(p^2+p_0^2)^{-1/2(l+m+\gamma+2)} \\ &\quad\times{}_2F_1((l+m+\gamma+2)/2,\ (l-m-\gamma)/2,\ l+\tfrac{3}{2}\ ,p^2/(p^2+p_0^2)) . \end{aligned} \tag{5}$$

Using the identities[11,12]

$${}_2F_1(a,b,a+b+\tfrac{1}{2},4z(1-z))={}_2F_1(2a,2b,a+b+\tfrac{1}{2},z) \text{ for } |z|\le\tfrac{1}{2} , \tag{6}$$

$$\frac{d^n}{dz^n}{}_2F_1(a,b,c,z)=\frac{(a)_n(b)_n}{(c)_n}{}_2F_1(a+n,b+n,c+n,z) , \tag{7}$$

$${}_2F_1(a,2-a,\tfrac{3}{2},\sin^2 z)=\frac{\sin[(2a-2)z]}{(a-1)\sin 2z} . \tag{8}$$

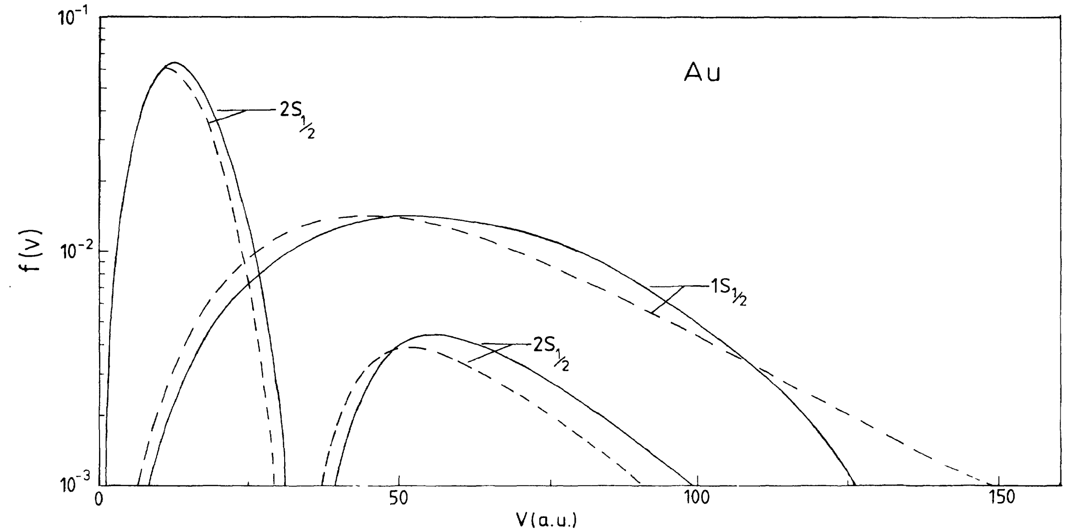

FIG. 1. Calculated velocity distribution function $f(v)$ as a function of velocity v for $1s_{1/2}$ and $2s_{1/2}$ electrons in Au. Full curve Dirac relativistic wave functions and broken curve nonrelativistic wave functions.

We get,

$$K(l,n)=-\Gamma(n+1)\Gamma(2\gamma+1)2^{1/2}\pi^{1/2}p^{l+1/2}\times\sum_{m=0}^{n}\frac{(-2p_0)^m(p^2+p_0^2)^{-1/2(l+m+\gamma+2)}}{\Gamma(m+1)\Gamma(n-m+1)\Gamma(2\gamma+m+1)\Gamma(l-m-\gamma)\sin[\pi(m+\gamma)]}\times\left(\frac{1}{\sin x}\frac{d}{dx}\right)^l[\sin\{(m+\gamma)x\}\cot x+\cos\{(m+\gamma)x\}]\ , \tag{9}$$

where $x=\tan^{-1}(p/p_0)$. Therefore, we have the final expressions,

$$G(p)=i^l(1+\epsilon)^{1/2}p^{-1/2}(2p_0)^{\gamma-1}C_{nx}\times[-n_rK(l,n_r-1)+(N-\kappa)K(l,n_r)]\ , \tag{10}$$

$$F(p)=i^{\bar{l}}(1-\epsilon)^{1/2}p^{-1/2}(2p_0)^{\gamma-1}C_{N\kappa}\times[n_rK(\bar{l},n_r-1)+(N-\kappa)K(\bar{l},n_r)]\ , \tag{11}$$

with the normalization condition

$$\int_0^\infty dp\,p^2(|G|^2+|F|^2)=1\ ,$$

where

$$N=[(n_r+|\kappa|)^2-2n_r(|\kappa|-\gamma)]^{1/2}\ ,$$

$$n_r=\text{radial quantum number}=0,1,2,\cdots\ ,$$

$$C_{N\kappa}=\frac{[(2\gamma+n_r+1)]^{1/2}(2p_0)^{3/2}}{\Gamma(2\gamma+1)[4N(N-\kappa)\Gamma(n_r+1)]^{1/2}}\ ,$$

$$p_0=\frac{Z}{Na_0},\quad \gamma=[\kappa^2-(\alpha Z)^2]^{1/2}\ ,$$

$$\epsilon=\left[1+\frac{(\alpha Z)^2}{(n_r+\gamma)^2}\right]^{-1/2}\ . \tag{12}$$

It is evident from Eq. (9) that the expressions of Eqs. (10) and (11) reduce to simple form for most of the practical applications.

For example, for K shell, we get,

$$G(p)=\frac{C}{p}(1+\epsilon)^{1/2}(p^2+p_0^2)^{-(\gamma+1)/2}\sin[(\gamma+1)x]\ , \tag{13}$$

$$F(p)=-\frac{C}{p\gamma}(1-\epsilon)^{1/2}(p^2+p_0^2)^{-(\gamma+1)/2}\times\left\{(\gamma+1)\cos[(\gamma+1)x]-\frac{p_0}{p}\sin[(\gamma+1)x]\right\} \tag{14}$$

where

$$C=\frac{\Gamma(\gamma+1)(2p_0)^{\gamma+1/2}}{\pi^{1/2}\sqrt{\Gamma(2\gamma+1)}}\ .$$

In the nonrelativistic limit, i.e., $\gamma\to 1$ and $\epsilon\to 1$ we get

$$G(p)=\frac{(2p_0)^{5/2}}{\pi^{1/2}(p^2+p_0^2)^2}\ , \tag{15}$$

which coincides with the nonrelativistic result.[9]

Figure 1 presents the velocity distribution function $f(v)$ with the normalization condition $\int f(v)dv=1$ for $1s_{1/2}$ and $2s_{1/2}$ electrons in Au. A comparison with nonrelativistic distribution function is also shown. It may be noted that $f(v)\to 0$ as $v\to c$ (the velocity of light in vacuum) in the relativistic case, whereas $f(v)\to 0$ as $v\to\infty$ in the nonrelativistic case.

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