Relativistic Klein–Gordon charge effects by information-theoretic measures

D Manzano\(^1,2,4\), R J Yáñez\(^1,3,4\) and J S Dehesa\(^1,2,4\)

1 Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071 Granada, Spain
2 Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, 18071 Granada, Spain
3 Departamento de Matemática Aplicada, Universidad de Granada, 18071 Granada, Spain
E-mail: manzano@ugr.es, ryanez@ugr.es and dehesa@ugr.es

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Abstract. The charge spreading of the ground and excited states of Klein–Gordon particles moving in a Coulomb potential is quantitatively analysed by means of ordinary moments and the Heisenberg measure as well as by using the most relevant information-theoretic measures of global (Shannon entropic power) and local (Fisher information) types. The dependence of these complementary quantities on the nuclear charge \(Z\) and the quantum numbers characterizing the physical states is carefully discussed. The comparison of relativistic Klein–Gordon and non-relativistic Schrödinger values is made. Non-relativistic limits at large principal quantum number \(n\) and for small values of \(Z\) are also reached.

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\(^4\) Author to whom any correspondence should be addressed.
1. Introduction

The interplay of quantum mechanics, relativity theory and information theory is a very important topic in present-day theoretical physics [1]–[7]. While the link between the former two theories is well known, information theory has not yet percolated sufficiently in the scientific community as a whole. Today, however, it is well established that the information-theoretic approach provides deeper insights for numerous other physical problems and raises new unsolved issues. Information is physical [8]. We refer to the excellent monographs of Peres and Terno [2] and Nalewajski [9], where the physical interest of this approach in relativistic quantum-mechanical phenomena and the quantum theory of electronic structure is explicitly shown and discussed in detail, respectively. Let us just mention, for illustration, the recent information-theoretic interpretations of the paradox of quantum black holes [10], the natural ultraviolet cutoff at the Planck scale [11] and numerous physical phenomena (avoided crossings of atoms in external fields [12], periodicity and shell structure throughout the periodic table [13], molecular similarities [14], etc). In particular, the information-theoretic treatment gives rise to the information representation of molecular states, which complements the conventional energy representation of the density-functional and wave-function theories. Recently, the information-theoretic approach has allowed us to (i) predict the transition state structure and other stationary points so as to reveal the bond breaking/forming regions of chemical reactions [15, 16], (ii) explain the growing behaviour of nanostructured molecules of polyamidoamine dendrimers, starting from monomers, dimers, trimers and tetramers up to generations of G0 (with 84 atoms), G1 (228 atoms), G2 (516 atoms), G2 (1092 atoms) and G3 (1092 atoms) [17], and (iii) study the entanglement properties of many-fermion systems [18].

Special relativity imposes both important restrictions on the transfer of information between distant systems [2] and severe changes on the integral structure of physical systems [19]. This is mainly because the relativistic effects produce a spatial redistribution of the single-particle density $\rho(\vec{r})$ of the corresponding quantum-mechanical states, which substantially alters the spectroscopic and macroscopic properties of the systems. The quantitative study of the relativistic modification of the spatial extent of the charge density of atomic and molecular systems by information-theoretic means is quite an open field [3, 9]. The only works published to date have calculated the ground-state relativistic effects on hydrogenic [3] and many-electron neutral atoms [5, 7] in different settings by use of the renowned standard deviation (or Heisenberg measure) as well as various information-theoretic measures.

In this paper, we quantify the relativistic effects of the ground and excited states of spinless single-particle charge spreading by comparing the Klein–Gordon and Schrödinger values for three qualitatively different measures: the Heisenberg measure $\sigma[\rho]$, the Shannon entropic power $N[\rho]$ [20] and the Fisher information $I[\rho]$ [21, 22]. While the Heisenberg quantity gives spreading with respect to the centroid of the charge distribution, the Shannon and Fisher measures do not refer to any specific point.

