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2008 J. Phys. A: Math. Theor. 41 055306

(http://iopscience.iop.org/1751-8121/41/5/055306)

J. Phys. A: Math. Theor. **41** (2008) 055306 (12pp) doi:10.1088/1751-8113/41/5/055306

Radial position–momentum uncertainties for Klein–Gordon hydrogen-like atoms

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Received 26 August 2007, in final form 7 December 2007
Published 23 January 2008
Online at stacks.iop.org/JPhysA/41/055306

Abstract

We show how the radial position–momentum uncertainty product can be obtained analytically for Klein–Gordon hydrogen-like atoms. Some interesting features of this quantum system are found. First, for the same principal quantum number n, when the angular momentum quantum number l increases, the uncertainties Δp_r and $\Delta r \Delta p_r$ decrease. However, Δr does not always decrease, which is different from the non-relativistic hydrogen-like atoms case, where it always decreases. Second, for same l both Δr and $\Delta r \Delta p_r$ increase as n increases. Third, all uncertainties for same n and $l = n - 1$ are smallest in comparison with those for same n but $l \neq n-1$. Fourth, $\Delta r \Delta p_r$ is independent of the value of charge Z in the non-relativistic case, while it is related to the value of charge Z in the relativistic case. Fifth, the relativistic corrections to the non-relativistic uncertainties are very small when the values of the charge Z are not too big. However, relativistic corrections to them will appear explicitly for large Z.

PACS numbers: 03.65.−w, 03.65.Pm, 03.65.Ta

1. Introduction

The great physicist Heisenberg introduced into physics a famous 'uncertainty principle', which is one of the deepest philosophical contributions in quantum mechanics. The frequently quoted statement of this principle is: 'it is impossible to know both the position and the momentum of a particle at a given momentum to an arbitrary degree of accuracy' [1], which is expressed as $\Delta x \Delta p \geqslant \hbar/2$.

It is usually known that the position–momentum uncertainty products for the harmonic oscillator and non-relativistic hydrogen atom were obtained analytically 76 years ago [2].

Many decades later, the position–momentum uncertainty relations for several exactly solvable potentials such as the symmetric Pöschl–Teller, symmetric Rosen–Morse and Morse potentials were discussed [3]. It should be noted that almost all contributions to this topic are limited to the one-dimensional Schrödinger equation. Recently, the radial position–momentum uncertainties of the non-relativistic hydrogen-like atoms in three dimensions have been studied [4]. On the other hand, we have investigated the radial position–momentum uncertainties of the Dirac hydrogen-like atoms in three dimensions [5]. However, the radial position–momentum uncertainties of the Klein–Gordon equation in a Coulomb potential field was not considered before. The purpose of this work is to show how the position–momentum uncertainty relations for the relativistic hydrogen-like atoms can be obtained analytically and then to investigate their properties.

This paper is organized as follows. In section 2, we present the exact uncertainty relations Δr, Δp_r and $\Delta r \Delta p_r$ for the relativistic hydrogen-like atoms by using recently developed MATHEMATICA package INTEPFFLL [6, 7]. Section 3 is devoted to the study of some interesting properties of these position–momentum uncertainties by taking a few typical values of the charge Z. In section 4, we study two special cases for $l = 0$ and $l = n - 1$. The non-relativistic limit is carried out in section 5. Some concluding remarks are given in section 6.

2. Analytical position–momentum uncertainty

Let us first review the exact solutions of the relativistic hydrogen-like atoms described by the Klein–Gordon equation before studying the mean values of the radial position r and momentum p_r.

Generally speaking, we can write down the Klein–Gordon equation with a central potential $V(r)$ as follows [8]:

$$\left[(E - V(r))^2 - m_0^2c^4 + \hbar^2c^2\nabla^2\right]\psi(\mathbf{r}) = 0. \tag{1}$$

If taking $\psi(\mathbf{r}) = \frac{R(r)}{r}Y_{lm}(\theta,\phi) \equiv u(r)Y_{lm}(\theta,\phi)$ and the Coulomb potential $V(r) = -Ze^2/r$, we obtain the radial Klein–Gordon equation as

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1) - (Z\alpha)^2}{r^2} + \frac{2EZ\alpha}{\hbar cr} + \frac{E^2 - m_0^2c^4}{\hbar^2c^2}\right]R(r) = 0, \qquad \alpha = \frac{e^2}{\hbar c}, \tag{2}$$

whose solution is given by [8]

$$R_{nl}(\rho) = N_{nl}\rho^{\mu+1/2}\,\mathrm{e}^{-\rho/2}{}_1F_1(-n_r, 2\mu+1, \rho), \tag{3}$$

where

$$\rho = \beta r, \qquad \beta = \frac{2}{\hbar c}\sqrt{m_0^2c^4 - E_{nl}^2}, \qquad \mu = \sqrt{\left(l+\frac{1}{2}\right)^2 - (Z\alpha)^2}. \tag{4}$$

The corresponding energy spectrum is written as

$$\begin{aligned} E_{nl} &= m_0c^2\left[1 + \frac{(Z\alpha)^2}{\left(n_r + \frac{1}{2} + \mu\right)^2}\right]^{-1/2} \\ &= m_0c^2\left[1 + \frac{(Z\alpha)^2}{\left(n - l - \frac{1}{2} + \sqrt{\left(l+\frac{1}{2}\right)^2 - (Z\alpha)^2}\right)^2}\right]^{-1/2}, \end{aligned} \tag{5}$$

$$n = n_r + l + 1 = 1, 2, 3, \ldots, \qquad l = 0, 1, 2, \ldots (n-1),$$

where n_r is the radial quantum number, n the principal quantum number and l the azimuthal quantum number. It should be noted that this energy spectrum is first given by Miromontes and Pajares [9]. The N_{nl} is the normalization constant to be given below. For convenience and the later use, we express β as another form

$$\begin{aligned}\beta &= \frac{2}{Za_0}\sqrt{\frac{1}{\left(\frac{1}{2}+l-n-\mu\right)^2+Z^2\alpha^2}}\\ &= \frac{2}{Za_0}\sqrt{\frac{1}{\left(\frac{1}{2}+n_r+\mu\right)^2+Z^2\alpha^2}},\\ a_0 &= \frac{\hbar^2}{m_0e^2}.\end{aligned} \tag{6}$$

