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The relativistic hydrogen atom : a theoretical laboratory for structure functions*

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ABSTRACT

Thanks to the Dirac equation, the hydrogen-like atom at high Z offers a precise model of relativistic bound state, allowing to test properties of unpolarized and polarized structure functions analogous to the hadronic ones, in particular: Sivers effect, sum rules for the vector, axial, tensor charges and for the magnetic moment, positivity constraints, sea contributions and fracture functions.

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1 INTRODUCTION

In this work we will study the hydrogen-like atom, treated by the Dirac equation, as a precise model of relativistic two-particle bound states when one of the constituent is very massive. We consider the case of large Z so that $Z\alpha \sim 1$ and relativistic effects are enhanced. What we neglect is

- the nuclear recoil
- the nuclear spin (but not necessarily the nuclear size)
- radiatives corrections, e.g. the Lamb shift $\sim \alpha(Z\alpha)^4 m_e$.

In analogy with the quark distributions, we will study:

- the electron densities $q(k^+)$, $q(\mathbf{k}_T, k^+)$ or $q(\mathbf{b}, k^+)$ where $\mathbf{b} = (x, y)$ is the impact parameter;
- the corresponding polarized densities;
- the sum rules for the vector, axial and tensor charges and for the atom magnetic moment;
- the positivity constraints;
- the electron - positron sea and the fracture functions.

We use $k^+ = k^0 + k_z$ instead of the Björken scaling variable k^+/P_{atom}^+ which would be of order m_e/M_{atom} , hence very small. $|k^+|$ can run up to M_{atom} , but typically $|k^+ - m| \sim Z\alpha m$.

2 Deep-inelastic probes of the electron state

Deep-inelastic reactions on the atom are, for instance:

- Compton scattering: $\gamma_i + e^-(\text{bound}) \rightarrow \gamma_f + e_f^-(\text{free})$,
- Moeller or Bhabha scattering (replacing the γ by a e^\pm),
- annihilation: $e^+ + e^-(\text{bound}) \rightarrow \gamma + \gamma$,

the Mandelstam invariants \hat{s} , \hat{t} and \hat{u} being large compared to m_e^2 . In Compton scattering for instance, taking the z axis along $\mathbf{Q} = \mathbf{k}_f^\gamma - \mathbf{k}_i^\gamma$, the particles γ_i , γ_f and e_f^- move almost in the $-z$ direction and we have

$$k^+ \simeq Q^+, \quad (1)$$

$$\mathbf{k}_T \simeq \mathbf{k}_{fT}^e + \mathbf{k}_{fT}^\gamma - \mathbf{k}_{iT}^\gamma = -\mathbf{P}_{fT}(\text{nucleus}). \quad (2)$$

3 Joint (\mathbf{b}, k^+) distribution

In the "infinite momentum frame" $P_z \gg M$, deep inelastic scattering measures the gauge-invariant *mechanical* longitudinal momentum

$$k_z = (P_z/M_{atom}) k_{rest\ frame}^+ = p_z - A_z \quad (3)$$

and not the canonical one $p_z = -i\partial/\partial z$. It is not possible to define a joint distribution $q(\mathbf{k}_T, k_z)$ in a gauge invariant way, since the three quantum operators $k_i = -i\partial_i - A_i(t, x, y, z)$ are not all commuting. On the other hand we can define unambiguously the joint distribution $q(\mathbf{b}, k_z)$. Note that $q(\mathbf{b}, k^+)$ can be measured in atom + atom collisions where two hard sub-collisions occur simultaneously: $\{e_1^- + e_2^- \text{ and } N_1 + N_2\}$ or: $\{e_1^- + N_2 \text{ and } e_2^- + N_1\}$.