The Shannon entropic power $N[\rho]$, which is essentially given by the exponential of the Shannon entropy $S[\rho] = -\langle \log \rho(\vec{r}) \rangle$, measures the total extent to which the distribution is in fact concentrated [22, 23]. This quantity has various relevant features. Firstly, it avoids the dimensionality troubles of $S[\rho]$, highlighting its physical meaning. Secondly, it exists when $\sigma$ does not. Thirdly, it is finite whenever $\sigma$ is. Thus, as a measure of uncertainty the use of the Shannon entropic power allows a wider quantitative range of applicability than
the Heisenberg measure \[24\]. Contrary to the Shannon and Heisenberg measures, which are insensitive to electronic oscillations, the translationally invariant Fisher information \[21\] has a locality property because it is a gradient functional of the density, so that it measures the pointwise concentration of the electronic cloud and quantifies its gradient content, providing a quantitative estimation of the oscillatory character of the density. Moreover, Fisher information measures the bias to particular points of the space, i.e. it gives a measure of local disorder.

To calculate the measures of charge spreading in a relativistic quantum-mechanical system, we have to tackle the problem of the very concept of quantum probability consistent with Lorentz covariance. The general formulation and interpretation of this problem are still currently discussed issues \[25\]. In this work, we avoid this problem in following relativistic quantum mechanics \[19\] by restricting ourselves to studying the stationary states of a spinless relativistic particle with a negative electric charge in a spherically symmetric Coulomb potential \[V(r) = -\frac{Ze^2}{r}\], which are solutions of the relativistic scalar wave equation, usually called the Klein–Gordon equation \[26\],

\[
[\epsilon - V(r)] \psi(\vec{r}) = \left(-\hbar^2 c^2 \nabla^2 + m_0^2 c^4\right) \psi(\vec{r}),
\]

appropriately normalized to particle charge. The symbols \(m_0\) and \(\epsilon\) denote mass and relativistic energy eigenvalue, respectively. We work in spherical coordinates, taking the ansatz \(\psi(r, \theta, \phi) = r^{-1} u(r) Y_{lm}(\theta, \phi)\), where \(Y_{lm}(\theta, \phi)\) denotes the spherical harmonics of order \((l, m)\). Then, to highlight the resemblance with the non-relativistic Schrödinger equation, we let

\[
\beta = \frac{\hbar c}{m_0 c^2 - \epsilon^2} = \frac{2m_0 c^2}{\hbar c} \sqrt{1 - \left(\frac{\epsilon}{m_0 c^2}\right)^2},
\]

\[
\lambda = \frac{2\epsilon Ze^2}{\hbar^2 c^2 \beta},
\]

and substitute the radial variable \(r\) by the dimensionless variable \(s\) through the transformation

\[
r \to s: \quad s = \beta r.
\]

Hence, the radial Klein–Gordon equation satisfied by \(u(s)\) can be written in the form \[20, 27\]

\[
\frac{d^2 u(s)}{ds^2} - \left[\frac{l'(l' + 1)}{s^2} - \frac{\lambda}{s} + \frac{1}{4}\right] u(s) = 0,
\]

where we have used the notation

\[
l' = \sqrt{\left(l + \frac{1}{2}\right)^2 - \gamma^2} - \frac{1}{2}, \quad \text{with} \quad \gamma = Z\alpha,
\]

\(\alpha = \frac{e^2}{\hbar c}\) being the fine structure constant. The physical solutions corresponding to the bound states (whose energy eigenvalues fulfil \(|\epsilon| < m_0 c^2\)) require that the radial eigenfunctions \(u_{nl}(r)\) vanish both at the origin and at infinity, so that they have the form \[20\]

\[
u_{nl}(s) = \mathcal{N} s^{(l'+1)} e^{-s/2} l_{n-l-1}^{2l'+1}(s),
\]
where \( \tilde{L}_k^{(\omega)}(s) \) denotes the orthonormal Laguerre polynomials of degree \( k \) and parameter \( \alpha \). The energy eigenvalues \( \epsilon \equiv \epsilon_n(Z) \) of the stationary bound states with wavefunctions \( \Psi_{nlm}(\vec{r}, t) = \psi_{nlm}(\vec{r}) \exp(-i/\hbar)(\epsilon t) \) are known to have the form [20]

\[
\epsilon = \frac{m_0c^2}{\sqrt{1 + (\gamma /(n-l+l'))^2}}.
\]  