Before proceeding further, let us introduce our recently developed MATHEMATICA package INTEPFFLL. As its name implies, this package can be used to calculate the integration containing exponential function, power function and two confluent hypergeometric functions or associated Laguerre polynomials [6, 7]

$$I_{FF}(n,\Delta n,m,\Delta m,\lambda) = \int_0^\infty \mathrm{e}^{-x}x^{m+\lambda}F(-n,m;x)F[-(n+\Delta n),m+\Delta m;x]\,\mathrm{d}x, \tag{7}$$

where n and m are symbols, but Δn, Δm and λ are integers and $\Delta n \geqslant 0$. As shown in [5–7], the tedious task to calculate the above integration can be performed easily and quickly by this MATHEMATICA package. From the normalization condition $\int_0^\infty u(r)^2r^2\,\mathrm{d}r = \frac{1}{\beta}\int_0^\infty R(\rho)^2\,\mathrm{d}\rho = 1$ and using INTEPFFLL, we can easily obtain the normalization constant as

$$N_{n_rl} = \frac{1}{\Gamma(1+2\mu)}\sqrt{\frac{\beta\Gamma(1+n_r+2\mu)}{(1+2n_r+2\mu)n_r!}}. \tag{8}$$

We now derive the uncertainty Δr for the relativistic hydrogen-like atoms. To this end, from equation (3) we can evaluate the expectation values of r^s as follows:

$$\begin{aligned}\langle r^s\rangle &= \int_0^\infty R_{nl}(r)^2r^s\,\mathrm{d}r = \frac{1}{\beta^{s+1}}\int_0^\infty R_{nl}(\rho)^2\rho^s\,\mathrm{d}\rho\\ &= \frac{N_{n_rl}^2}{\beta^{1+s}}I_{FF}(n_r,0,2\mu+1,0,s),\end{aligned} \tag{9}$$

from which we obtain the mean values of r and r^2 for an electron in the relativistic hydrogen-like atoms as

$$\langle r\rangle = \frac{2\left[3n_r^2+3n_r(1+2\mu)+(1+\mu)(1+2\mu)\right]}{\beta(1+2nr+2\mu)}, \tag{10}$$

$$\langle r^2\rangle = \frac{2[3+5n_r(1+nr)+5\mu+10n_r\mu+2\mu^2]}{\beta^2}. \tag{11}$$

The uncertainty Δr in the measurement of the distance of the electron from the nucleus can be obtained as

$$\begin{aligned}\Delta r = \sqrt{\langle r^2\rangle-\langle r\rangle^2} &= \frac{2}{\beta(1+2n_r+2\mu)}\big\{2n_r^4+n_r^3(4+8\mu)+n_r^2[7+12\mu(\mu^2+1)]\\ &\quad +n_r[5+2\mu(7+6\mu+4\mu^2)]+(1+\mu)(1+2\mu)^2\big\}^{1/2}\end{aligned}$$

$$= \frac{a_0\sqrt{(1+2n_r+2\mu)^2+4Z^2\alpha^2}}{2\sqrt{2}Z(1+2n_r+2\mu)}\big\{2n_r^4+n_r^3(4+8\mu)+n_r^2[7+12\mu(\mu^2+1)] + n_r[5+2\mu(7+6\mu+4\mu^2)]+(1+\mu)(1+2\mu)^2\big\}^{1/2}, \tag{12}$$

which means that Δr is inversely proportional to the value of charge Z except for its dependence on the principal quantum number n ($n = n_r + l + 1$) and azimuthal quantum number l. On the other hand, the relative dispersion $\Delta r/\langle r\rangle$ in the measurement of radial position, which also depends on the quantum numbers n and l as well as the value of the charge Z, gives us a possible estimate of how indeterminate the measurement in radial position r is relative to the average radial position $\langle r\rangle$ for an electron in the relativistic hydrogen-like atoms.

In order to obtain the product $\Delta r\Delta p_r$ of the uncertainties Δr and Δp_r, we have to study the radial momentum uncertainty Δp_r. To this end, we start by considering the definition of the radial momentum [10]

$$p_r = -\mathrm{i}\hbar\frac{1}{r}\frac{\partial}{\partial r}r = -\mathrm{i}\hbar\left(\frac{\partial}{\partial r}+\frac{1}{r}\right), \tag{13}$$

from which we can obtain $\langle p_r\rangle = 0$. This coincides with the result for other exactly solvable systems [2]–[5].

Now, let us derive the mean value of p_r^2

$$\langle p_r^2\rangle = (-i\hbar)^2\int_0^\infty r^2u(r)\frac{1}{r}\frac{\partial^2}{\partial r^2}[ru(r)]\,\mathrm{d}r = -\hbar^2\int_0^\infty R(r)\frac{\partial^2}{\partial r^2}R(r)\,\mathrm{d}r. \tag{14}$$

By substituting equation (3) into equation (14) we can obtain a very complicated expression for $\langle p_r^2\rangle$, which includes six integrals $I_{FF}(n, \Delta n, m, \Delta m, \lambda)$ with different n, Δn, m and Δm (see appendix). By using package INTEPFFLL [6, 7] and greatly simplifying, we can finally obtain the uncertainty $\triangle p_r$ for radial momentum p_r as follows:

$$\begin{aligned}\triangle p_r &= \sqrt{\langle p_r^2\rangle - \langle p_r\rangle^2}\\ &= \frac{\hbar\beta}{2}\sqrt{\frac{1+2\mu(1+2n_r)}{2\mu(1+2n_r+2\mu)}}\\ &= \frac{\hbar Z}{a_0}\sqrt{\frac{2(1+2\mu+4n_r\mu)}{\mu(1+2n_r+2\mu)[4Z^2\alpha^2+(1+2n_r+2\mu)^2]}}\\ &= \frac{\sqrt{2}\hbar Z}{a_0}\sqrt{\frac{2\mu(2n-2l-1)+1}{\mu[2(n-l+\mu)-1]\{4Z^2\alpha^2+[2(n-l+\mu)-1]^2\}}},\end{aligned} \tag{15}$$

which also depends on the quantum numbers n and l and is proportional to the value of charge Z.

