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# Radial Matrix Elements for the Hydrogen Atom

M. Enciso-Aguilar, J. López-Bonilla*, M. Sánchez-Meraz

*Sección de Estudios de Posgrado e Investigación*
*Escuela Superior de Ingeniería Mecánica y Eléctrica*
*Instituto Politécnico Nacional*
*Edif. Z-4, 3er. Piso, Col. Lindavista, C.P. 07738 México DF*

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**Abstract:** It is known that the hydrogenlike atom can be studied as a Morse oscillator, then here we show that these fact leads to an interesting method to obtain the matrix elements for the Coulomb potential.


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## 1. Introduction

For the hydrogenic atom its radial wave function $\frac{1}{r}g_{nl}$ depends of the total $(n)$ and orbital $(l)$ quantum numbers, which are associated to eigenvalues for energy and angular momentum, respectively. Lee [1] showed that the Langer transformation [2] permits to study a non-relativistic hydrogenlike system as a vibrational Morse oscillator $(MO)$ [3], such that $n$ gives the parameters of the Morse well and $l$ determines an energy level in these well. In Sec.2 we exhibit this result of Lee.

In according with [1] the function $g_{nl}$ is proportional to the corresponding $(MO)$ wave function, which means that the matrix elements $\left\langle nl_2 \left| r^k \right| nl_1 \right\rangle$ of the hydrogenic atom are equivalent to $\left\langle N_2 \left| e^{-\gamma u} \right| N_1 \right\rangle$,$\gamma = k+2$, of its $MO$. Thus the knowledge on Morse matrix elements can be used to determine $\left\langle r^k \right\rangle$ for the Coulomb potential. In Sec.3 we apply this approach to obtain $\left\langle nl_2 \left| r^k \right| nl_2 \right\rangle$, $k =$*integer* $\geq -2$, without factorization techniques [4, 5] as in [6]; we reproduce, as particular cases, the elements $\left\langle nl \left| r^k \right| nl \right\rangle$, $k = \pm 1, \pm 2$, deduced analytically by Landau-Lifshitz [7].

* jlopezb@ipn.mx

## 2. Hydrogenlike Atom As A Morse Oscillator

Here we exhibit the result of Lee [1]: The motion of an electron into the Coulomb field generated by a nucleus with charge Ze, is equivalent to the vibrational dynamics of a $MO$.

It is very well known [7] that the radial wave function $\frac{1}{r}g_{nl}$ satisfies the Schrödinger equation (in natural units $\hbar = m = 1$):

$$-\frac{1}{2}\left[\frac{d^2}{dr^2} - \frac{l\,(l+1)}{r^2}\right] g_{nl} - \frac{Ze^2}{4\pi\varepsilon_0 r} g_{nl} = -\frac{Z^2e^2}{32\pi^2\varepsilon_0^2 n^2} g_{nl} \tag{1}$$

where $n = 1,\ 2, ...$ and $l = 0,\ 1, ..., n-1$. Now the quantities $r$, $g_{nl}$ are changed to $u$, $\psi_N$ via the Langer transformation [1, 2]:

$$g_{nl} = \frac{e^{-\frac{u}{2}}}{\left[bn\left(l+\frac{1}{2}\right)\right]^{\frac{1}{2}}} \Psi_N\,(u) \tag{2}$$

with $r = bn^2e^{-u}$, and $b = \frac{4\pi\varepsilon_0}{Ze^2}$, then (1) adopts the form:

$$-\frac{1}{2}\frac{d^2}{du^2}\Psi_N + D\left(e^{-2u} - 2e^{-u}\right)\ \Psi_N = E\,\Psi_N \tag{3}$$

which is the Schrödinger equation for a $MO$ [3, 5] with parameters:

$$\tilde{k} = \frac{2}{a}\sqrt{2D} = 2n, D = \frac{n^2}{2}, a = 1, \tag{4}$$

$$E = -\frac{1}{8}(\tilde{k} - 2N - 1)^2 = -\frac{1}{2}\left(l + \frac{1}{2}\right)^2,$$

$$N = n - l - 1,$$

thus each $n$ generates one $MO$ with width $a = 1$, depth $D = \frac{n^2}{2}$ and vibrational frequency $\frac{a}{2\pi}\sqrt{2D} = \frac{n}{2\pi}$. Finally, the value of $l$ determines the eigenstate $\psi_N$, $N = n - l - 1$, with energy $E = -\frac{1}{2}(l+\frac{1}{2})^2$.