Given the Dirac wave function $\Psi(\mathbf{r})$ at $t = 0$ in the atom frame, we have

$$dN_{e^-}/[d^2\mathbf{b} dk^+/(2\pi)] \equiv q(\mathbf{b}, k^+) = \Phi^\dagger(\mathbf{b}, k^+) \Phi(\mathbf{b}, k^+), \quad (4)$$

$$\Phi(\mathbf{b}, k^+) = \int dz \exp\{-ik^+z + iE_n z - i\chi(\mathbf{b}, z)\} \Phi(\mathbf{r}), \quad (5)$$

$$\Phi(\mathbf{r}) = \begin{pmatrix} \Psi_1(\mathbf{r}) + \Psi_3(\mathbf{r}) \\ \Psi_2(\mathbf{r}) - \Psi_4(\mathbf{r}) \end{pmatrix}, \quad (6)$$

$$\chi(\mathbf{b}, z) = \int_{z_0}^z dz' V(x, y, z') = -Z\alpha \left[\sinh^{-1}\left(\frac{z}{b}\right) - \sinh^{-1}\left(\frac{z_0}{b}\right) \right]. \quad (7)$$

The two-component spinor Φ represents $(1+\alpha_z)\Psi$. The "gauge link" $\exp\{-i\chi(\mathbf{b}, z)\}$ transforms Ψ in the Coulomb gauge to Ψ in the gauge $A^+ = 0$ ($A_z = 0$ in the infinite momentum frame). The choice of z_0 corresponds to a residual gauge freedom.

One can check that (4) is invariant under the gauge transformation $V(\mathbf{r}) \rightarrow V(\mathbf{r}) + \text{Constant}$, $E_n \rightarrow E_n + \text{Constant}$. Such a transformation may result from the addition of electrons in outer shells; it does not change the mechanical 4-momentum of a K-shell electron.

4 Joint (\mathbf{k}_T, k^+) distribution

The amplitude of the Compton reaction is given, modulo α matrices, by

$$\langle \Psi_f | e^{-i\mathbf{Q}\cdot\mathbf{r}} | \Psi_i \rangle \propto \int d^3\mathbf{r} e^{-i\mathbf{Q}\cdot\mathbf{r} - i\mathbf{k}_f\cdot\mathbf{r} - i\chi(\mathbf{b}, z)} \Phi(\mathbf{r}) = \Phi(\mathbf{k}_T, k^+) \quad (8)$$

with $z_0 = -\infty$. $\exp\{-i\mathbf{k}_f\cdot\mathbf{r} - i\chi\}$ is the final wave function distorted by the Coulomb potential, in the eikonal approximation. Equivalently,

$$\Phi(\mathbf{k}_T, k^+) = \int d^3\mathbf{r} e^{-i\mathbf{k}_T\cdot\mathbf{b} - ik^+z - i\chi(\mathbf{r})} \Phi(\mathbf{r}) = \int d^2\mathbf{b} e^{-i\mathbf{k}_T\cdot\mathbf{b}} \Phi(\mathbf{b}, k^+), \quad (9)$$

with the identification $k^+ = E_n + k_{f,z} + Q_z$. [*check*: in a semi-classical approach, $k^0(\mathbf{r}) = E_n - V(\mathbf{r})$ and $k_{f,z} + Q_z = k_z(\mathbf{r}) - V(\mathbf{r})$ at the collision point]. For the annihilation reaction, the *incoming positron* wave is distorted, then $z_0 = +\infty$. Thus, the gauge link takes into account either an initial or a final state interaction [1, 2, 3]. The quantity

$$q(\mathbf{k}_T, k^+) = \Phi^\dagger(\mathbf{k}_T, k^+) \Phi(\mathbf{k}_T, k^+) \quad (10)$$

depends on the deep inelastic probe, contrary to $q(\mathbf{b}, k^+)$ and

$$q(k^+) = \int q(\mathbf{b}, k^+) d^2\mathbf{b} = \int q(\mathbf{k}_T, k^+) d^2\mathbf{k}_T / (2\pi)^2. \quad (11)$$