Based on the results (12) and (15), we finally obtain a complicated expression of the product of the radial position–momentum uncertainties

$$\Delta r\Delta p_r = \frac{\hbar}{2+4n_r+4\mu}\sqrt{\frac{1+2\mu+4n_r\mu}{\mu(1+2n_r+2\mu)}}\big\{2n_r^4+n_r^3(4+8\mu)+n_r^2[7+12\mu(\mu^2+1)] + n_r[5+2\mu(7+6\mu+4\mu^2)]+(1+\mu)(1+2\mu)^2\big\}^{1/2}, \tag{16}$$

from which we find that the product $\Delta r\Delta p_r$ of the radial position–momentum uncertainty relations is analytical. Also, it depends on the value of the charge Z as shown in equation (4). We study some properties of these uncertainties by taking a few typical values of the charge Z as shown below.

Table 1. Some uncertainties of the Klein–Gordon hydrogen-like atom H ($Z = 1$).

(nl)	$\left(\frac{\langle r\rangle}{a_0}\right)_R$	$\left(\frac{\langle r\rangle}{a_0}\right)_N$	$\left(\frac{\Delta r}{a_0}\right)_R$	$\left(\frac{\Delta r}{a_0}\right)_N$	$\left(\frac{\Delta r}{\langle r\rangle}\right)_R$	$\left(\frac{\Delta r}{\langle r\rangle}\right)_N$	$\left(\frac{\Delta p_r a_0}{\hbar}\right)_R$	$\left(\frac{a_0 \Delta p_r}{\hbar}\right)_N$	$\left(\frac{\Delta r \Delta p_r}{\hbar}\right)_R$	$\left(\frac{\Delta r \Delta p_r}{\hbar}\right)_N$
(10)	1.499 907	1.500 000	0.865 987	0.866 025	0.577 361	0.577 350	1.000 080	1.000 000	0.866 056	0.866 025
(20)	5.999 747	6.000 000	2.449 397	2.449 489	0.408 250	0.408 248	0.500 023	0.500 000	1.224 756	1.224 745
(21)	4.999 953	5.000 000	2.236 055	2.236 068	0.372 692	0.447 214	0.288 677	0.288 675	0.645 499	0.645 497
(30)	13.499 59	13.500 00	4.974 791	4.974 937	0.368 514	0.368 514	0.333 344	0.333 333	1.658 318	1.658 312
(31)	12.499 90	12.500 00	4.873 362	4.873 397	0.389 872	0.389 872	0.248 454	0.248 452	1.210 805	1.210 805
(32)	10.499 96	10.500 00	3.968 619	3.968 627	0.377 965	0.377 965	0.149 072	0.149 071	0.591 608	0.591 608
(40)	23.999 43	24.000 00	8.485 082	8.485 281	0.353 554	0.353 554	0.250 006	0.250 000	2.121 323	2.121 320
(41)	22.999 85	23.000 00	8.426 095	8.426 149	0.366 354	0.366 354	0.204 125	0.204 124	1.719 979	1.719 981
(42)	20.999 93	21.000 00	7.937 232	7.937 254	0.377 965	0.377 965	0.158 114	0.158 114	1.254 990	1.254 990
(43)	17.999 97	18.000 00	5.999 993	6.000 000	0.333 334	0.333 333	0.094 491	0.094 491	0.566 947	0.566 947
(50)	37.499 27	37.500 00	12.990 13	12.990 38	0.346 410	0.346 410	0.200 004	0.200 000	2.598 078	2.598 076
(51)	36.499 80	36.500 00	12.951 76	12.951 83	0.354 845	0.354 845	0.171 271	0.171 270	2.218 255	2.218 258
(52)	34.499 90	34.500 00	12.639 19	12.639 23	0.366 354	0.366 354	0.144 222	0.144 222	1.822 854	1.822 855
(53)	31.499 95	31.500 00	11.521 70	11.521 72	0.365 769	0.365 769	0.112 123	0.112 122	1.291 842	1.291 843
(54)	27.499 97	27.500 00	8.291 557	8.29156	0.301 512	0.301 511	0.066 667	0.066 667	0.552 771	0.552 772
(60)	53.999 11	54.000 00	18.492 94	18.493 24	0.342 467	0.342 467	0.166 667	0.166 667	3.082 208	3.082 207
(61)	52.999 75	53.000 00	18.466 09	18.466 19	0.348 419	0.348 419	0.146 987	0.146 986	2.714 271	2.714 274
(62)	50.999 87	51.000 00	18.248 24	18.248 29	0.357 810	0.357 810	0.129 100	0.129 099	2.355 842	2.355 844
(63)	47.999 93	48.000 00	17.492 83	17.492 86	0.364 435	0.364 435	0.109 109	0.109 109	1.908 626	1.908 627
(64)	43.999 95	44.000 00	15.556 34	15.556 35	0.353 553	0.353 554	0.084 863	0.084 863	1.320 151	1.320 152
(65)	38.999 97	39.000 00	10.816 65	10.816 65	0.277 350	0.277 350	0.050 252	0.050 252	0.543 557	0.543 557

Table 2. Some uncertainties of the Klein–Gordon hydrogen-like atom Na ($Z = 11$).

