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Relativistic calculations of pionic and kaonic atoms hyperfine structure

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We present the relativistic calculation of the hyperfine structure in pionic and kaonic atoms. A perturbation method has been applied to the Klein-Gordon equation to take into account the relativistic corrections. The perturbation operator has been obtained via a multipole expansion of the nuclear electromagnetic potential. The hyperfine structure of pionic and kaonic atoms provide an additional term in the quantum electrodynamics calculation of the energy transition of these systems. Such a correction is required for a recent measurement of the pion mass.

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I. INTRODUCTION

In the last few years transition energies in pionic \[ \pi \] and kaonic atoms \[ K \] have been measured with an unprecedented precision. The spectroscopy of pionic and kaonic hydrogen allows to study the strong interaction at low energies \[ \pi^+ p \rightarrow \pi^0 n \] by measuring the energy and natural width of the ground level with a precision of few meV \[ 1, 3, 4 \]. Besides, light pionic atoms can additionally be used to define new low-energy X-ray standards \[ 5, 6 \] and to evaluate the pion mass using high accuracy X-ray spectroscopy \[ 7, 8, 9 \]. Similar endeavour are in progress with kaonic atoms \[ 2 \].

In this paper we present the calculation of the hyperfine structure in pionic and kaonic atoms considering the perturbation term due to the interaction between the pion or kaon orbital moment with the magnetic momentum of the nucleus. Non-relativistic calculations for the pionic atom hyperfine structure can be found in Ref. \[ 11, 12, 13 \]. Other theoretical predictions for HFS including relativistic corrections can be found only for spin-\( \frac{1}{2} \) nucleus \[ 14, 15, 16 \]. Contrary to these methods, our technique is not restricted to this case and it can be used for an arbitrary value of the nucleus spin including automatically the relativistic effects. In particular, we calculate the HFS energy splitting for pionic nitrogen, which has been used for a recent measurement of the pion mass aiming at an accuracy of few ppm \[ 17, 18 \], and for kaonic nitrogen that has been proposed for the kaon mass measurement \[ 19 \].

This article is organized as follows. In Sec. II we calculate the first energy correction applying a perturbation method for the Klein-Gordon equation. In Sec. III we will obtain the perturbation term using the multipole expansion of the nuclear electromagnetic potential. Section IV is dedicated to the numerical calculations for some pionic and kaonic atoms.

II. CALCULATION OF THE ENERGY CORRECTION

The relativistic dynamic of a spinless particle is described by the Klein-Gordon equation. The electromagnetic interaction between a negatively charged spin-0 particle with a charge equal to \( q = -e \) and the nucleus can be taken into account introducing the nuclear potential \( A_\nu \) in the KG equation via the minimal coupling \( p_\nu \rightarrow p_\nu - qA_\nu \) \[ 20 \]. In particular, in the case of a central Coulomb potential \( (V_0(r), 0) \), the KG equation for a particle with a mass \( m \) is:

\[
m^2 c^2 \Psi_0(x) = \frac{1}{c^2} \left[ i \hbar \partial_t + ev_0(r) \right]^2 + \hbar^2 \nabla^2 - m^2 c^2 \Psi_0(x), \quad (1)
\]

where \( \hbar \) is the Planck constant, \( c \) the velocity of the light and the scalar wavefunction \( \Psi_0(x) \) depends on the space-time coordinate \( x = (ct, r) \). We consider here the stationary solution of Eq. (1). In this case, we can write:

\[
\Psi_0(x) = \exp(-iE_0t/\hbar) \varphi_0(r) \quad (2)
\]

and Eq. (1) becomes:

\[
\left\{ \frac{1}{c^2} \left[ E_0 + eV_0(r) \right]^2 + \hbar^2 \nabla^2 - m^2 c^2 \right\} \varphi_0(r) = 0, \quad (3)
\]

where \( E_0 \) is the total energy of the system (sum of the mass energy \( mc^2 \) and binding energy \( E_0 \)).

