3-1-1988

Limitation of the semirelativistic approach in sum rules and related calculations in atomic physics

M. L. Rustgi
PT. Leung
Portland State University
S. A. Long

Citation Details

This Article is brought to you for free and open access. It has been accepted for inclusion in Physics Faculty Publications and Presentations by an authorized administrator of PDXScholar. For more information, please contact pdxscholar@pdx.edu.
Limitation of the semirelativistic approach in sum rules
and related calculations in atomic physics

M. L. Rustgi and P. T. Leung*
Department of Physics, State University of New York, Buffalo, New York 14260

S. A. T. Long
National Aeronautics and Space Administration, Langley Research Center, Hampton, Virginia 23665
(Received 14 September 1987)

It is shown that the semirelativistic approach, when applied consistently to atomic calculations
involving the Thomas-Reiche-Kuhn sum rule or its applications, may lead to very inaccurate results.

In spite of the availability of the fully relativistic (Dirac-type) treatment for atomic calculations, the
semirelativistic approach (SA) is still applied many times to problems dealing with inner-shell ionizations\(^1\) and
sum-rule calculations\(^2\)–\(^7\) both because of its simplicity and accuracy. Especially for the latter type of calcula-
tions which are encountered in problems on photoabsorption in atomic systems, the SA has been found to be
extremely efficient and leads to reasonably accurate results with tremendous simplifications as compared to a fully
relativistic state-to-state calculation.\(^8\),\(^9\) The SA or the projection operator approach\(^6\) is used not just for its sim-

plicity but because of its necessity to get rid of the negative energy states in the sum-rule calculations for a rela-
тивistic system, as had been noted first by Levinger, Rust-
gi, and Okamoto.\(^2\)

In this report, we shall point out that the SA as applied
to sum-rule calculations can yield very inaccurate results
for the high-Z systems, and that the seemingly good
agreement reported earlier is fortuitous due to the applica-
tion of an approximate eigenstate of the semirelativistic
Hamiltonian. The SA can hardly be expected to be very
accurate for \(Z = 100\) and in general one expects the cor-
duction due to the next term, the order of \((\alpha/c)^4\), to
be roughly of the order \((\alpha Z)^4\), and we shall see that
this is indeed the case. We shall limit ourselves mainly to
the one-electron atomic systems and shall discuss the im-

(1)


dictions of our results to the many-electron systems.

We shall start by defining clearly what we mean by the
SA. By the SA, we mean that the system is described by
the Foldy-Wouthuysen (FW) Hamiltonian to the lowest
order in \(\beta = \alpha/c\). Thus, for a one-electron system with
nuclear charge \(Z\epsilon\), we have, in standard notation, the
eigenvalue equation\(^10\),\(^11\)

\[
H_{FW} \psi_{FW} = E \psi_{FW},
\]

where

\[
H_{FW} = \frac{p^2}{2m} + eV - \frac{p^4}{8m^3c^2} + \frac{e\hbar}{4m^2c^2} \frac{1}{r} \frac{\partial}{\partial r} \sigma \cdot L
+ \frac{e\hbar^2}{8m^2c^2} \vec{p}^2 V ,
\]

and

\[
V = - \frac{Ze}{r} .
\]

In Eq. (1), the \(\psi_{FW}\) form a complete set of two-spinor
wave functions. The solutions for the eigenenergies of \(E\)
of Eq. (1) are well known; however, the eigenfunctions
\(\psi_{FW}\) are less familiar.\(^10\) Consequently, in some previous
sum-rule calculations\(^7\) the eigenfunction \(\psi_{FW}\) had been
approximated by the hydrogenic Schrödinger-type wave
function. Recently, we have discovered that Berestetskii
and Landau\(^12\) (BL) had actually obtained the exact (non-
perturbative) form of \(\psi_{FW}\) even before FW published
their work\(^13\) The solution by BL can be expressed as\(^11\),\(^12\)

\[
\psi_{FW}(r) = \left[ 1 - \frac{\hbar^2}{8m^2c^2} \frac{1}{r} \right] \phi_D(r) ,
\]

where \(\phi_D(r)\) denotes the large components of the well-
known exact Dirac wave function.\(^10\)