The constant \( \mathcal{N} \) is determined not by the normalization of the wavefunction to unity as in the non-relativistic case, but by the charge conservation carried out by \( \int_{\mathbb{R}^3} \rho(\vec{r}) \, d^3r = e \) to preserve the Lorentz invariance [19], where the charge density of the negatively charged particle (e.g. a \( \pi^- \)-meson; \( q = -e \)) is given by

\[
\rho_{nlm}(\vec{r}) = \frac{e}{m_0c^2} [\epsilon - V(r)] |\psi_{nlm}(\vec{r})|^2.
\]  

Then, the charge normalization imposes the following restriction on the radial eigenfunctions:

\[
1 = \int_0^\infty \frac{\epsilon - V(r)}{m_0c^2} u_{el}^2(r) \, dr = \frac{1}{m_0c^2} \int_0^\infty \left( \frac{\epsilon}{\beta} + \frac{\gamma \hbar c}{\rho} \right) u_{el}^2(s) \, ds.
\]  

The substitution of expression (7) for \( u_{el}(s) \) into equation (10) provides the following normalization constant:

\[
\mathcal{N}^2 = m_0c^2 \left[ \frac{2\epsilon}{\beta (n+l'-l) + \gamma \hbar c} \right]^{-1} = \frac{m_0c^2 \gamma}{\hbar c} \frac{1}{(n+l'-l)^2 + \gamma^2},
\]  

where we have used for the second equality the relation

\[
\frac{\epsilon}{\beta} = \frac{\hbar c}{2} \frac{n+l'-l}{\gamma}.
\]  

Let us emphasize that the resulting Lorentz-invariant charge density \( \rho_{LI}(\vec{r}) \) given by equation (9) is always (i.e. for any observer’s velocity \( v \)) appropriately normalized while the density \( \rho_{NLI}(\vec{r}) = |\psi_{nlm}(\vec{r})|^2 \) (used in [27]) is not. This is numerically illustrated in figure 1 for a pionic atom with nuclear charge \( Z = 68 \) in the infinite nuclear mass approximation (\( \pi^- \)-meson mass = 273.132054 au).

For completeness, we have plotted in figure 2 the radial density of the charge distribution for two different states \((n=1, l=0)\) and \((n=4, l=1)\) of a pionic system with nuclear charge \( Z = 68 \) in the infinite nuclear mass approximation. Moreover, in these figures we have also made a comparison with the corresponding Schrödinger density functions [28]. We observe that the relativistic effects other than spin (i) tend to compress the charge towards the origin and (ii) are most apparent for states \( S \).

In this paper, we quantify this relativistic charge compression by three different means. First, in section 2, we compute the ordinary moments or radial expectation values \( \langle r^k \rangle \) for

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general \((n, l, m)\) states, with emphasis on the Heisenberg measure for circular \((l = n - 1)\) and S-states \((l = 0)\). These quantities, which are well known in the Dirac case [31, 32], are, strikingly, only known [27] for the non-Lorentz-invariant density \(\rho_{\text{NLI}}(\vec{r})\) in the Klein–Gordon case. Here, we will study them for the Lorentz-invariant Klein–Gordon density \(\rho_{\text{LI}}(\vec{r})\). Then, in section 3 we study numerically the most relevant charge information-theoretic measures of the system; Shannon entropy and Fisher information.

2. Radial expectation values and Heisenberg’s measure

The charge distribution of the Klein–Gordon particles in a Coulomb potential can be completely characterized by means of the ordinary radial expectation values \(\langle r^k \rangle, k \in \mathbb{N}\), given by

\[
\langle r^k \rangle := \int_{\mathbb{R}^3} r^k \rho_{nm}(\vec{r}) \, d^3 r
= \frac{1}{m_0 c^2} \int_0^\infty \left( \epsilon + \frac{Ze^2}{r} \right) r^k u_{nm}^2(r) \, dr
\]
\[ S = \frac{1}{m_0 c^2} \frac{1}{\beta} \int_0^\infty \left( \frac{\epsilon}{\beta} + \frac{\gamma \hbar c}{s} \right) s^k u_n^2(s) ds \]

\[ \frac{\mathcal{N}}{m_0 c^2} \frac{1}{\beta^k} \left[ \frac{\epsilon}{\beta} I_n(k) + \gamma \hbar c J_n(k-1) \right], \]  

where we have used equations (7) and (9), and the symbol \( J_n(k) \) denotes the integral [20]

\[ J_n(k) := \int_0^\infty x^{2l'+k+2} e^{-x} \left[ \tilde{L}_{n-l-1}(x) \right]^2 dx \]

\[ = \frac{(n-l-1)!}{\Gamma(n-l+2l'+1)} \sum_{j=n-l-k-2}^{n-l-1} \left( \frac{k+1}{n-l-j-1} \right)^2 \frac{\Gamma(2l'+k+j+3)}{j!}. \]  