The perturbation correction \( E_1 \) can be deduced introducing an additional operator \( W \) in the zeroth order equation:

\[
\left\{ \frac{1}{c^2} \left[ E + eV_0(r) \right]^2 + \hbar^2 \nabla^2 - m^2 c^2 - W(r) \right\} \varphi(r) = 0. \quad (4)
\]

\( W(r) \) is in general non-linear. In the case of a correction \( V_1 \) to the Coulomb potential \( V_0 \), we have:

\[
W(r) = -\frac{1}{c^2} \left[ 2e^2 V_0(r) V_1(r) + 2eE V_1(r) \right] \quad (5)
\]

If we consider the interaction with the nuclear magnetic field as a perturbation, we have:

\[
W(r) = i\hbar e \left[ 2A_\nu(r) \partial^r + [\partial^r, A^r(r)] \right] - e^2 A^I(r) A_I(r). \quad (6)
\]
The correction to the energy due to $W$ can be calculated perturbatively with some manipulation of Eqs. (3) and (7), or via a linearization of the KG equation using the Feeshbach-Villars formalism [23, 24]. In both cases we have

$$E_1 = \frac{\epsilon^2\langle W \rangle}{2\left(E_{nl}^0 + (\epsilon E_0)\right)},$$

(7)

where we define

$$\langle A \rangle = \int V \varphi^*(r) A(r, t) \varphi(r) \, d^3r.$$  \hspace{1cm} (8)

Equation (8) is valid for any wavefunction normalization.

III. CALCULATION OF THE HYPERFINE STRUCTURE OPERATOR

The expression for $W(r)$ in the HFS case is derived using the multipole development of the vector potential $A(r)$ in the Coulomb gauge [23, 24, 25]. We neglect here the effect due to the spatial distribution of the nuclear magnetic moment in the nucleus [28] (Bohr-Weisskopf effect), while effect due to the charge distribution (Bohr-Rosenthal effect) are included in the numerical results of Sec. IV.

The hyperfine structure due to the magnetic dipole interaction is obtained by taking into account the first magnetic multipole term. Using the Coulomb gauge we have [23, 24]:

$$A(r) = -i\frac{\mu_0}{4\pi} \sqrt{2} r^{-2} C_1^{11} \cdot M^1,$$

where the symbol “·” indicates here the general scalar product between tensor operators. $M^1$ operates only on the nuclear part $|nmI\rangle$ and $C_1^{11}$ is the vector spherical harmonic [21, 22] acting on the pion part $|nlm\rangle$ of the wavefunction. We can decompose the perturbation term $W(r)$ as:

$$W(r) = W_1(r) + W_2(r),$$

(10)

where

$$W_1(r) = +i\epsilon A^0(r) \partial^0 + \left[\partial_t, A^0(r)\right]$$

(11)

is the linear part and

$$W_2(r) = -\epsilon^2 A^0(r) A^0(r),$$

(12)

is the quadratic part.

We study first the operator $W_1$. We note that $[\partial_t, A^0(r)] = -\nabla \cdot A(r) = 0$ since we are using the Coulomb gauge. In this case we have:

$$W_1(r) = +2i\epsilon \mu_0 h \sqrt{2} r^{-2} \left(C_1^{11} \cdot \nabla\right) M^1,$$

(13)

Using the properties of the spherical tensor [26, 27], we can show that:

$$C_1^{11} \cdot \nabla = -\frac{r^{-3}}{\sqrt{2}} L_q,$$

(14)

where $L_q$ is the dimensionless angular momentum operator in spherical coordinates. The perturbation operator can be written as a scalar product in spherical coordinate of the operator $T^1$ acting on the pion wavefunction, and the nuclear operator $M^1$:

$$W_1(r) = \frac{\epsilon \mu_0 h}{2\pi} r^{-3} (L \circ M^1) = T^1 \circ M^1$$

(15)

with

$$T^1_q = \frac{\epsilon \mu_0 h}{2\pi} r^{-3} L_q.$$  \hspace{1cm} (16)

The expected value of the operator $W_1$ can be evaluated applying the scalar product properties in spherical coordinates [26, 27]:

$$\langle n'l'\bar{l}m'|W_1|nlIm_Im_f\rangle = (-1)^{l'+l} F_{F'F} \delta_{m_f m'_f} \delta_{l'l'} \times \left\{ F 1 1 \right\} \langle n'l'\bar{l}m'||n|l||F|M^1||I\rangle,$$

(17)

where $\{a b c\}$ represents a Wigner 6-j symbol. The reduced operator $\langle n'l'\bar{l}m'||n|l||F|M^1||I\rangle$ is calculated from the matrix elements $\langle n'l'm'|T^1|nlm\rangle$ by a particular choice of the quantum numbers $m$ and $q$ applying the Wigner-Eckart theorem:

$$\langle n'l'\bar{l}m'||n|l||F|M^1||I\rangle = \delta_0 \left(\begin{array}{ccc} I & 1 & l \\ -1 & 0 & 1 \end{array}\right),$$

(18)

where $\{a b c\}$ indicates the Wigner 3-j symbol.