In the following, we shall illustrate with some simple
examples how these eigenfunctions \(\psi_{FW}\), when consistent-
ly applied, may lead to large deviations from the exact
relativistic results for hydrogenlike systems with a large
nuclear charge \(Z\). We shall mainly deal with the
ground-state wave function

\[
\phi_D^0(r) = Nr^{-1} \psi_D^0(r) \chi_{\pm} ,
\]

where \(\psi_D^0(r)\) is the ground-state Schrödinger wave
function and is written as \(\exp(-Zr/a_0)\); \(a_0\) denotes the Bohr
radius, \(\chi_+ = (\psi^0)\) and \(\chi_- = (\psi^1)\) are the up and down spin-
ors, and \(\gamma\) is defined as

\[
\gamma = \left[ 1 - (Z\alpha)^2 \right]^{1/2} .
\]

In (6), \(\alpha\) is the fine-structure constant and \(N\) in (5) is the
normalization constant given by

\[
N = \frac{1}{\sqrt{2}} \left[ \pi \Gamma(2\gamma + 1) \right]^{-1/2} \left[ \frac{2Z}{a_0} \right]^{\gamma + 1/2}
\times \left[ 1 + \frac{1}{4} \frac{\hbar^2 Z^2}{a_0^2} \frac{1}{(2\gamma - 1)} \right]^{-1/2} .
\]
The $V^2$ term in (4) involves the ratio of the kinetic energy to the rest energy of the atomic electron and hence should be negligible for small $Z$. However, this term may contribute significantly to the high-$Z$ systems.

As illustrations, let us calculate the mean-square radius

$$
\langle r^2 \rangle_{SA} = \int \psi_{FW}^0 \psi_{FW}^0 \psi_{FW}^0 dr
$$

$$
= 4\pi N^2 \left[ \frac{a_0}{2Z} \right]^{2\gamma+3} \frac{\Gamma(2\gamma+3)}{1-\frac{1}{4}\frac{\hbar^2}{m^2c^2}} \left[ \frac{Z}{a_0} \right]^2 \frac{1-3\gamma}{(1+\gamma)(1+2\gamma)}
$$

and

$$
F_{SA}(q,Z) = \int \psi_{FW}^0 e^{iq\cdot r} \psi_{FW}^0 \psi_{FW}^0 dr
$$

$$
= \frac{4\pi}{\pi} \frac{N^2}{Z} \left[ \frac{\Gamma(2\gamma)}{\frac{2Z}{a_0} + q^2} \right]^\gamma \left[ 1 - \frac{\hbar^2}{4m^2c^2} \frac{Z^2}{a_0^2} \right] \sin \left[ 2\gamma \tan^{-1} \left[ \frac{qa_0}{2Z} \right] \right]
$$

$$
- (\gamma - 1) \left[ \frac{\Gamma(2\gamma-2)}{\frac{2Z}{a_0} + q^2} \right]^\gamma \sin \left[ 2(\gamma-1) \tan^{-1} \left[ \frac{qa_0}{2Z} \right] \right].
$$

On the other hand, on using the exact Dirac wave function, we get the fully relativistic results

$$
\langle r^2 \rangle_R = 2(a_0/2Z)^2 (2\gamma+1)(\gamma+1)
$$

and

$$
F_R(q,Z) = \frac{1}{(2\gamma q)} \left[ \frac{2Z}{a_0} \right]^{2\gamma+1} \left[ \frac{2Z}{a_0^2} + q^2 \right]^\gamma \sin \left[ 2\gamma \tan^{-1} \left[ \frac{qa_0}{2Z} \right] \right].
$$

We have carried out numerical calculations for each of the results in Eqs. (8)-(11). A comparison of $\langle r^2 \rangle_{SA}$ and $\langle r^2 \rangle_R$ is shown in Table 1. It can be seen from Table 1 that the SA yields considerably smaller values of the mean-square radius in comparison with the relativistic ones. These results differ by as much as 25% for $Z = 100$.