For the lowest values of \( k \), we have

\[ J_n(0) = 2(n+l'-l), \]

\[ J_n(1) = 2 \left[ 3(n-l)^2 + l'(6n+2l'-6l-1) \right], \]

\[ J_n(2) = 4(n+l'-l) \left[ 1 + 5(n-l)^2 + l'(10n+2l'-10l-3) \right]. \]

Then, besides the normalization \( \langle r^0 \rangle = 1 \), we have

\[ \langle r \rangle = \frac{\mathcal{N}}{m_0 c^2} \frac{1}{\beta} \left[ \frac{\epsilon}{\beta} I_n(1) + \gamma \hbar c J_n(0) \right] \]

for the centroid of the charge density, and

\[ \langle r^2 \rangle = \frac{\mathcal{N}}{m_0 c^2} \frac{1}{\beta^2} \left[ \frac{\epsilon}{\beta} I_n(2) + \gamma \hbar c J_n(1) \right] \]

for the second-order moment, so that the Heisenberg measure \( \sigma_{nl} \), which quantifies charge spreading around the centroid, is given by

\[ \sigma_{nl}^2 \equiv \sigma \left[ \rho_{nlm} \right] = \langle r^2 \rangle - \langle r \rangle^2 \]

\[ = \frac{\mathcal{N}}{m_0 c^2} \frac{1}{\beta^2} \left\{ \frac{\epsilon}{\beta} I_n(2) + \gamma \hbar c J_n(1) - \frac{\mathcal{N}}{m_0 c^2} \left[ \frac{\epsilon}{\beta} I_n(1) + \gamma \hbar c J_n(0) \right] \right\}^2. \]  

To gain insight into these general expressions, we will now discuss two particular classes of quantum-mechanical states, the circular (i.e. \( l = n-1 \)) states and the ns-states (i.e. \( l = 0 \)).

For circular states, we have

\[ l' = \sqrt{(n-\frac{1}{2})^2 - \gamma^2 - \frac{1}{4}}, \]

\[ \epsilon = \frac{m_0 c^2}{\sqrt{1 + (\gamma/(l'+1))^2}}, \quad \frac{\epsilon}{\beta} = \frac{\hbar c}{2\gamma} (l'+1), \]
so that
\[
\sqrt{\frac{\mathcal{A}^2}{m_0 c^2}} = \frac{\gamma}{\hbar c} \frac{1}{(l' + 1)^2 + \gamma^2},
\]
and the integrals
\[
\mathcal{J}_{n l}(0) = 2l' + 2,
\]
\[
\mathcal{J}_{n l}(1) = (2l' + 2)(2l' + 3),
\]
\[
\mathcal{J}_{n l}(2) = (2l' + 2)(2l' + 3)(2l' + 4).
\]

Then, the centroid of the charge distribution is, according to equation (15),
\[
\langle r \rangle = \frac{\hbar c}{4m_0 c^2} \frac{1}{\gamma \sqrt{1 + (\gamma/(l' + 1))^2}} \left[ (2l' + 2)(2l' + 3) + 4\gamma^2 \right] \]
and the second-order moment, according to equation (16), becomes
\[
\langle r^2 \rangle = \left( \frac{\hbar c}{m_0 c^2} \right)^2 \frac{1}{2\gamma^2} \frac{(l' + 1)(2l' + 3)}{(l' + 1)(l' + 2) + \gamma^2}.
\]

so that the Heisenberg measure for circular states \(\sigma^2_n = \sigma^2_{n,n-1}\) has the following value:
\[
\sigma^2_n = \left( \frac{\hbar c}{m_0 c^2} \right)^2 \left( \frac{l' + 1}{4\gamma^2} \right) \frac{(l' + 1)(2l' + 3)}{(l' + 1)^2 + \gamma^2} + 2\gamma^4.
\]

These expressions for circular states and the corresponding ones for ns-states are discussed and compared with the Schrödinger values as a function of the principal quantum number \(n\) for the pionic system with nuclear charge \(Z = 68\) in figure 3. We observe that both centroid and variance ratios increase very rapidly with \(n\), the rate of this behaviour being much faster for
circular than for S-states. This indicates that the charge compression provoked by relativity in a given system (i.e. for fixed $Z$) decreases when $n$ ($l$) is increasing for fixed $l$ ($n$). This can also be noticed in figure 4, where the two previous ratios have been plotted as a function of $l$ for different values of $n$.