The nuclear operator can be related to the magnetic moment on the nucleus by $\langle I| M_N^1 |I\rangle = \mu_1 \mu_N$ [26, 27] where $\mu_1$ is the nuclear dipole momentum in units of the nuclear magneton $\mu_N = e\hbar/2m_p c$:

$$\langle I|M^1|I\rangle = \frac{\mu_1 \mu_N}{I 1 1} \times \left(-1\right)^{l'+l} \left(\begin{array}{ccc} I & 1 & l \\ -1 & 0 & 1 \end{array}\right).$$

(19)

Considering Eq. (14), the total expression for $W_1(r)$ becomes:

$$\langle n'l'\bar{l}m'|W_1|nlIm_Im_f\rangle = \delta_{F'F} \delta_{m_f m'_f} \delta_{l'l'} \mu_1 \mu_N \times \frac{\epsilon \mu_0 h}{2\pi} F(F + 1) - (l + 1) - l(l + 1) \langle n'|r^{-3}|nl\rangle.$$  \hspace{1cm} (20)
which, as expected, is equal to zero for $l = 0$ (then $I = F$).

To find the final expression of the HFS energy shift, we have to evaluate the contribution of the operator $W_2(r) = -e^2 A'(r) A_z(r)$ in the $\langle W \rangle$ diagonal terms. Using Eq. (20), we have:

\[
\langle nlIFmF'|W_2|nlIFmF \rangle = +2 \left( \frac{e\mu_0}{4\pi} \right)^2 \times \\
\langle nlIFmF|(r^{-2}C^{11}_l \circ M^1_l) \cdot (r^{-2}C^{11}_l \circ M^1_l)\rangle |nlIFmF\rangle.
\] (21)

We are in presence of three independent scalar products: two scalar products between the tensor $C^{11}_l$ and the vector $M^1_l$, and the scalar product between the vectorial operators $C^{11}_l \circ M^1_l$. The "\) scalar product in $W_2$ can be decomposed using the reduced matrix elements of a generic operator product $X^K$, of rank $K$, between non-commuting tensor operators $U^k$ and $V^k$ of rank $k$. For our case, this scalar product corresponds to a tensor product with $K = 0$, and $k = 1$:

\[
X^0 = U^1 \cdot V^1 = (r^{-2}C^{11}_l \circ M^1_l) \cdot (r^{-2}C^{11}_l \circ M^1_l),
\] (22)

\[
U^1 = V^1 = (r^{-2}C^{11}_l \circ M^1_l).
\] (23)

We have [29]:

\[
\langle nlIF|X^0|nlIF \rangle = \sum_{F'} \left\{ \begin{array}{ccc}
1 & 1 & 0 \\
F & F & F'
\end{array} \right\} \times \\
\langle nlIF|U^1|nlIF \rangle \langle nlIF'|V^1\rangle |nlIF\rangle.
\] (24)

$V^1$ and $U^1$ are scalar products between commutative tensor operators, and their reduced matrix element $\langle F'\rangle |V^1\rangle$ can be calculated applying again the Wigner-Eckart theorem for the component $q = 0$:

\[
\langle nlIF'|V^1\rangle |nlIF\rangle = \langle nlIF'|V^1_0|nlIF\rangle \left( \frac{F}{F'} \frac{1}{1} \frac{F}{0} \right).
\] (25)

where [31]:

\[
V^1_0 = U^1_0 = r^{-2}(C^{11}_l \circ M^1_l) = r^{-2} \sum_q (-1)^q \frac{g}{\sqrt{2}} C^{11}_q M^{1,-q}_q.
\] (26)