5 Spin dependence of the electron density

Ignoring nuclear spin, the atom spin is $\mathbf{j} = \mathbf{L} + \mathbf{s}$. We will consider a $j = 1/2$ state and denote by $\bar{\mathbf{S}}^A = 2\langle \mathbf{j} \rangle$ and $\bar{\mathbf{S}}^e = 2\langle \mathbf{s} \rangle$ the atom and electron polarization vectors. \mathbf{S}^A and \mathbf{S}^e without bar indicate pure spin states. The *unpolarized* electron density in (\mathbf{b}, k^+) space from a *polarized* atom is

$$q(\mathbf{b}, k^+; \mathbf{S}^A) = \Phi^\dagger(\mathbf{b}, k^+; \mathbf{S}^A) \Phi(\mathbf{b}, k^+; \mathbf{S}^A) \quad (12)$$

and the electron polarisation is given by

$$\bar{\mathbf{S}}^e(\mathbf{b}, k^+; \mathbf{S}^A) q(\mathbf{b}, k^+; \mathbf{S}^A) = \Phi^\dagger(\mathbf{b}, k^+; \mathbf{S}^A) \vec{\sigma} \Phi(\mathbf{b}, k^+; \mathbf{S}^A). \quad (13)$$

Taking into account the conservations of parity and angular momentum, the fully polarized density can be written as

$$q(\mathbf{b}, k^+, \mathbf{S}^e; \mathbf{S}^A) = q(b, k^+) [1 + C_{0n} (\mathbf{S}^A \cdot \hat{\mathbf{n}}) + C_{n0} (\mathbf{S}^e \cdot \hat{\mathbf{n}}) + C_{nn} (\mathbf{S}^e \cdot \hat{\mathbf{n}})(\mathbf{S}^A \cdot \hat{\mathbf{n}})]$$

$$+ C_{ll} S_z^e S_z^A + C_{l\pi} S_z^e (\mathbf{S}^A \cdot \hat{\pi}) + C_{\pi l} (\mathbf{S}^e \cdot \hat{\pi}) S_z^A + C_{\pi\pi} (\mathbf{S}^e \cdot \hat{\pi})(\mathbf{S}^A \cdot \hat{\pi})] \quad (14)$$

where $\hat{\pi} = \mathbf{b}/b$ and $\hat{\mathbf{n}} = \hat{\mathbf{z}} \times \hat{\pi}$. The $C_{i,j}$'s are functions of b and k^+ .

Similar equations work for \mathbf{k}_T instead of \mathbf{b} . The link with Amsterdam notations [4] is, omitting kinematical factors,

$$q(k_T, k^+) = f_1 \quad f_1 C_{0n} = f_{1T}^\perp \quad (15)$$

$$f_1 C_{ll} = g_1 \quad f_1 C_{n0} = -h_1^\perp \quad (16)$$

$$f_1 C_{nn} = h_1 - h_{1T}^\perp \quad f_1 C_{l\pi} = g_{1T} \quad (17)$$

$$f_1 C_{\pi\pi} = h_1 + h_{1T}^\perp \quad f_1 C_{\pi l} = h_{1L}^\perp, \quad (18)$$

The \mathbf{b} - or \mathbf{k}_T integration washes out all correlations but C_{ll} and $C_{TT} = \frac{1}{2}[C_{nn} + C_{\pi\pi}]$, giving

$$q(k^+, \mathbf{S}^e; \bar{\mathbf{S}}^A) = q(k^+) + \Delta q(k^+) S_z^e \bar{S}_z^A + \delta q(k^+) \mathbf{S}_T^e \cdot \bar{\mathbf{S}}_T^A. \quad (19)$$

5.1 Sum rules

Integrating (19) over k^+ , one obtains the vector, axial and tensor charges

$$q = \int_{-\infty}^{\infty} q(k^+) dk^+ / (2\pi) = \int d^3\mathbf{r} \Psi^\dagger(\mathbf{r}; \mathbf{S}^A) \Psi(\mathbf{r}; \text{any } \mathbf{S}^A) \quad (20)$$

$$\Delta q = \int \Delta q(k^+) dk^+ / (2\pi) = \int d^3\mathbf{r} \Psi^\dagger(\mathbf{r}; \mathbf{S}^A) \Sigma_z \Psi(\mathbf{r}; \mathbf{S}^A = \hat{\mathbf{z}}) \quad (21)$$

$$\delta q = \int \delta q(k^+) dk^+ / (2\pi) = \int d^3\mathbf{r} \Psi^\dagger(\mathbf{r}; \mathbf{S}^A) \beta \Sigma_x \Psi(\mathbf{r}; \mathbf{S}^A = \hat{\mathbf{x}}). \quad (22)$$

