Complexity analysis of Klein-Gordon single-particle systems

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Abstract – The Fisher-Shannon complexity is used to quantitatively estimate the contribution of relativistic effects to the internal disorder of Klein-Gordon single-particle Coulomb systems which is manifest in the rich variety of three-dimensional geometries of its corresponding quantum-mechanical probability density. It is observed that, contrary to the non-relativistic case, the Fisher-Shannon complexity of these relativistic systems does depend on the potential strength (nuclear charge). This is numerically illustrated for pionic atoms. Moreover, its variation with the quantum numbers \((n, l, m)\) is analysed in various ground and excited states. It is found that the relativistic effects enhance when \(n\) and/or \(l\) are decreasing.

Numerous phenomena and properties of many-electron systems have been qualitatively characterized by information-theoretic means. In particular, various single and composite information-theoretic measures have been proposed to identify and analyze the multiple facets of the internal disorder of non-relativistic quantum systems; see, e.g., refs. [1–9].

They are often expressed as products of two quantities of local (e.g. the Fisher information) and/or global (e.g. the variance or Heisenberg measure, the Shannon entropy, the Rényi and Tsallis entropies and the disequilibrium or linear entropy \(\rho\)) character, which describe the charge spreading of the system in a complementary and more complete manner than their individual components. This is the case of the disequilibrium-Shannon or Lopez-Ruiz-Mancini-Calvet (LMC in short) [2], disequilibrium-Heisenberg [4], Fisher-Shannon [5,8] and the Cramer-Rao [5,10] complexities, which have their minimal values at the extreme ordered and disordered limits.

Recently these studies have been extended to take into account the relativistic effects in atomic physics. Relativistic quantum mechanics [11] tells us that special relativity provokes (at times, severe) spatial modifications of the electron density of many-electron systems, what produces fundamental and measurable changes in their physical properties. The qualitative and quantitative evaluation of the relativistic modification of the spatial redistribution of the electron density of ground and excited states in atomic and molecular systems by information-theoretic means is a widely open field. In the last three years the relativistic effects of various single and composite information-theoretic quantities of the ground states of hydrogenic [12] and neutral atoms [13–15] have been investigated in different relativistic settings.

First Borgoo et al. [13] (see also [16]), in a Dirac-Fock setting, find that the LMC shape complexity of the ground-state atoms i) has an increasing dependence on the nuclear charge (also observed by Katriel and Sen [12] in Dirac ground-state hydrogenic systems), ii) manifest shell and relativistic effects, the latter being specially relevant in the disequilibrium ingredient (which indicates that they are dominated by the innermost orbital). Then, Sañudo and López-Ruiz [14] (see also [15]) show a similar trend for both LMC and Fisher-Shannon complexities in a different setting which uses the fractional occupation probabilities of electrons in atomic orbitals instead of the continuous electronic wave functions; so, they use discrete forms for the information-theoretic ingredients of the complexities. Moreover, their results allow to identify the shell structure of noble gases and the irregular shell filling of some specific elements; this phenomenon is specially striking in the Fisher-Shannon case as the authors explicitly point out.

The present work contributes to this new field with the quantification of the relativistic compression of both...
ground and excited states of the Klein-Gordon single-particle wave functions in a Coulombian well by means of the Fisher-Gordon complexity. This quantity is defined by

\[ C_{FS} [\rho] := I [\rho] \times J [\rho], \tag{1} \]

where

\[ I [\rho] = \int \rho \left[ \frac{d}{dx} \ln \rho (\vec{r}) \right]^2 d\vec{r}, \quad J [\rho] = \frac{1}{2 \pi e} \exp(2S [\rho] / 3), \tag{2} \]

are the Fisher information and the Shannon entropic power of the density \( \rho (\vec{r}) \), respectively. The latter quantity, which is an exponential function of the Shannon entropy \( S [\rho] = - \ln \rho \), measures the total extent to which the single-particle distribution is in fact concentrated [10]. The Fisher information \( I [\rho] \), which is closely related to the kinetic energy [17], is a local information-theoretic quantity because it is a gradient functional of the density, so being sensitive to the single-particle oscillations. Then, contrary to the remaining complexities published in the literature up until now, the Fisher-Shannon complexity has a property of locality and it takes simultaneously into account the spatial extent of the density and its (strong) oscillatory nature.