(nl)	$\left(\frac{\langle r\rangle}{a_0}\right)_R$	$\left(\frac{\langle r\rangle}{a_0}\right)_N$	$\left(\frac{\Delta r}{a_0}\right)_R$	$\left(\frac{\Delta r}{a_0}\right)_N$	$\left(\frac{\Delta r}{\langle r\rangle}\right)_R$	$\left(\frac{\Delta r}{\langle r\rangle}\right)_N$	$\left(\frac{\Delta p_r a_0}{\hbar}\right)_R$	$\left(\frac{a_0 \Delta p_r}{\hbar}\right)_N$	$\left(\frac{\Delta r \Delta p_r}{\hbar}\right)_R$	$\left(\frac{\Delta r \Delta p_r}{\hbar}\right)_N$
(10)	0.135 333	0.136 364	0.078 304	0.078 730	0.578 603	0.577 350	11.108 18	11.000 00	0.869 813	0.866 025
(20)	0.542 654	0.545 455	0.221 658	0.222 681	0.408 470	0.408 248	5.531 467	5.500 000	1.226 094	1.224 745
(21)	0.454 032	0.454 546	0.203 137	0.203 279	0.374 340	0.447 214	3.178 560	3.175 426	0.645 683	0.645 497
(30)	1.222 702	1.227 273	0.450 652	0.452 267	0.368 571	0.368 514	3.681 300	3.666 667	1.658 986	1.658 312
(31)	1.135 305	1.136 364	0.442 653	0.443 036	0.389 898	0.389 872	2.735 129	2.732 972	1.210 714	1.210 805
(32)	0.954 125	0.954 546	0.360 692	0.360 784	0.378 034	0.377 965	1.640 324	1.639 783	0.591 652	0.591 608
(40)	2.175 478	2.181 818	0.769 183	0.771 389	0.353 570	0.353 553	2.758 412	2.750 000	2.121 723	2.121 320
(41)	2.089 278	2.090 909	0.765 414	0.766 014	0.366 353	0.366 354	2.246 825	2.245 366	1.719 752	1.719 981
(42)	1.908 362	1.909 091	0.721 323	0.721 569	0.377 980	0.377 965	1.739 772	1.739 253	1.254 936	1.254 990
(43)	1.635 982	1.636 364	0.545 383	0.545 455	0.333 367	0.333 333	1.039 569	1.039 402	0.566 963	0.566 947
(50)	3.400 981	3.409 091	1.178 146	1.180 944	0.346 414	0.346 410	2.205 453	2.200 000	2.598 346	2.598 076
(51)	3.359 710	3.318 182	1.176 633	1.177 439	0.354 838	0.354 845	1.885 002	1.883 967	2.217 955	2.218 258
(52)	3.135 303	3.136 364	1.148 635	1.149 020	0.366 355	0.366 354	1.586 868	1.586 443	1.822 732	1.822 855
(53)	2.863 043	2.863 636	1.047 244	1.047 429	0.365 780	0.365 769	1.233 535	1.233 346	1.291 813	1.291 843
(54)	2.499 639	2.500 000	0.753 718	0.753 778	0.301 531	0.301 511	0.733 402	0.733 333	0.552 779	0.552 771
(60)	4.899 211	4.909 091	1.677 816	1.681 204	0.342 466	0.342 467	1.837 152	1.833 333	3.082 403	3.082 207
(61)	4.815 388	4.818 182	1.677 735	1.678 744	0.348 411	0.348 419	1.617 614	1.616 848	2.713 929	2.714 274
(62)	4.634 962	4.636 364	1.658 419	1.658 935	0.357 806	0.357 810	1.420 435	1.420 094	2.355 676	2.355 844
(63)	4.362 813	4.363 636	1.589 971	1.590 260	0.364 437	0.364 435	1.200 372	1.200 198	1.908 556	1.908 627
(64)	3.999 479	4.000 000	1.414 064	1.414 214	0.353 562	0.353 553	0.933 574	0.933 488	1.320 133	1.320 151
(65)	3.545 106	3.545 455	0.983 280	0.983 332	0.277 363	0.277 350	0.552 805	0.552 771	0.543 562	0.543 557

3. Some properties of uncertainties in radial position and momentum

Due to the complicated expressions for the uncertainties Δr, Δp_r, relative dispersion $\Delta r/\langle r\rangle$ and the product $\Delta r \Delta p_r$, we attempt to show some interesting properties of these uncertainties in radial position and momentum by doing some typical calculations. Some useful results for principal quantum number $n \in [1, 6]$ and $Z = 1, 11, 37, 55$ with different azimuthal quantum number l are listed in tables 1–4, in which we denote by $()_N$ and $()_R$ as the non-relativistic and relativistic results for simplicity. We do not list the results of other values of charge Z for simplicity. On the other hand, for better visualization some properties of these uncertainties are illustrated in figures 1–4. We find that the relativistic corrections to the non-relativistic

Table 3. Some uncertainties of the Klein–Gordon hydrogen-like atom Rb ($Z = 37$).

(nl)	$\left(\frac{\langle r\rangle}{a_0}\right)_R$	$\left(\frac{\langle r\rangle}{a_0}\right)_N$	$\left(\frac{\Delta r}{a_0}\right)_R$	$\left(\frac{\Delta r}{a_0}\right)_N$	$\left(\frac{\Delta r}{\langle r\rangle}\right)_R$	$\left(\frac{\Delta r}{\langle r\rangle}\right)_N$	$\left(\frac{\Delta p_r a_0}{\hbar}\right)_R$	$\left(\frac{a_0 \Delta p_r}{\hbar}\right)_N$	$\left(\frac{\Delta r \Delta p_r}{\hbar}\right)_R$	$\left(\frac{\Delta r \Delta p_r}{\hbar}\right)_N$
(10)	0.036 847	0.040 541	0.021 859	0.023 406	0.593 227	0.577 350	42.031 70	37.000 00	0.918 764	0.866 025
(20)	0.152 038	0.162 162	0.062 514	0.066 202	0.411 174	0.408 249	19.917 45	18.500 00	1.245 119	1.224 745
(21)	0.133 399	0.135 135	0.059 953	0.060 434	0.394 328	0.447 214	10.802 49	10.680 98	0.647 639	0.645 497
(30)	0.348 316	0.364 865	0.128 629	0.134 458	0.369 288	0.368 514	12.982 93	12.333 33	1.669 979	1.658 312
(31)	0.334 254	0.337 838	0.130 417	0.131 713	0.390 174	0.389 872	9.276 154	9.192 724	1.209 770	1.210 805
(32)	0.282 368	0.283 784	0.106 949	0.107 261	0.378 757	0.377 965	5.536 347	5.515 634	0.592 105	0.591 608
(40)	0.625 677	0.648 649	0.221 359	0.229 332	0.353 791	0.353 553	9.620 438	9.250 000	2.129 569	2.121 320
(41)	0.616 098	0.621 622	0.225 704	0.227 734	0.366 344	0.366 354	7.608 975	7.552 593	1.717 373	1.719 981
(42)	0.565 110	0.567 568	0.213 691	0.214 520	0.378 140	0.377 965	5.870 077	5.850 214	1.254 381	1.254 990
(43)	0.485 200	0.486 487	0.161 921	0.162 162	0.333 721	0.333 333	3.502 538	3.496 171	0.567 135	0.566 947
(50)	0.984 119	1.013 514	0.340 974	0.351 091	0.346 477	0.346 410	7.638 917	7.400 000	2.604 675	2.598 076
(51)	0.978 998	0.986 487	0.347 319	0.350 050	0.354 770	0.354 845	6.376 894	6.336 981	2.214 814	2.218 258
(52)	0.928 855	0.932 432	0.340 302	0.341 601	0.366 367	0.366 354	5.352 482	5.336 216	1.821 460	1.822 855
(53)	0.849 352	0.851 351	0.310 776	0.311 398	0.365 897	0.365 769	4.155 749	4.148 528	1.291 506	1.291 843
(54)	0.742 027	0.743 243	0.223 895	0.224 096	0.301 734	0.301 511	2.469 294	2.466 667	0.552 862	0.552 771
(60)	1.423 642	1.459 460	0.487 557	0.499 817	0.342 472	0.342 467	6.333 403	6.166 667	3.087 896	3.082 207
(61)	1.422 968	1.432 432	0.495 670	0.499 086	0.348 335	0.348 419	5.468 030	5.438 489	2.710 339	2.714 274
(62)	1.373 651	1.378 378	0.491 456	0.493 197	0.357 773	0.357 810	4.789 723	4.776 679	2.353 937	2.355 844
(63)	1.294 525	1.297 297	0.471 809	0.472 780	0.364 465	0.364 435	4.043 646	4.037 031	1.907 826	1.908 627
(64)	1.187 436	1.189 189	0.419 938	0.420 442	0.353 651	0.353 553	3.143 202	3.139 913	1.319 950	1.320 151
(65)	1.052 881	1.054 054	0.292 166	0.292 342	0.277 492	0.277 350	1.860 614	1.859 320	0.543 608	0.543 557