For the hydrogen ground state,

$$q = 1, \quad \Delta q = (1 - \xi^2/3)/(1 + \xi^2), \quad \delta q = (1 + \xi^2/3)/(1 + \xi^2) \quad (23)$$

where $\xi = Z\alpha/(1 + \gamma)$, $\gamma = E/m_e = \sqrt{1 - (Z\alpha)^2}$.

Note the large "spin crisis" $\Delta q = 1/3$ for $Z\alpha = 1$.

5.2 Results for the polarized densities in (\mathbf{b}, k^+)

The 2-component wave functions of a $j_z = +1/2$ state write

$$\Phi(\mathbf{b}, k^+) = \begin{pmatrix} w \\ -iv e^{i\phi} \end{pmatrix}, \quad \Phi(\mathbf{k}_T, k^+) = \begin{pmatrix} \tilde{w} \\ -\tilde{v} e^{i\phi} \end{pmatrix}. \quad (24)$$

Other orientations of \mathbf{S}^A can be obtained by rotation in spinor space.

For the (\mathbf{b}, k^+) representation we can ignore the second term of (7). Then $v(\mathbf{b}, k^+)$ and $w(\mathbf{b}, k^+)$ are real and given by

$$\begin{pmatrix} v \\ w \end{pmatrix} = \int_{-\infty}^{\infty} dz \begin{pmatrix} \xi b \\ r + i\xi z \end{pmatrix} e^{-ik^+z + iEz - i\chi(\mathbf{b}, z)} f(r)/r \quad (25)$$

where $f(r) \propto r^{\gamma-1} \exp(-mZ\alpha r)$ is the radial wave function. Then,

$$\begin{aligned} q(b, k^+) &= w^2 + v^2 \\ C_{nn}(b, k^+) &= 1 \\ C_{0n}(b, k^+) = C_{n0}(b, k^+) &= -2wu/(w^2 + v^2) \\ C_{ll}(b, k^+) = C_{\pi\pi}(b, k^+) &= (w^2 - v^2)/(w^2 + v^2) \\ C_{l\pi}(b, k^+) = C_{\pi l}(b, k^+) &= 0. \end{aligned} \quad (26)$$

5.2.1 Sum rule for the atom magnetic moment

Consider a classical object at rest, of mass M , charge Q , spin \mathbf{J} and time-averaged magnetic moment $\vec{\mu}$. Its center of mass \mathbf{r}_G and the average center of charge $\langle \mathbf{r}_C \rangle$ coincide, say at $\mathbf{r} = 0$. Upon a boost of velocity \mathbf{v} , the center of energy \mathbf{r}_G and $\langle \mathbf{r}_C \rangle$ are displaced laterally by

$$\mathbf{b}_G = \mathbf{v} \times \mathbf{J}/M, \quad \langle \mathbf{b}_C \rangle = \mathbf{v} \times \vec{\mu}/Q. \quad (27)$$

\mathbf{b}_G and $\langle \mathbf{b}_C \rangle$ coincide if the gyromagnetic ratio has the Dirac value Q/M . For the hydrogen atom, \mathbf{b}_G is negligible and the magnetic moment is almost fully anomalous. In the infinite momentum frame ($\mathbf{v} \simeq \hat{\mathbf{z}}$), we have an electric dipole moment [5]

$$-e \langle \mathbf{b} \rangle = \mu_A \hat{\mathbf{z}} \times \bar{\mathbf{S}}^A, \quad (28)$$

the transverse asymmetry of the \mathbf{b} distribution coming from the C_{0n} term of (14). We recover the atom magnetic moment

$$\mu_A = -e (1 + 2\gamma)/(6m_e) \quad (29)$$

(the anomalous magnetic moment of the electron being omitted).