Here we use the Fisher-Shannon complexity to quantify the relativistic charge spreading of Klein-Gordon particles moving in a Coulomb potential \( V (\vec{r}) = - \frac{Z e}{r} \). We study the dependence of these quantities on the potential strength \( Z \) and on the quantum numbers \((n, l, m)\) which characterize the stationary states of a spinless relativistic particle with a negative electric charge.

The Klein-Gordon wave equation was introduced in 1926 and constituted the first theoretical description of particle dynamics in a relativistic quantum setting [18]. Since then, the study of its properties for different potentials of various dimensionalities has been a problem of increasing interest [19–22]. Many efforts were addressed to obtain the spectrum of energy levels and the ordinary moments or expectation values \( \langle r^n \rangle \) of the charge distribution of numerous single-particle systems (such as, e.g., muonic and pionic atoms [23]). Only recently, Chen and Dong [22] have been able to calculate explicit expressions for these moments and some off-diagonal matrix elements of \( r^k \) for a Klein-Gordon single-particle of mass \( m_0 \) in the Coulomb potential \( V (\vec{r}) = - \frac{Z e}{r} \). These authors, however, do not use the Lorentz-Invariant (LI) Klein-Gordon charge density

\[ \rho_{LI} (\vec{r}) = \frac{e}{m_0 c^2} \left[ e - V (r) \right] |\Psi_{nlm} (\vec{r})|^2, \tag{3} \]

but just the Non-Lorentz-Invariant (NLI) expression

\[ \rho_{NLI} (\vec{r}) = |\Psi_{nlm} (\vec{r})|^2 \] as in the non-relativistic case, where \( e \) and \( \Psi (\vec{r}) \) denote the physical solutions of the Klein-Gordon equation [19,22]

\[ |e - V (r)| \Psi (\vec{r}) = (-\hbar^2 c^2 \nabla^2 + m_0^2 c^4) \Psi (\vec{r}), \tag{4} \]

which characterizes the wave functions \( \Psi_{nlm} (\vec{r}, \alpha) = \psi_{nlm} (\vec{r}) \exp(-\frac{i}{\hbar} \alpha t) \) of the stationary states of our system.

In spherical coordinates \( \vec{r} = (\alpha, \theta, \phi) \), the eigenfunction \( \psi (r, \theta, \phi) = r^{-1} u(r) Y_{lm} (\theta, \phi) \), where the \( Y \)-symbol denotes the spherical harmonics of order \((l, m)\). Making the change \( r \to s \), with \( s = \beta r \) in eq. (4), and using the notations

\[ \beta \equiv \frac{2}{\hbar c} \sqrt{m_0^2 c^4 - e^2}, \quad \lambda \equiv \frac{2 e Z e^2}{\hbar^2 c^3 \beta}, \tag{5} \]

one has the radial Klein-Gordon equation

\[ \frac{d^2 u(s)}{ds^2} - \left[ \ell' (\ell' + 1) - \frac{\lambda}{s} + \frac{1}{4} \right] u(s) = 0, \tag{6} \]

where the following additional notations:

\[ \ell' = \sqrt{\left( l + 1 \right)^2 - \gamma^2} - \frac{1}{2}, \quad \text{with } \gamma \equiv Z \alpha, \tag{7} \]

have also been used, being the fine-structure constant \( \alpha \equiv e^2 / \pi \). It is known (see, e.g., eq. (21a) on page 39 of ref. [11] and eq (5.12) with \( N = 1 \) of ref. [19]) duly corrected for the inappropriate location of the \( \frac{1}{2} \)-power in it) that the bound states have the energy eigenvalues

\[ \epsilon = \sqrt{\left( m_0 c^2 \right)^2 + \frac{\gamma^2}{1 + \left( \frac{\gamma}{2} \right)^2}}, \tag{8} \]

and the eigenfunctions

\[ u_{nl}(s) = \mathcal{N}_s \ell' (\ell' + 1) e^{-\frac{\gamma}{2} L_{n-l-1}^2} (s). \tag{9} \]