The results for the form factor, however, do not show any significant differences. This is so because for small values of $q$, $F(q,Z) \approx 1 - q^2 \langle r^2 \rangle /6$, and though $\langle r^2 \rangle_{SA}$ and $\langle r^2 \rangle_R$ differ significantly for large $Z$, the deviation of $F(q,Z)$ from 1 is almost negligible because of the presence of $q^2$. For large values of $q$, the exponential factor in the expression for the form factor oscillates so rapidly that the form factor becomes very small and almost identical in both the approximations. This example explains to a certain extent the occasional success of the SA.

As a more interesting example, let us refer to the calculation of the real part of the forward scattering amplitude $f(\omega)$ for a $K$-electron in the high-photon-energy limit. While numerical results from an exact Dirac-type calculation are available, the problem has also been treated by the much simpler sum-rule approach. Nonrelativistically one would just expect, in units of $e^2/mc^2$, employing the Thomas-Reiche-Kuhn (TRK) sum rule, $f(\infty) = 1$.

<table>
<thead>
<tr>
<th>$Z$</th>
<th>$\langle r^2 \rangle_{SA}$</th>
<th>$\langle r^2 \rangle_R$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>$8.363 \times 10^{-19}$</td>
<td>$8.375 \times 10^{-19}$</td>
</tr>
<tr>
<td>40</td>
<td>$4.873 \times 10^{-20}$</td>
<td>$4.987 \times 10^{-20}$</td>
</tr>
<tr>
<td>60</td>
<td>$1.949 \times 10^{-20}$</td>
<td>$2.067 \times 10^{-20}$</td>
</tr>
<tr>
<td>80</td>
<td>$9.147 \times 10^{-21}$</td>
<td>$1.040 \times 10^{-20}$</td>
</tr>
<tr>
<td>100</td>
<td>$4.093 \times 10^{-21}$</td>
<td>$5.579 \times 10^{-21}$</td>
</tr>
</tbody>
</table>
higher-order terms in $\beta$ not included in the semirelativistic Hamiltonian should contribute significantly to such sum-rule calculations for the $K$ electrons of heavy elements. Thus we can conclude from the above examples that the SA, when consistently applied, may lead to results considerably smaller than the exact relativistic ones for large-$Z$ systems.

Recently, Smith has considered a similar comparison for the many-electron systems. Adopting an independent particle description, Smith has generalized the result derived in Ref. 2 to a system with $Z$ electrons to obtain

$$f(\infty) = Z - \langle 0 | T | 0 \rangle / m c^2,$$

which turns out to be in agreement with previous results from direct calculations by Cromer and Liberman and Smith. Smith then argued that usually the reduction of the forward atomic scattering factor from $Z$ is reported by applying the nonretarded $E1$ approximation which leads to an extra factor $\frac{1}{3}$ in the correction term to $f(\infty)$ in (16), but with the inclusion of the $E2$ oscillator strength and the retardation correction to the electric-dipole transitions as in Eq. (13), the sum-rule calculations show good agreement with the measured anomalous scattering factor (see Fig. 1 of Ref. 7). However, in light of our present investigation for the one-electron system, we believe that Smith’s agreement is again somewhat fortuitous, and a consistent evaluation of Eq. (16) using the Foldy-Wouthuysen-type wave function will lead to further deviation from the exact results. Moreover, the many-electron problem is further complicated for one is not clear regarding the relative importance of the contributions due to the correlation effects among the electrons and their effect on the $E2$ oscillator strength and retardation correction to the $E1$ transition. A further investigation of these effects would surely be interesting and would lead to a deeper understanding of the validity and limitation of the sum-rule approach.

The authors are grateful to Professor Joseph S. Leger and Professor William McKinley for their comments on the earlier version of the manuscript and to Professor W. McKinley and Professor D. Y. Smith for the details of their calculations. This work was partially supported by the National Aeronautics and Space Administration under Grant No. NAG1577.
673 (1949).


16 G. Breit, Rev. Mod. Phys. 4, 504 (1932); 5, 91 (1933); M. Gell-Mann, M. L. Goldberger, and W. Thirring, Phys. Rev. 95, 1612 (1954).

17 Note that in this case the $\nabla^2$ term in Eq. (4) can be ignored since this would lead to a correction of order $\beta^2$ in $f(\infty)$. See Ref. 5 for more details.