Table 4. Some uncertainties of the Klein–Gordon hydrogen-like atom Cs ($Z = 55$).

(nl)	$\left(\frac{\langle r\rangle}{a_0}\right)_R$	$\left(\frac{\langle r\rangle}{a_0}\right)_N$	$\left(\frac{\Delta r}{a_0}\right)_R$	$\left(\frac{\Delta r}{a_0}\right)_N$	$\left(\frac{\Delta r}{\langle r\rangle}\right)_R$	$\left(\frac{\Delta r}{\langle r\rangle}\right)_N$	$\left(\frac{\Delta p_r a_0}{\hbar}\right)_R$	$\left(\frac{a_0 \Delta p_r}{\hbar}\right)_N$	$\left(\frac{\Delta r \Delta p_r}{\hbar}\right)_R$	$\left(\frac{\Delta r \Delta p_r}{\hbar}\right)_N$
(10)	0.021 083	0.027 273	0.013 085	0.015 746	0.620 641	0.577 350	79.743 40	55.000 00	1.04346	0.866 025
(20)	0.091 844	0.109 091	0.038 284	0.044 536	0.416 832	0.408 248	34.048 30	27.500 00	1.30349	1.224 745
(21)	0.088 309	0.090 909	0.039 932	0.040 656	0.434 785	0.447 214	16.286 70	15.877 13	0.650 367	0.645 497
(30)	0.217 186	0.245 455	0.080 551	0.090 453	0.370 883	0.368 514	21.254 50	18.333 33	1.71207	1.658 312
(31)	0.221 898	0.227 273	0.086 662	0.088 607	0.390 550	0.389 872	13.945 10	13.664 86	1.20851	1.210 805
(32)	0.188 798	0.190 909	0.071 692	0.072 157	0.379 729	0.377 965	8.267 560	8.198 892	0.592 718	0.591 608
(40)	0.397 078	0.436 364	0.140 705	0.154 278	0.354 352	0.353 553	15.392 00	13.750 00	2.16574	2.121 320
(41)	0.409 895	0.418 182	0.150 157	0.153 203	0.366 331	0.366 354	11.415 80	11.226 83	1.71417	1.719 981
(42)	0.378 154	0.381 818	0.143 076	0.144 314	0.378 353	0.377 965	8.762 030	8.696 264	1.25364	1.254 990
(43)	0.325 358	0.327 273	0.108 732	0.109 091	0.334 192	0.333 333	5.218 020	5.197 012	0.567 365	0.566 947
(50)	0.631 516	0.681 818	0.218 943	0.236 189	0.346 694	0.346 410	12.049 60	11.000 00	2.63818	2.598 076
(51)	0.652 398	0.663 636	0.231 391	0.235 488	0.354 678	0.354 845	9.553 430	9.419 837	2.21058	2.218 258
(52)	0.621 939	0.627 273	0.227 867	0.229 804	0.366 382	0.366 354	7.986 040	7.932 213	1.81976	1.822 855
(53)	0.569 751	0.572 727	0.208 559	0.209 486	0.366 053	0.365 769	6.190 550	6.166 731	1.2911	1.291 843
(54)	0.498 190	0.500 000	0.150 456	0.150 756	0.302 004	0.301 511	3.675 320	3.666 667	0.552 972	0.552 771
(60)	0.920 500	0.981 818	0.315 321	0.336 241	0.342 554	0.342 467	9.894 770	9.166 667	3.12003	3.082 207
(61)	0.949 432	0.963 636	0.330 624	0.335 749	0.348 234	0.348 419	8.183 010	8.084 240	2.7055	2.714 274
(62)	0.920 224	0.927 273	0.329 191	0.331 787	0.357 729	0.357 810	7.143 610	7.100 469	2.35161	2.355 844
(63)	0.868 600	0.872 727	0.316 605	0.318 052	0.364 501	0.364 435	6.022 800	6.000 992	1.90685	1.908 627
(64)	0.797 391	0.800 000	0.282 093	0.282 843	0.353 770	0.353 553	4.678 270	4.667 438	1.31971	1.320 151
(65)	0.707 346	0.709 091	0.196 404	0.196 666	0.277 664	0.277 350	2.768 110	2.763 854	0.543 669	0.543 557

values of these uncertainties are very small when the value of charge Z is not too big, while the relativistic corrections to them will appear for large Z (e.g. $Z = 55$).