To preserve Lorentz invariance, according to relativistic quantum mechanics [11], we calculate the constant \( \mathcal{N} \) by taking into account the charge conservation \( \int_{\mathbb{R}^3} \rho (\vec{r}) d^3 r = e \), which yields the value [24]

\[ \mathcal{N}^2 = \frac{m_0 c^2 \gamma}{\hbar c} (n - l + l')^2 + \gamma^2. \tag{10} \]

Let us emphasize that the resulting Lorentz-invariant charge density \( \rho_{LI} (\vec{r}) \) given by eqs. (3)–(10) is always (i.e., for any observer’s velocity \( v \)) appropriately normalized, while the non-Lorentz-invariant density \( \rho_{NLI} (\vec{r}) \) used by Chen and Dong [22] is not. This was numerically discussed in ref. [24] for some pionic atoms in the infinite nuclear mass approximation.

Let us now numerically discuss the relativistic effects in the Fisher-Shannon complexity of a pionic system. First, we center our attention on the dependence on the nuclear charge of the system. As we can see in fig. 1, the Fisher-Shannon complexity of the Klein-Gordon case depend on the nuclear charge \( Z \), contrary to the non-relativistic description. The Schrödinger or non-relativistic value of the Fisher-Shannon complexity has been recently shown to be independent of the nuclear charge \( Z \) for any hydrogenic system ([25], see also [8]). It is apparent that this quantity is a very good indicator of the relativistic effects as has been recently pointed out by Sañudo and López-Ruiz [14,15] in other relativistic settings. These effects are bigger when the nuclear charge increases, so the relativistic Fisher-Shannon complexity enhances this.
and number are practically negligible when the magnetic quantum completeness, let us point out that the relativistic effects big. This dependence on is different from zero even when the nuclear charge is practically negligible when the angular quantum number increasing. Third, this decreasing behaviour with principal quantum number is increasing. Second, the relativistic effects decrease when the principal quantum number is increasing. Third, this decreasing behaviour with \( n \) has a strong dependence with \( Z \), being slower as bigger is the nuclear charge.

In fig. 3 we can observe that the relativistic effects are practically negligible when the angular quantum number is different from zero even when the nuclear charge is big. This dependence on \( l \) is more important than the dependence on the principal quantum number \( n \). For completeness, let us point out that the relativistic effects are practically negligible when the magnetic quantum number \( m \) varies for \( (Z, n, l) \) fixed.

In conclusion, we have explored relativistic effects on the behaviour of the Fisher-Shannon complexity of pionic systems with nuclear charge \( Z \) in the Klein-Gordon framework. We have done it for both ground and excited states. First we found that the relativistic Fisher-Shannon complexity grows when the nuclear charge increases in contrast with the non-relativistic case for both ground and excited states. A similar behaviour has been recently observed in the case of the ground state of systems governed by the Dirac equation [13–16]. We found that this trend remains for excited states in a damped way, so that the relativistic effects enhance with \( Z \) for a given \((n, l, m)\) state and, for a given Z, decrease when the principal and/or orbital quantum numbers are increasing. Let us also highlight that the non-relativistic limits at large principal quantum number \( n \) for a given \( Z \) (see fig. 2) and at small values of \( Z \) (see fig. 1) are reached. On the other hand, it is pertinent to underline that the finite nuclear volume effects are very tiny for any information-theoretic and complexity measure because of its macroscopic character.

It is worthwhile noting that the Fisher-Shannon complexity given by eq. (1) is a much better qualitative and quantitative measure of relativistic effects than any other single information-theoretic measure, including the Shannon entropy and Fisher information recently studied [24], because it grasps both the total extent and the gradient content of the quantum-mechanical probability densities which characterize the hydrogenic states. Moreover, contrary to the Shannon and Fisher quantities, the Fisher-Shannon complexity better reflects the usual understanding of complexity of the system because of its special properties; namely, minimization at the extreme ordered and disordered limits and invariance under replication, translation and rescaling transformations.

Let us finally say for completeness that we have also investigated the relativistic Klein-Gordon effects in pionic atoms by means of the LMC shape complexity [2] \( C(LMC) = \langle \rho \rangle \exp S[\rho] \). We found that the relativistic effects are also identified by this quantity but in a much weaker way than the Fisher-Shannon complexity \( C(FS) \). Apparently this is because of the property of locality of \( C_{FS} \) coming through its gradient-dependent
oscillatory condition of the pionic densities.

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