We have plotted these two ratios in terms of the nuclear charge $Z$ of the system in figure 5 for states 1S, 2S and 2P. We find that both the centroid and the variance ratios monotonically decrease as the nuclear charge $Z$ increases. Moreover, the decreasing rate is much faster for states 1S than for states 2S and 2P. These two observations illustrate that the relativistic charge compression effect is greater in heavier systems for a given ($nl$)-state. Moreover, we see here again that for a given system it increases both when $n$ decreases for fixed $l$ and when $l$ decreases for fixed $n$. The quantum number $m$ does not affect both ratios because the radial part of the density is not a function of it.

Finally, let us highlight that in all figures the Klein–Gordon values tend toward the Schrödinger values in the non-relativistic limit of large $n$ or small $Z$.

3. Shannon and Fisher information measures

Here we study numerically the relativistic effects on the charge spreading of pionic systems of hydrogenic type by means of the following information-theoretic measures of the associated

Figure 4. Comparison of the Klein–Gordon and Schrödinger values for the centroid (left) and the variance (right), as a function of quantum number $l$ varying from 0 to $n - 1$, for different values of $n$.

Figure 5. Comparison of the Klein–Gordon and Schrödinger values for the centroid (left) and the variance (right) as a function of nuclear charge $Z$ for pionic states 1S, 2S and 2P.
charge distribution $\rho_{nlm}(\vec{r})$ given by equation (9): Shannon entropy power and Fisher information.

The Shannon entropic power of a negatively charged Klein–Gordon particle characterized by the charge density $\rho_{nlm}(\vec{r})$ is defined by [22]

$$N_{nlm} \equiv N[\rho_{nlm}] = \frac{1}{2\pi e} \exp \left( \frac{2}{3} S_{nlm} \right),$$

where $S_{nlm}$ is the Shannon entropy of $\rho_{nlm}(\vec{r})$ given by the expectation value of $-\log(\rho_{nlm}(\vec{r}))$, i.e.

$$S_{nlm} \equiv S[\rho_{nlm}] = -\int_{\mathbb{R}^3} \rho_{nlm}(\vec{r}) \log \rho_{nlm}(\vec{r}) \, d^3r,$$

which quantifies the total extent of the charge spreading of the system. Taking into account the above-mentioned ansatz for $\psi(\vec{r})$ and equations (7), (9) and (22), this expression can be separated into radial and angular parts,

$$S_{nlm} = S[R_{nl}] + S[Y_{lm}],$$

and is explained in full detail in [29], $R_{nl}$ and $Y_{lm}$ being the radial and angular parts of the density. We should keep in mind that the angular part is the same for both Klein–Gordon and Schrödinger cases.

Fisher information is defined by [21]

$$I_{nlm} \equiv I[\rho_{nlm}] = \int_{\mathbb{R}^3} \frac{[\nabla \rho(\vec{r})]^2}{\rho(\vec{r})} \, d^3r.$$  

Note that we are not using here the parameter-dependent Fisher information originally introduced (and much used) by statisticians [33], but its translationally invariant form, which does not depend on any parameter; see [21, 30] for further details. It is worth pointing out that Fisher information is a measure of the gradient content of the charge distribution. Therefore, when $\rho(\vec{r})$ has a discontinuity at a certain point, the local slope value changes drastically and Fisher information varies strongly. This indicates that it is a local quantity, in contrast to the Heisenberg measure $\sigma_{nl}^2$ and the Shannon entropy $S_\rho$ (and its associated power), which have global character because they are power-like and logarithmic functionals of the density, respectively.