By analyzing tables 1–4 and figures 1–4 carefully, we find that there are a few kinds of change rules. First, for the same principal quantum number n, the analytical uncertainties Δp_r and the product $\Delta r \Delta p_r$ decrease as l increases. It should be pointed out that, in the non-relativistic hydrogen-like atoms case, the average radial position $\langle r\rangle$ and the uncertainty Δr also decrease as l increases except for uncertainties Δp_r and $\Delta r \Delta p_r$, as discussed in [4]. On the other hand, for same n the $\langle r\rangle$ first increases and then decreases as l increases for large values $Z = 37, 55$, namely, $\langle r\rangle$ for states $(n, l = 1)(n \in [3, 6])$ are biggest. This kind of property does not exist at all in the non-relativistic hydrogen-like atom case. The

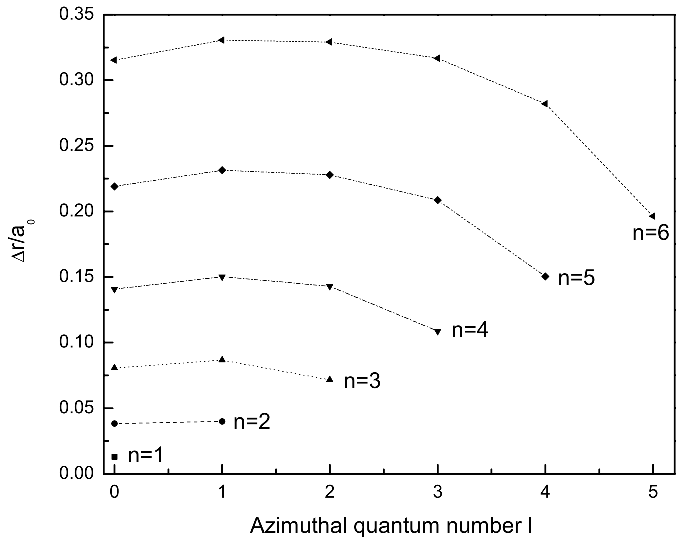

Figure 1. The change rule in the uncertainty $\triangle r$ with respect to quantum numbers n and l for $Z = 55$. For the same l, this uncertainty increases as n increases.

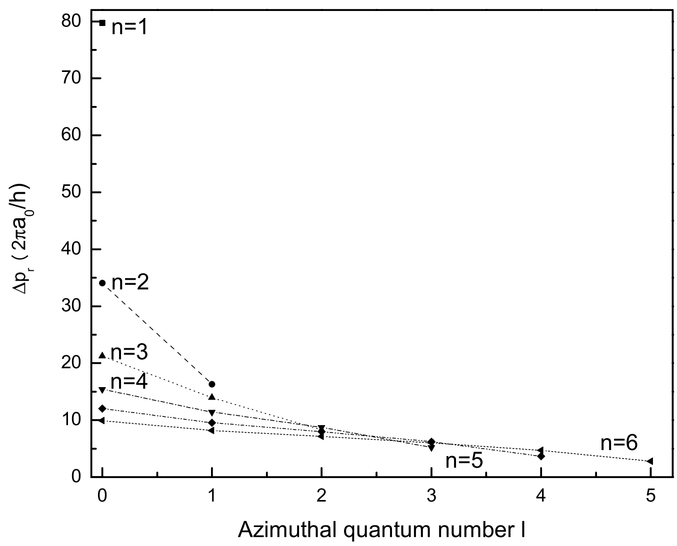

Figure 2. The change rule in the uncertainty $\triangle p_r$ with respect to quantum numbers n and l for $Z = 55$. For the same n, this uncertainty decreases as l increases. Here $\hbar = h/2\pi$ is used.

difference between them arises from the relativistic corrections to the non-relativistic values of these uncertainties. Second, all uncertainties for same n and $l = n - 1$ are smallest in comparison with those for same n but $l \neq n - 1$. This property is not new since it also exists in the non-relativistic case. Third, it is found that for the same state (n, l), the relativistic corrections to non-relativistic values of these uncertainties are very small when the values of charge Z are not too big, while the relativistic corrections to them will appear when Z is very

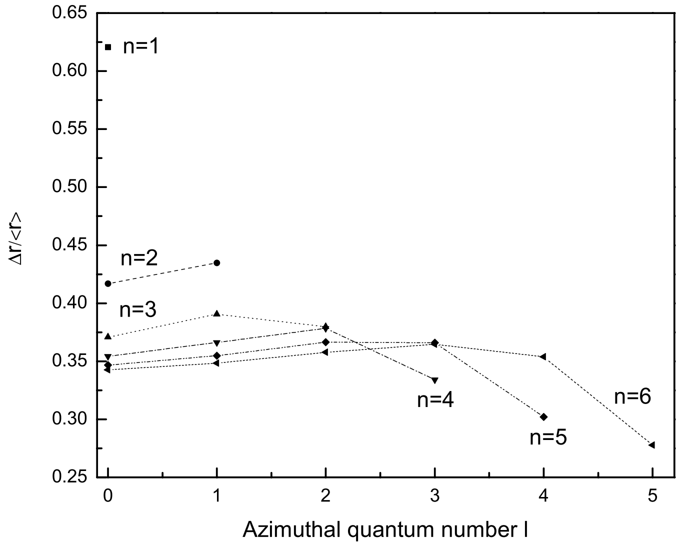

Figure 3. The change rule in the relative dispersion $\triangle r/\langle r\rangle$ with respect to quantum numbers n and l for $Z = 55$. It is found that there does not exist explicit change rule for same n or l.

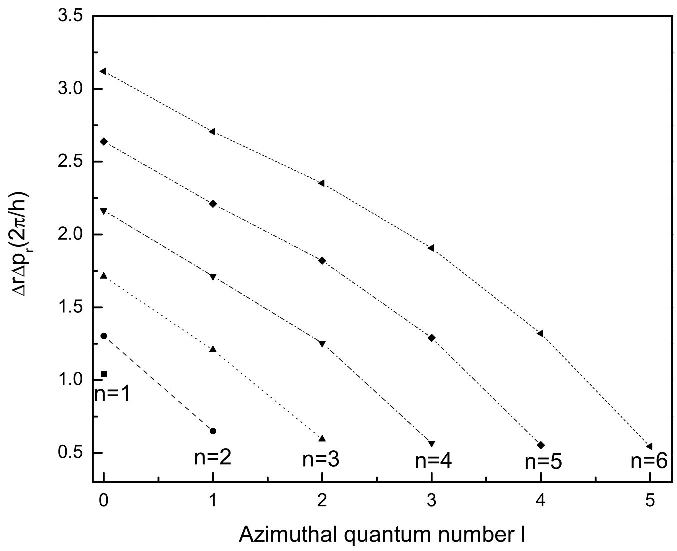

Figure 4. The change rule in the uncertainty $\triangle r\triangle p_r$ with respect to quantum numbers n and l for $Z = 55$. For same l, this uncertainty increases as n increases, while for same n, it decreases as l increases.