5.3 Results for the polarized densities in (\mathbf{k}_T, k^+)

For the (\mathbf{k}_T, k^+) representation we should take $z_0 = \pm\infty$ but then (7) diverges. In practice we assume some screening of the Coulomb potential and take $|z_0|$ large but finite, which gives

$$\chi(\mathbf{b}, z) = -Z\alpha \left[\pm \ln(2|z_0|/b) + \sinh^{-1}(z/b) \right], \quad (30)$$

the upper sign corresponding to Compton scattering and the lower sign to annihilation. Modulo an overall phase,

$$\begin{pmatrix} \tilde{w} \\ \tilde{v} \end{pmatrix} = 2\pi \int_0^\infty b db b^{\mp iZ\alpha} \begin{pmatrix} J_0(k_T b) w(b, k^+) \\ J_1(k_T b) v(b, k^+) \end{pmatrix}, \quad (31)$$

$$\begin{aligned} q(k_T, k^+) &= |\tilde{w}|^2 + |\tilde{v}|^2 \\ C_{nn}(k_T, k^+) &= 1 \\ C_{0n}(k_T, k^+) = C_{n0}(k_T, k^+) &= 2\Im(\tilde{v}^* \tilde{w}) / (|\tilde{w}|^2 + |\tilde{v}|^2) \\ C_{ll}(k_T, k^+) = C_{\pi\pi}(k_T, k^+) &= (|\tilde{w}|^2 - |\tilde{v}|^2) / (|\tilde{w}|^2 + |\tilde{v}|^2) \\ C_{l\pi}(k_T, k^+) = -C_{\pi l}(k_T, k^+) &= 2\Re(\tilde{v}^* \tilde{w}) / (|\tilde{w}|^2 + |\tilde{v}|^2). \end{aligned} \quad (32)$$

The factor $b^{-iZ\alpha}$ (Compton case) behaves like a converging cylindrical wave. Multiplying $\Phi(\mathbf{r})$, it mimics an additional momentum of the electron toward the z axis. In fact it takes into account the "focusing" of the final particle by the Coulomb field [5]. It also provides the relative phase between \tilde{w} and \tilde{v} which gives non-zero $C_{0n}(k_T, k^+)$ and $C_{n0}(k_T, k^+)$ (Sivers and Boer-Mulders-Tangerman effects). Similarly, $b^{+iZ\alpha}$ (annihilation case) takes into account the defocusing of the incoming positron.

5.4 Positivity constraints

The spin correlations between the electron and the atom can be encoded in a "grand density matrix" R [6], which is the final density matrix of the crossed reaction $nucleus \rightarrow atom(\mathbf{S}^A) + e^+(-\mathbf{S}^e)$.

Besides the trivial conditions $|C_{ij}| \leq 1$ the positivity of R gives

$$(1 \pm C_{nn})^2 \geq (C_{n0} \pm C_{0n})^2 + (C_{ll} \pm C_{\pi\pi})^2 + (C_{\pi l} \mp C_{l\pi})^2 \quad (33)$$

These two inequalities as well as $|C_{ll}| \leq 1$ are saturated by (26) and (32). In fact R is found to be of rank one. It means that the spin information of the

atom is fully transferred to the electron, once the other degrees of freedom (k^+ and \mathbf{b} or \mathbf{k}_T) have been fixed. If there is additional electrons or if we integrate over k^+ , for instance, some information is lost and some positivity conditions get non-saturated. Conversely, the hypothesis that R is of rank one leaves only two possibilities:

$$C_{nm} = \pm 1, \quad C_{0n} = \pm C_{n0}, \quad C_{\pi\pi} = \pm C_{ll}, \quad C_{l\pi} = \mp C_{\pi l}, \quad (34)$$

with (33) saturated. The hydrogen ground state chooses the upper sign. After integration over \mathbf{b} or \mathbf{k}_T , we are left with the *Soffer inequality*,

$$2 |\delta q(k^+)| \leq q(k^+) + \Delta q(k^+) \quad (35)$$

which in our case is saturated, even after integration over k^+ , see (23).