To evaluate the matrix element $\langle nlIF'|V^1_0|nlIF\rangle$ we can explicitly decompose $|nlIF\rangle$ as a function of the eigenfunctions $|nlm\rangle$ and $|Im_l\rangle$ using the Clebsch-Gordan coefficients. We have

\[
\langle nlIF'|V^1_0|nlIF\rangle = \\
-\frac{1}{r^2\sqrt{2}} \sum_{m',m,m,m} |\langle lmIm_{l}'|lIF\rangle\langle lmIm_{l}|IFF\rangle| \\
\times \left[ \langle lm'|r^{-2}C^{11}_{L1}nlm\rangle|lm_{l}'\rangle M^{11}_{l}\langle lm_{l}\rangle - \\
\langle lm'|r^{-2}C^{11}_{L1}nlm\rangle|lm_{l}'\rangle M^{10}_{l}\langle lm_{l}\rangle \right].
\] (27)

Applying the Wigner-Eckart theorem we obtain

\[
\langle nlIF'|V^1_0|nlIF\rangle = \\
-\frac{1}{r^2\sqrt{2}} \langle nl|r^{-2}C^{11}_l|nl\rangle \langle I|M^1_l|I\rangle \times \\
\sum_{m',m_{l}'m_{l},m_{l}} |\langle lmIm_{l}'|lIF\rangle\langle lmIm_{l}|IFF\rangle| \\
\times \left[ \left( \begin{array}{ccc}
l & 1 & l \\
-m_{l}' & 1 & m
\end{array} \right) \left( \begin{array}{ccc}
I & 1 & I \\
-m_{l} & -1 & m_{l}
\end{array} \right) \right] \\
\times \left( \begin{array}{ccc}
-l & l & 1 \\
-m_{l}' & -1 & m_{l}
\end{array} \right) \left( \begin{array}{ccc}
I & 1 & I \\
-m_{l}' & +1 & m_{l}
\end{array} \right). \] (28)

The reduced matrix element $\langle nl|r^{-2}C^{11}_l|nl\rangle$ can be decomposed in a radial and angular part

\[
\langle nl|r^{-2}C^{11}_l|nl\rangle = \langle nl|r^{-2}|nl\rangle \langle l|C^{11}_l|l\rangle.
\] (29)

Due to the symmetry properties, $\langle l|C^{11}_l|l\rangle$ is equal to zero for any $l \geq 2$. This result implies that the reduced matrix elements of $U^1$ and $V^1$ are always equal to zero. As a consequence, the diagonal elements $\langle A'(r)A_z(r)\rangle = 0$ for any wavefunction, i.e., $W_2$ does not contribute to the HFS energy shift.

We can now write the final expression for the HFS energy correction:

\[
E^{nl}_{nlIF} = \frac{\mu_1\mu_\eta\mu_3\hbar^2}{4\pi (E^{nl}_{nlIF} - \langle V^1_0|nl|V^1_0\rangle)} \times \\
\left[ \frac{F(F+1) - ll + 1 - l(l+1)}{2l} \right] \langle nl|r^{-3}|nl\rangle.
\] (30)

This formula is obtained by a perturbation approach of the KG equation. For this reason, all the relativistic effects are automatically included in Eq. [29]. In the non-relativistic limit $c \to \infty$, $(E_0 - V)/c^2 \to m$ and we find the usual expression of the HFS for the Schrödinger equation [32].

IV. NUMERICAL RESULTS AND BEHAVIORS

We present here some calculations for a selection of pionic and kaonic atom transitions. Such calculations are obtained solving numerically the Klein-Gordon equation using the multi-configuration Dirac-Fock code developed by one of the author (P.I.) and J.-P. Desclaux [33, 34, 35, 36] that has been modified to include spin-0 particles case, even in the presence of electrons [37]. The first part is dedicated to the $5 \to 4$ and $8 \to 7$ transitions in pionic and kaonic nitrogen, respectively. In the second part we will study the dependence of the HFS splitting against the nuclear charge $Z$ to observe the role of the relativistic corrections.
TABLE I: Energy (in eV) contribution for the selected levels in pionic nitrogen. The first error takes into account neglected next order QED corrections. The second is due to the accuracy of the pion mass (±2.5 ppm).