## 3. Matrix Elements for the Coulomb Potential

The principal aim of our work is the calculation of the matrix elements:

$$\langle nl_2|\, r^k\, |nl_1\rangle = \int_0^\infty g_{nl_2} r^k g_{nl_1} dr, \quad k = \text{ integer } \geq -2 \tag{5}$$

The factorization method [4, 6] calculates (5) using ladder operators for the proper states $g_{nl}$; the analytical approach [7] employs the explicit expression of $g_{nl}$ and determines directly the integral (5). Here we apply the Langer transformation [1, 2] to obtain (5) via the relationship between the Coulomb and Morse interactions.

In fact, if we put (2) into (5):

$$\langle nl_2| \, r^k \, |nl_1\rangle = n^{2k+1} b^k \left[ \left( l_1 + \frac{1}{2} \right) \left( l_2 + \frac{1}{2} \right) \right]^{-\frac{1}{2}} \langle N_2| \, e^{-\gamma u} \, |N_1\rangle \tag{6}$$

with $N_j = n - l_j - 1$, $j = 1, 2$ and $\gamma = k + 2 = 0, 1, 2, ...$, which means that any $\langle r^k \rangle$ for the Coulomb potential is proportional to a matrix element of the corresponding $MO$. The elements $\langle e^{-\gamma u} \rangle$ are determined in [8, 9]:

$$\begin{gathered} \langle N_2| \, e^{-\gamma u} \, |N_1\rangle = \frac{(-1)^{N_1+N_2}}{\tilde{k}^{\gamma}} \left[ \frac{Q_1 Q_2 N_2! \, \Gamma\left(\tilde{k} - N_2\right)}{N_1! \, \Gamma\left(\tilde{k} - N_1\right)} \right]^{\frac{1}{2}} \bullet \\ \bullet \sum_{j=0}^{N_2} \frac{(-1)^j \Gamma\left(N_1 + \gamma - j\right) \Gamma\left(\tilde{k} - N_1 - 1 + \gamma - j\right)}{j! \, \left(N_2 - j\right)! \, \Gamma\left(\tilde{k} - N_2 - j\right) \Gamma\left(\gamma - j\right)} \end{gathered} \tag{7}$$

where $\Gamma$ denotes the gamma function, $Q_c = \tilde{k} - 2N_c - 1$, $c = 1, \ 2$, and without loss of generality we have accepted $N_1 \geq N_2$(that is, $l_2 \geq l_1$). Then (6) and (7) with $\tilde{k} = 2n$ imply the exact expression:

$$\begin{gathered} \langle nl_2| \, r^k \, |nl_1\rangle = \frac{(-1)^{l_1+l_2}}{2n} \left(\frac{bn}{2}\right)^k \left[ \frac{(n-l_2-1)! \, (n+l_2)!}{(n-l_1-1)! \, (n+l_1)!} \right]^{\frac{1}{2}} \bullet \\ \bullet \sum_{j=0}^{n-l_2-1} \frac{(-1)^j (n+k-l_1-j)! \, (n+k+l_1-j+1)!}{j!(n-l_2-1-j)! \, (n+l_2-j)! \, (k+1-j)!} \end{gathered} \tag{8}$$

which is not explicitly in the literature, and it is more simple than the corresponding relation deduced in [6] using factorization techniques. Special applications of (6) and (8) are:

a) $k = -2$.

In this case$\gamma = 0$, then from (6) it is immediate that:

$$\langle nl_2| \, r^{-2} \, |nl_1\rangle \propto \langle N_2 \mid N_1\rangle = \delta_{N_1 N_2} \tag{9}$$

therefore only if $l_1 = l_2$ we have$\langle r^2 \rangle \neq 0$, which is the result of Pasternack-Sternheimer mentioned in [6].

b) $l_1 = l_2 = l, \quad k = \pm 1, \ \pm 2$

The general expression (8) reproduces easily the following particular examples of Landau-Lifshitz [7]:

$$\begin{gathered} \left\langle r^{-2} \right\rangle = \frac{b^{-2}}{n^3 \left( l + \frac{1}{2} \right)}, \\ \langle r \rangle = \frac{b}{2} \left[ 3n^2 - l\left(l+1\right) \right], \\ \left\langle r^{-1} \right\rangle = \frac{b^{-1}}{n^2}, \\ \left\langle r^2 \right\rangle = \frac{b^2 n^2}{2} \left[ 5n^2 + 1 - 3l\left(l+1\right) \right]. \end{gathered} \tag{10}$$

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