Unlike the moment-based quantities discussed in the previous section, these complementary measures do not depend on a special point, either the origin as ordinary moments or the centroid as the Heisenberg measure. These quantities, first used by statisticians and electrical engineers and later by quantum physicists, have been shown to be measures of disorder or smoothness of the density $\rho_{nlm}(\vec{r})$ [21, 22]. Let us highlight that Fisher information not only measures the charge spreading of the system in a complementary and qualitatively different manner to the Heisenberg and Shannon measures but also quantifies their oscillatory character, indicating the local charge concentration all over space [21].

The relativistic (Klein–Gordon) and non-relativistic (Schrödinger) values of the Shannon entropic power are numerically discussed and compared in figure 6 for the pionic system. Therein, on the left, we plot the ratio $N_{nl}(KG)/N_{nl}(Sch)$ between these two values as a function

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of the principal quantum number $n$ for the system with nuclear charge $Z = 68$. We notice that the Shannon ratio systematically increases when $n$ increases, approaching unity for large $n$, for both circular and S-states. Moreover, we find that this approach is much faster for circular states, which indicates once more that the relativistic effects are much more important for S-states. In addition, on the right of figure 6, we show the dependence of the Shannon ratio with nuclear charge $Z$ for the 1S, 2S and 2P states. We observe here again that the ratio is a decreasing function of $Z$ for any state, indicating that the relativistic effects are much more important for heavy systems. Moreover, for a given system (i.e. fixed $Z$) the relativistic effects increase when $n$ ($l$) decreases for fixed $l$ ($n$). The quantum number $m$ affects the absolute value of the Shannon entropic power but it does not affect the ratio.

Figure 7 shows the dependence of the ratio of the non-relativistic and relativistic values of Fisher information for various states with $l \neq 0$ on their quantum numbers $(n, l, m)$ for the pionic system with $Z = 68$ (left graph) and on nuclear charge $Z$ (right graph). The Fisher information for S-states is not defined because the involved integral diverges. Firstly, we should remark here that, contrary to the previous quantities considered in this work, the Schrödinger values are always smaller than the Klein–Gordon; this is strongly related to the local character of Fisher information, indicating that the localized internodal charge concentration is always larger.
in the relativistic case. Secondly, we observe that for fixed $l$ the Fisher ratio $I_{nl}^{\text{(Sch)}}/I_{nl}^{\text{(KG)}}$ monotonically increases when $n$ increases, approaching unity at a rate that grows as $l$ increases. Thirdly, we find that the Fisher ratio decreases for all states in a systematic way as nuclear charge increases. Moreover, for a given $Z$ value this ratio increases as the quantum numbers $n$ and/or $l$ increase.

For completeness, the behaviour of the Shannon and Fisher ratios in terms of the orbital quantum number $l$ for a fixed $n$ is more explicitly shown on the left- and right-hand graphs, respectively, of figure 8.

Finally, in figure 9, the dependence of the Fisher ratio on the magnetic quantum number $m$ is studied. Notice that the ratio is greater when $|m|$ is increasing, indicating that the lower the $|m|$, the more concentrated the charge density of the state and the more important the relativistic effects.

Figure 8. Comparison of the Klein–Gordon and Schrödinger values for Shannon entropic power as a function of $l$ varying from 0 to $n-1$ (left) and Fisher information as a function of $l$ varying from 1 to $n-1$ (right) for different values of $n$.

Figure 9. Comparison of the Klein–Gordon and Schrödinger values for Fisher information as a function of $m$ varying from 0 to $l$, for different values of $l$. 

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4. Conclusions

The relativistic charge compression of spinless Coulomb particles has been quantitatively investigated by means of the Heisenberg, Shannon and Fisher spreading measures. These three complementary quantities show that the relativity effects are greater (i.e. the charge compresses more towards the origin) for the lower energetic states and when the Coulomb strength (i.e. nuclear charge $Z$) increases. Moreover, a detailed analysis of these quantities on the quantum numbers $(n, l, m)$ characterizing the physical states of a given system (i.e. for a fixed $Z$) indicates that the relativistic effects increase when $n$ ($l$) decreases for fixed $l$ ($n$). Furthermore, the study of the Fisher information shows that the relativistic effects also increase when the magnetic quantum number $|m|$ increases for fixed $(n, l)$.

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