large, in particular for $Z = 55$. Fourth, for same l when n increases, the change rules of $\langle r\rangle$, the uncertainties $(\Delta r)_R$ and $(\Delta p_r)_R$ are almost same as those in the non-relativistic case. However, it should be noted that the product $\Delta r\Delta p_r$ in the non-relativistic case is independent of the value of charge Z (see equation (22) below), while in the relativistic case it is related to the value of the charge Z, in particular when Z is very large, say $Z = 55$, the relativistic corrections to the non-relativistic values of these uncertainties will appear. On the other hand, $(\Delta p_r)_R$ and $(\Delta r \Delta p_r)_R$ are almost equal to those in the non-relativistic case when n is large. That is to say, the relativistic corrections to the non-relativistic values become very small and can be ignored when one analyzes the behavior of the uncertainties of the radial position r and radial momentum p_r or their product for large n. Fifth, for same l both Δr and $\Delta r \Delta p_r$ increase as n increases, while both Δp_r and $\Delta r/\langle r\rangle$ decrease. This property exists both in the non-relativistic case and in the relativistic case. Finally, we find that the change of $\Delta r/\langle r\rangle$ is very small both in the non-relativistic hydrogen-like atoms case and in the relativistic case. The $\Delta r/\langle r\rangle$ is independent of charge Z in the non-relativistic case.

4. Special cases for $l = 0$ and $l = n - 1$

In order to have an insight into the features of those uncertainties, we attempt to study two special cases for $l = 0$ and $l = n - 1$, as shown in [4, 5].

First, let us consider the special case $l = 0$. For this case, we have

$$\begin{aligned}
\triangle r|_{l=0} &= \frac{a_0\sqrt{1+2n^2+2n(\omega-1)-\omega}}{2\sqrt{2}Z(-1+2n+\omega)}[4n^4+8n^3(\omega-1)+2n^2(7-6\omega+3\omega^2)\\
&\quad +2n(-5+7\omega-3\omega^2+\omega^3)-(\omega-2)(\omega-1)^2]^{1/2},\\
\left.\frac{\Delta r}{\langle r\rangle}\right|_{l=0} &= \frac{1}{6n^2+6n(\omega-1)+(\omega-2)(\omega-1)}\\
&\quad \times[4n^4+8n^3(\omega-1)+2n^2(7-6\omega+3\omega^2)\\
&\quad +2n(-5+7\omega-3\omega^2+\omega^3)-(\omega-2)(\omega-1)^2]^{1/2},\\
\triangle p_r|_{l=0} &= \frac{\sqrt{2}\hbar Z}{a_0}\sqrt{\frac{1+(2n-1)\omega}{\omega[4n^3+6n^2(\omega-1)+2n(\omega-2)(\omega-1)-(\omega-1)^2]}},\\
\triangle r\triangle p_r|_{l=0} &= \frac{\hbar}{2}\sqrt{\frac{1+(2n-1)\omega}{\omega(2n+\omega-1)^3}}[4n^4+8n^3(\omega-1)+2n^2(7-6\omega+3\omega^2)\\
&\quad +2n(-5+7\omega-3\omega^2+\omega^3)-(\omega-2)(\omega-1)^2]^{1/2},
\end{aligned} \tag{17}$$

where

$$\omega = \sqrt{1-4Z^2\alpha^2}. \tag{18}$$

Second, let us study the special case $l = n - 1$. For this case, however, we have

$$\begin{aligned}
\triangle r|_{l=n-1} &= \frac{a_0\sqrt{(2+\zeta)(1-2n+2n^2+\zeta)}}{2\sqrt{2}Z}, \qquad \left.\frac{\Delta r}{\langle r\rangle}\right|_{l=n-1} = \frac{1}{\sqrt{2+\zeta}},\\
\triangle p_r|_{l=n-1} &= \frac{\sqrt{2}\hbar Z}{a_0\sqrt{\zeta(1-2n+2n^2+\zeta)}}, \qquad \triangle r\triangle p_r|_{l=n-1} = \frac{\hbar}{2}\sqrt{\frac{2+\zeta}{\zeta}},
\end{aligned} \tag{19}$$

where

$$\zeta = \sqrt{(1-2n)^2-4Z^2\alpha^2}. \tag{20}$$

5. Non-relativistic limit

We now study the non-relativistic limit. If we expand μ in equation (4) and β in equation (6) as series of Z and neglect terms higher than second order, we obtain

$$\beta = \frac{2Z}{a_0 n}, \qquad \mu = l + \frac{1}{2}. \tag{21}$$

Substitution of them into equations (10), (12), (15) and (16) allows us to obtain the following uncertainties in the non-relativistic hydrogen-like atoms case,

$$\Delta r = \frac{a_0}{2Z}\sqrt{n^2(2+n^2) - l^2(l+1)^2}, \qquad \frac{\Delta r}{\langle r\rangle} = \frac{\sqrt{n^2(2+n)^2 - l^2(l+1)^2}}{3n^2 - l(l+1)},$$
$$\Delta p_r = \frac{Z\hbar}{na_0}\sqrt{1 - \frac{2l(l+1)}{n(1+2l)}}, \qquad \Delta r\,\Delta p_r = \frac{\hbar}{2}\sqrt{1 - \frac{2l(l+1)}{n(1+2l)}}\sqrt{(2+n^2) - \frac{l^2(l+1)^2}{n^2}}. \tag{22}$$

Similarly, if expanding ω in equation (18) and ζ in equation (20) as series of Z and neglecting terms higher than second order, for $l = 0$ we have

$$\Delta r = \frac{na_0}{2Z}\sqrt{2+n^2}, \qquad \frac{\Delta r}{\langle r\rangle} = \frac{\sqrt{2+n^2}}{3n},$$
$$\Delta p_r = \frac{\hbar Z}{a_0 n}, \qquad \Delta r\,\Delta p_r = \frac{\hbar}{2}\sqrt{n^2+2}. \tag{23}$$

For $l = n - 1$ case, however, we have

$$\Delta r = \frac{a_0 n\sqrt{1+2n}}{2Z}, \qquad \frac{\Delta r}{\langle r\rangle} = \frac{1}{\sqrt{1+2n}},$$
$$\Delta p_r = \frac{\hbar Z}{a_0 n\sqrt{2n-1}}, \qquad \Delta r\,\Delta p_r = \frac{\hbar}{2}\sqrt{\frac{2n+1}{2n-1}}. \tag{24}$$

It is found that equations (22)–(24) are all agreement with those of [4, 5].

