Simple Analytical Eigenfunctions of Electrons in Thomas–Fermi Atoms

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Analytical solutions of the Schrödinger equation for the approximate Thomas–Fermi potential have been given by KERNER 1 and others 2. The author 2 has obtained his functions using a more accurate approximate potential, but the obtained eigenfunctions are not simple for practical purposes. It is the purpose of this note to give analytical solutions for practical use of the Schrödinger equation for the approximate Thomas–Fermi potential of the author. The Schrödinger equation for the author’s approximate potential in atomic units is

\[ yi'' + \left[ -\alpha^2 + \frac{2Z}{r(1+A)r} \right] y_i = 0, \quad (1) \]

where \( Z \) = atomic number and \( A = 0.64309 Z^{1/4} \). The radial part \( R_i(r) = y_i(r)/r \) may be written in the form

\[ y_i(r) = e^{-\alpha r} \left( \frac{A}{1+A^2 r} \right)^{1/2} f(x), \quad (2) \]

where \( x = A r/(1+A^2 r) \). Substituting \( y_i(r) \) in the Schrödinger equation, we see that \( f(x) \) fulfills the differential equation

\[ x(x-1)^2 f'' + 2\left[ (l+1) - (2l+3) + \frac{x}{A} \right] f' + \frac{2Z}{A^2} \left[ -2(l+1)^2 - \frac{2\alpha}{A} (l+1) + (l+1)(l+2) x - \frac{2Z}{A} x \right] f = 0. \quad (3) \]

If we set \( f(x) = \sum_{v=0}^{\infty} c_v x^v \) we obtain the following recurrence formulas for the \( c_v \):

\[ \left[ (v-1)(v+2l+2) + (l+1)(l+2) - \frac{2Z}{A} \right] c_v = -2Z \left[ (l+1)^2 - \frac{2\alpha}{A} (l+v+1) - v(2l+v+2) \right] c_{v+1} \]

valid for \( v = 0, 1, 2, \ldots \) and \( c_{-1} = 0 \). Setting \( A = 0 \) we obtain the well known recurrence formulas for an electron in the field of a bare nucleus where \( n = l+1+v \) is the principal quantum number. Rewriting the recurrence formulas given by Eq. (4) in the quantum numbers \( n, l \) we have

\[ n(n-1) - \frac{2Z}{A} c_{n-1} = 2 \left[ \frac{A}{Z} - \frac{\alpha n}{A} - n^2 \right] c_{n-1} + (n-l)(n+l+1) c_{n-l} = 0. \quad (5) \]

Neglecting the coefficient \( c_{n-l} \) in Eq. (5) gives us the zero approximation for the eigenvalue \( \alpha_0 = Z/n - n A \). In order to obtain the first approximation of the eigenvalue \( \alpha_1 \) we apply the same procedure which has been previously used by the author 3. At first we write the following determinant

\[ 2 \left[ \frac{Z}{A} \frac{\alpha n}{A} (n-1) - (n-1)^2 \right] \frac{(n-l)\,(n+l)}{2} - 2 \frac{Z}{A} \frac{(n-l)\,(n+l+1)}{2} = 0 \quad (6) \]

which follows directly from the recurrence formulas given by Eq. (5). If we set \( z = \alpha_0 \) in the corner terms of this determinant we then obtain the first order equation for \( \alpha_1 \)

\[ \alpha_1 = \frac{Z}{n} - n A - \frac{(n-l)(n+l+1)[2Z-n(n+1)] A}{4(n+l+1)(n-1)} = \frac{(n-l)(n+l+1)[2Z-n(n-1)] A}{4(n+l+1)} A. \quad (7) \]

1 E. H. KERNER, Phys. Rev. 83, 71 [1951].
3 For reference see ref. 2.
Table 1 gives a comparison of our results $\alpha_1$ for the 1s-state with Latter's results for several Z-values.

<table>
<thead>
<tr>
<th>Z</th>
<th>8</th>
<th>10</th>
<th>13</th>
<th>19</th>
<th>26</th>
<th>29</th>
<th>37</th>
<th>47</th>
<th>57</th>
<th>65</th>
<th>74</th>
<th>82</th>
<th>92</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>6.092</td>
<td>-</td>
<td>10.536</td>
<td>16.022</td>
<td>22.546</td>
<td>25.365</td>
<td>32.939</td>
<td>42.485</td>
<td>51.971</td>
<td>59.800</td>
<td>68.498</td>
<td>76.250</td>
<td>85.965</td>
</tr>
<tr>
<td>(b)</td>
<td>5.897</td>
<td>7.680</td>
<td>10.260</td>
<td>15.962</td>
<td>22.455</td>
<td>25.404</td>
<td>33.048</td>
<td>42.672</td>
<td>52.347</td>
<td>59.785</td>
<td>68.348</td>
<td>76.722</td>
<td>85.769</td>
</tr>
</tbody>
</table>

Table 1. A comparison of our results (b) with Latter's results (a) for the 1s-state and several Z-values.

Table 2 shows a comparison of our approximate eigenvalues $\alpha_1$ for $Z=80$ with the corresponding Hartree eigenvalues for several quantum numbers.

<table>
<thead>
<tr>
<th>States</th>
<th>$1s$</th>
<th>$2s$</th>
<th>$2p$</th>
<th>$3s$</th>
<th>$3p$</th>
<th>$3d$</th>
<th>$4s$</th>
<th>$4p$</th>
<th>$4d$</th>
<th>$4f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_1$ Eq. (7)</td>
<td>74.728</td>
<td>30.794</td>
<td>30.348</td>
<td>15.218</td>
<td>14.713</td>
<td>13.702</td>
<td>7.521</td>
<td>7.041</td>
<td>6.079</td>
<td>4.638</td>
</tr>
<tr>
<td>Hartree</td>
<td>74.48</td>
<td>30.41</td>
<td>29.87</td>
<td>14.76</td>
<td>14.19</td>
<td>13.08</td>
<td>6.87</td>
<td>6.34</td>
<td>5.27</td>
<td>3.09</td>
</tr>
</tbody>
</table>

Table 2. A comparison of our approximate eigenvalues given by Eq. (7) for $Z=80$ with the corresponding Hartree-values.

Table 1 and 2 show that the approximate eigenvalues calculated by help of Eq. (7) give reasonable results. In order to obtain more accurate eigenvalues than those given by $\alpha_1$ we must solve a determinant of higher order than that in Eq. (6). The corresponding eigenfunctions for practical purpose are obtained from Eqs. (2) and (5) by respecting only finite numbers of the coefficients $c_{n-i}$ so that the eigenfunctions show the proper numbers of zeroes. Eq. (2) shows that the eigenfunctions have accurate behavior for $r=0$ and $r \to \infty$.

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Reactivity Indices in Benzotropones

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The present communication reports a theoretical study of the reactivity indices of tropones fused with a benzene ring; the so-called benzotropones. There are three possible benzotropones: 4,5-benzotropone, 2,3-benzotropone, and 3,4-benzotropone, shown in Fig. 1. Several research workers have reported the syntheses and properties of 4,5-benzotropone and 2,3-benzotropone. To our knowledge there is so far no synthesis of 3,4-benzotropone reported in literature. We have investigated these molecules regarding substitution and addition reactions, being interested in predict-

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