<table>
<thead>
<tr>
<th>Transition F-F'</th>
<th>Trans. rate (s⁻¹)</th>
<th>Trans. E (eV)</th>
<th>Shift (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5f → 4d</td>
<td>4-3</td>
<td>4.57×10⁻¹³</td>
<td>-0.00606</td>
</tr>
<tr>
<td>3-2</td>
<td>3.16×10⁻¹³</td>
<td>4057.6876</td>
<td>0.00341</td>
</tr>
<tr>
<td>3-3</td>
<td>2.98×10⁻¹³</td>
<td>4057.6845</td>
<td>-0.00910</td>
</tr>
<tr>
<td>2-1</td>
<td>2.13×10⁻¹³</td>
<td>4057.7031</td>
<td>0.00946</td>
</tr>
<tr>
<td>2-2</td>
<td>2.25×10⁻¹³</td>
<td>4057.6948</td>
<td>0.00112</td>
</tr>
<tr>
<td>2-3</td>
<td>0.01×10⁻¹³</td>
<td>4057.6822</td>
<td>-0.01138</td>
</tr>
</tbody>
</table>

Coulomb term in the Table includes the non-relativistic recoil correction using the reduced mass on the KG equation. The pion and nucleus charge distribution contribution are also included. The pion charge distribution radius contribution is included following [37, 40]. For the pion charge distribution radius we take r_π = 0.672 ± 0.08 [41]. For the nuclei we take values from Ref. [42]. The leading QED corrections, vacuum polarization, contribution is calculated self-consistently, thus taking into account the loop-after-loop contribution to all orders, at the Uehling approximation. This is obtained by including the Uehling potential into the KG equation [43]. Other higher-order vacuum polarization contribution are calculated as perturbation to the KG equations: Wichman-Kroll and Källén-Sabry [44, 85]. The self-energy is calculated using the expression in Ref. [43] and it includes the recoil correction. The Relativistic recoil term has been evaluated adapting the formulas from Refs. [45, 44] (more details can be found in Ref. [39]). The calculations presented here do not take into account second order recoil effects (Fig. 1 top), or higher QED corrections as vacuum polarization and self-energy mixed diagrams (Fig. 2 bottom). The contribution from these terms has been estimated using the formula for a spin-½ particle with a mass equal to the pion’s. For the 5 → 4 pionic nitrogen transitions, vacuum polarization and self-energy mixed diagrams contribute in the order of 1 meV for the diagram with the vacuum polarization loop in the nuclear photon line [47] (Fig. 2 bottom-left), and 0.0006 meV for the diagram with the vacuum polarization loop inside the self-energy loop [48] (Fig. 2 bottom-right). The second order recoil contributions are in the order of 0.04 meV [49] (Fig. 2 top). The largest contribution comes from the unevaluated diagram with the vacuum polarization loop in the nuclear photon line [17].

Assuming a statistical population distribution of the HFS sublevels, we can use Eq. (31) to calculate the mean value of the transitions using the results in Table I. Comparing this calculation with the one without the HFS, we obtain a value for the HFS shift. For transitions 5g → 4f and 5f → 4d we obtain shifts of 0.8
FIG. 1: Diagrams relative to the unevaluated QED contributions: second order recoil correction (top), and vacuum polarization and self-energy mixed diagrams (bottom). Their effects are estimated using the available formulas for spin-\(\downarrow\) particles.

and 2.2 meV, respectively. These values correspond to a correction to the pion mass between 0.2 and 0.6 ppm.

The transition energies for the 8 \(\rightarrow\) 7 transitions in kaonic nitrogen are presented in Tables III and IV. As for the pionic nitrogen, the error contribution due to the QED correction not considered is dominated by the un-evaluated diagram with the vacuum polarization loop in the nuclear photon line \[47\], the associated correction is estimated in the order of 0.5 meV. For \(8k \rightarrow 7i\) and \(8i \rightarrow 7h\) transitions we have a HFS shift of 0.6 and 0.8 meV, respectively, which correspond to a correction of the kaon mass between 0.2 and 0.3 ppm.

As a general note, we remark that if we assume a statistical distribution of the initial state sublevels populations, transitions \(nl \rightarrow n's\) with a s orbital as final state have an average HFS shift equal to zero due to an exact cancellation between the weighted excited sublevels energy shifts as seen from Eq. \([42]\).