6. Concluding remarks

By using the MATHEMATICA package INTEPFFLL we have shown that the radial position–momentum uncertainties Δr, Δp_r, the relative dispersion $\Delta r/\langle r\rangle$ and the product $\Delta r\Delta p_r$ for the Klein–Gordon hydrogen-like atoms can be obtained analytically. All these quantities are found to depend on the quantum numbers n and l as well as the value of charge Z. However, it should be pointed out that $\Delta r\Delta p_r$ in the non-relativistic case is independent of the value of charge Z. On the other hand, we have found that the relativistic corrections to the non-relativistic values of these uncertainties are very small when the value of charge Z is not too big, while the relativistic corrections to them will appear for large Z (e.g. $Z = 55$). In addition, we have also found that the average radial position $\langle r\rangle$ for states $(n, l = 1)(n \in [3, 6])$ is biggest. This property does not exist at all in the non-relativistic case. It should be mentioned that these properties are new in comparison with those in the non-relativistic case. Some other properties of these uncertainties are given explicitly in section 3.

The fact that the uncertainties Δr and Δp_r presented in this work are found to be analytical suggests that both the position and momentum of an electron in the Klein–Gordon hydrogen-like atoms can be measured simultaneously with known uncertainties if the wavefunctions of that electron could be specified. The similar results both in the non-relativistic case and in the Dirac equation case were also obtained in [4, 5], in which the inequality '$\geqslant$' appearing in the uncertainty relation of Heisenberg are explained in detail. Before ending this work, we make three useful remarks here. First, the present case tells us that we can obtain the analytical uncertainties because the wavefunctions of this quantum system are put into the calculations of the position–momentum uncertainties. Second, it should be pointed out that there is a limit for the value of the charge Z, that is, $Z \leqslant 68.5$ due to the variable μ given in equation (5). This is unlike the Dirac hydrogen-like atom case [5], in which we have discussed the hydrogen-like atom Fr ($Z = 87$). Third, the present method is possible to be used to investigate these uncertainties for other solvable quantum systems.

Acknowledgments

This work was supported by Natural Science Basic Research Plan in Shaanxi Province of China (program no: 2005A22), NSF of the Education Bureau of Shaanxi Province of China under grant O5jk238, COFFA-IPN, project nos 20062088-SIP-IPN and 20070914-SIP-IPN, Mexico.

Appendix. Calculation of average radial momentum square $\langle p_r^2\rangle$

In this appendix, we are going to give the concrete expressions of the six integrals $I_{FF}(n, \Delta n, m, \Delta m, \lambda)$ appearing in the expectation value of p_r^2. After calculation, it is found that

$$\langle p_r^2\rangle = \sum_{i=1}^{6} \mathrm{INT}\, i, \tag{A.1}$$

where

$$\mathrm{INT}\,1 = \frac{\hbar^2\beta^2\Gamma(1+n_r+2\mu)}{(1+2n_r+2\mu)\Gamma(n_r)\Gamma(1+2\mu)^2} I_{FF}(n_r-1, 1, 2+2\mu, -1, -2), \tag{A.2}$$

$$\mathrm{INT}\,2 = -\frac{\hbar^2\beta^2(1+2\mu)\Gamma(1+n_r+2\mu)}{(1+2n_r+2\mu)\Gamma(n_r)\Gamma(2+2\mu)^2} I_{FF}(n_r-1, 1, 2+2\mu, -1, -1), \tag{A.3}$$

$$\mathrm{INT}\,3 = -\frac{2\hbar^2\beta^2(1+\mu)(1+2\mu)\Gamma(1+n_r+2\mu)}{(1+2n_r+2\mu)\Gamma(-1+n_r)\Gamma(3+2\mu)^2} I_{FF}(n_r-2, 2, 3+2\mu, -2, -2), \tag{A.4}$$

$$\mathrm{INT}\,4 = \frac{\hbar^2\beta^2(1+2\mu)\Gamma(1+n_r+2\mu)}{2(1+2n_r+2\mu)n_r!\Gamma(1+2\mu)^2} I_{FF}(n_r, 0, 1+2\mu, 0, -1), \tag{A.5}$$

$$\mathrm{INT}\,5 = -\frac{\hbar^2\beta^2(-1+4\mu^2)\Gamma(1+n_r+2\mu)}{4(1+2n_r+2\mu)n_r!\Gamma(1+2\mu)^2} I_{FF}(n_r, 0, 1+2\mu, 0, -2), \tag{A.6}$$

$$\mathrm{INT}\,6 = -\frac{\hbar^2\beta^2\Gamma(1+n_r+2\mu)}{4(1+2n_r+2\mu)n_r!\Gamma(1+2\mu)^2} I_{FF}(n_r, 0, 1+2\mu, 0, 0). \tag{A.7}$$

The summation of them, which can be obtained by equation (7), allows us to obtain the following result:

$$\begin{aligned}\langle p_r^2\rangle = {} & \frac{\hbar^2\beta^2}{4(1+2n_r+2\mu)n_r!\Gamma(n_r)\Gamma(1+2\mu)^2\Gamma(2+2\mu)} n_r![4(1+2\mu)n_r!\Gamma(1+2\mu)^3 \\ & + \Gamma(n_r)((2\mu-8\mu^3)\Gamma(2\mu)^2 + (1-2n_r+2\mu)\Gamma(1+2\mu)^2)\Gamma(2+2\mu)],\end{aligned} \tag{A.8}$$

which can be further simplified as

$$\langle p_r^2\rangle = \frac{\hbar^2\beta^2(1+2\mu+4n_r\mu)}{4(1+2n_r+2\mu)2\mu}. \tag{A.9}$$

The reader is suggested to refer to [6, 7] for more information about calculation (7).

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