6 The electron-positron sea

The charge rule (20) involves positive contributions of both positive and negative values of k^+ . So it seems that there is less than one electron (with $k^+ > 0$) in the atom. This paradox is solved by the introduction of the electron-positron sea.

Let $|n\rangle$ be an electron state in the Coulomb field. Negative n 's are assigned to negative energy scattering states. Positive n 's up to n_B label the bound states ($-m < E_n < +m$) and the remaining ones from $n_B + 1$ to $+\infty$ are assigned to unbound states of positive energy, $E_n > +m$, considered as discrete. Let $|k, s\rangle$ be the plane wave of four-momentum k and spin s , solution the free Dirac equation. The destruction and creation operators in these two bases are related by

$$\alpha_{k,s} = \sum_n \langle k, s | n \rangle a_n, \quad \alpha_{k,s}^\dagger = \sum_n a_n^\dagger \langle n | k, s \rangle. \quad (36)$$

In the Dirac hole theory, the hydrogen-like atom is in the Fock state

$$|H_n\rangle = a_n^\dagger a_{-1}^\dagger a_{-2}^\dagger \cdots a_{-\infty}^\dagger |\text{QED-bare nucleus}\rangle \quad (37)$$

The number of electrons in the state $|k, s\rangle$ is

$$N^{elec}(\mathbf{k}, s) = \langle \alpha_{k,s}^\dagger \alpha_{k,s} \rangle = |\langle k, s | n \rangle|^2 + \sum_{n' < 0} |\langle k, s | n' \rangle|^2 \quad (38)$$

For a nucleus alone (but "QED-dressed") the first factor a_n^\dagger of (37) is missing and the first term of (38) is absent. Therefore, passing to the continuum limit $\langle k, s|n\rangle \longrightarrow \Phi(\mathbf{k}_T, k^+)$,

$$N_{atom}^{elec} - N_{nucleus}^{elec} = \sum_{k, k^0 > 0} \sum_s |\langle k, s|n\rangle|^2 = \int_{k^+ > 0} \frac{dk^+}{2\pi} q(k^+). \quad (39)$$

One term n' of (38) corresponds, e.g., to Compton scattering on an electron of the Dirac sea, producing a fast electron plus the positron $|n'\rangle =$ vacant. It is the *fracture function* of reaction $\gamma_i + A \rightarrow \gamma_f + A + e^- + X$.

Similarly the number of positrons is (with $k^0 > 0$):

$$N^{posit}(\mathbf{k}, s) = \langle \alpha_{-k, -s} \alpha_{-k, -s}^\dagger \rangle = \sum_{0 < n' \neq n} |\langle -k, -s|n'\rangle|^2. \quad (40)$$

For a nucleus alone the condition $n' \neq n$ is relaxed. By difference,

$$N_{nucleus}^{posit} - N_{atom}^{posit} = \int_{k^+ < 0} \frac{dk^+}{2\pi} q(k^+) \quad (41)$$

One term of Eq.(40) corresponds to the extraction of an electron of large negative energy, giving a fast positron and an electron in $|n'\rangle$. Eqs.(39) + (41) and (20) tell that the atom and nuclear charges differ by e . But the charge of the electron-positron virtual cloud surrounding the nucleus is not zero (charge renormalisation).

7 CONCLUSION

We have seen that the leading twist structure functions of the hydrogen-like atom at large Z has many properties that are supposed or verified for the hadronic ones, in particular: sum rules, longitudinal "spin crisis", Sivers effect, transverse electric dipole moment in the P_∞ frame, etc. It remains to evaluate these effects quantitatively. With this "theoretical laboratory" one may also investigate spin effects in fracture functions, non-leading twist structure functions, Isgur-Wise form factors, etc. The electron-positron sea may deserve further studies: to what extent is it polarized or asymmetrical in charge? Is the charge renormalisation of the nucleus found in Sec.6 the same as in standard QED? Is it finite and calculable for an extended nucleus?

Finally it may be interesting to do or re-analyse experiments on deep inelastic Compton scattering ("Compton profile" measurements).

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