### B. General behavior of the hyperfine structure correction over \(Z\)

For the non-relativistic case, the HFS splitting normalized to the binding energy and to the nuclear magnetic moment, depends linearly on \(Z\alpha\). Any deviation from this linear dependence in the Klein-Gordon HFS can be attributed only to relativistic effects.

To study the behavior of the normalized HFS splitting \((E_{P=3/2}^{p} - E_{P=1/2}^{p})/(E_0\mu I)\) for the relativistic case, we calculated the HFS for a selected choice of pionic atoms with a stable nucleus of spin 1/2. The orbital 9p has been chosen to minimize the effect of the finite nuclear size and strong interaction shifts, particularly for high values of \(Z\). The results are summarized in Table V. For these calculations we used the nuclear mass values from Ref. \[31\], the nuclear radii from Refs. \[42, 50\] and the nuclear magnetic moments from Ref. \[51\].

For higher \(Z\) values a non-linear dependence on \(Z\alpha\) appears as we can see in Fig. 2. This non-linearity originates in the two different parts of Eq. \([34]\): the non-trivial dependency on \(E_0\) in the denominator and the expectation value \(\langle nl|r^{-3}|nl\rangle\).

### V. CONCLUSIONS

We presented a relativistic calculation of the hyperfine structure in pionic and kaonic atoms. The precise evaluation of the specific case of pionic and kaonic nitrogen is particularly important for the new measurement of the pion and kaon mass. The small error on the theoretical predictions, of the order of 1 meV for the 5 \(\rightarrow\) 4 transition, corresponds to a systematic error of \(\gtrsim 0.2\) ppm for the pion mass evaluation, considerably smaller than the error of previous theoretical predictions \[52\].
TABLE V: HFS separation of the F=1/2 and F=3/2 levels for the 9p orbital for pionic atoms with spin $\frac{1}{2}$ nucleus.

<table>
<thead>
<tr>
<th>Element</th>
<th>Z</th>
<th>9p energy (eV)</th>
<th>HFS splitting (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1</td>
<td>-39.93816</td>
<td>0.0001</td>
</tr>
<tr>
<td>$^4$He</td>
<td>2</td>
<td>-174.8370</td>
<td>-0.0009</td>
</tr>
<tr>
<td>$^{13}$C</td>
<td>6</td>
<td>-1633.402</td>
<td>0.0060</td>
</tr>
<tr>
<td>$^{15}$N</td>
<td>7</td>
<td>-2226.813</td>
<td>-0.0039</td>
</tr>
<tr>
<td>$^{19}$F</td>
<td>9</td>
<td>-3689.435</td>
<td>0.0767</td>
</tr>
<tr>
<td>$^{31}$P</td>
<td>15</td>
<td>-10286.63</td>
<td>0.1544</td>
</tr>
<tr>
<td>$^{57}$Fe</td>
<td>26</td>
<td>-53146.21</td>
<td>0.8293</td>
</tr>
<tr>
<td>$^{77}$Se</td>
<td>34</td>
<td>-69987.00</td>
<td>-0.3143</td>
</tr>
<tr>
<td>$^{89}$Y</td>
<td>39</td>
<td>-101681.20</td>
<td>-0.4266</td>
</tr>
<tr>
<td>$^{107}$Ag</td>
<td>47</td>
<td>-134178.0</td>
<td>-4.1295</td>
</tr>
<tr>
<td>$^{129}$Xe</td>
<td>54</td>
<td>-250634.4</td>
<td>1.2629</td>
</tr>
<tr>
<td>$^{183}$W</td>
<td>74</td>
<td>-306731.6</td>
<td>7.8662</td>
</tr>
</tbody>
</table>

The formalism presented in this article can be applied for other effect as the quadrupole nuclear moment which can not be negligible for mesonic atoms with high Z. In this case, HFS due to the quadrupole moment can be predicted using the next multipole in the development of the electric potential of the nucleus to evaluate the correspondent perturbation operator. This application is particularly important for the calculation of the atomic levels in heavy pionic ions, where relativistic and nucleus deformation effects can be taken into account at the same time.

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