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Analytical Expressions of Matrix Elements for Saxon-Woods Potential and Padé Approximations

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Abstract

The paper presents the analytical matrix elements of the kinetic hamiltonian in the oscillator base. The Padé approximations for the potential part (Saxon - Woods and alike) was used. From residue calculus the potential matrix elements are analytical. Many parts of these expressions can be computed once for ever. In this way the evaluation time can be reduced and the relations obtained are well suited for parallel computation.

The theory of electromagnetic emission is well known. In this way the interaction of radiation (γ radiation) with nuclei was more easy to study [1a, 1b, 2].

To obtain the reduced probability transition we need the wave functions. These can be obtained by solving the radial Schrödinger equation with the hamiltonian :

$$H = -(\hbar^2/2m)d^2/dr^2 + 2/rd/dr - \ell(\ell+1)/r^2 + V(r) \tag{1}$$

$$V(r) = V_c(r) + V_{\ell s}(r) + V_{coulomb}(r) \tag{2}$$

$$V_c(r) = -V_0^{N,Z}/1 + exp(\beta(r - R_0)) \tag{3}$$

$$V_{ls}(r) = -\aleph/r^\star(dV/dr)^\star \mathbf{l}^\star\mathbf{s}, \quad \mathbf{l}^\star\mathbf{s} = [j(j+1) - l(l+1) - s(s+1)]^{/2} \tag{4}$$

The coulombian part for a uniform charged sphere is

$$V_{coulombian}(r) = (Z-1)e^2/r^\star[(3/2)(r/R_o) - 1/2(r/R_o)^3] \quad for \quad r \leq R_o \tag{5}$$

$$V_{Coulombian}(r) = (Z-1)e^2/r \qquad for \quad r > R_o \tag{6}$$

The nuclear potential like inter-atomic potentials [3-5] can be evaluated by Padé approximants and minimax method. The sum of the central saxon-Woods (SW) potential and the coulombian part was evaluated by Padé approximants (unified potential) [6]. The harmonic oscillator wave functions [7] are:

$$R_{nl}(r) = [2^\star\alpha^{3/2}\star\Gamma(n+1)/\Gamma(n+l+3/2)]^{1/2}(\alpha\star r^2)^{\ell/2}\star L_n^{l+1/2}(\alpha^\star r^2)exp(-\alpha^\star r^2/2) \tag{7}$$

$$L_n^{l+1/2}(\alpha r^2) = \sum_{m=0}^{n}(-1)^m[\Gamma(n-m+1)^\star\Gamma(n+l+3/2)/(\Gamma(m+l+3/2)\Gamma(m+l))]^\star(\alpha r^2)^m, \tag{8}$$

Where θ is the Heaviside operator. The substitution u $=\sqrt{\alpha}\star r$ and the following relations were used [8]:

$$\int_0^\infty t^{2n}exp(-at^2)dt = \Gamma(n+1/2)/(2a^{n+1/2}) \qquad a>0 \qquad n=0,1,2,\cdots \tag{9}$$

$$\int_0^\infty t^{2n+1}exp(-at^2)dt = \Gamma(n+1)/(2a^{n+1}) \qquad a>0 \qquad n=0,1,2,\cdots \tag{10}$$

Then the matrix elements for the hamiltonian kinetic part (3-components) were obtained:

$$\int R_{n'l'}(r)(d^2/dr^2)R_{nl}(r)R^2dr = \alpha^\star 2^\star A^\star_{nl}A^\star_{n'l'}\sum_{m=0}^{n}B_{nlm}\sum_{m'=0}^{n'}B_{n'l'm'}$$

$$\begin{aligned}
&*\{[\theta(\ell'-2)*\ell'*(\ell'-1)*I(\ell,\ell',m,m',0) - (\theta(\ell'-1)*\ell'+(\ell'+1))\\
&*I(\ell,\ell',m,m',2) - I(\ell,\ell',m,m',4)] +\\
&+[(\theta(\ell'-1)*\theta(n'-1)*\ell'+\theta(n'-1)*\ell')*(2m')*I(\ell,\ell',m,m',0)] +\\
&+[\theta(n'-2)*(2m'*(2m'-1))*I(\ell,\ell',m,m',0)]\}
\end{aligned} \tag{11}$$

$$\int_0^\infty R_{n'l'}(2/r^\star d/dr)R_{nl}(r)r^2dr = \alpha^{2\star}4^\star A_{nl}A_{n'l'}$$

$$^\star \sum_{m=0}^{n} B_{nlm} \sum_{m'=0}^{n'} B_{n`l`m`} * \{\theta(l`-1)^\star l`^\star I(l,l`,m,m`0)$$
$$-I(l,l`,m,m`,2)+\theta(n`-1)^\star(2m`)^\star I(l,l`,m,m`,0)\} \quad (12)$$

$$\int_0^\infty R_{n`l`}(r)(l^\star(l+1)/r^2)R_{nl}(r)r^2dr = \alpha^\star 2^\star A_{nl}A_{n`l`}$$
$$^\star \sum_{m=0}^{n} B_{nlm} \sum_{m'=0}^{n'} B_{n`l`m`} I(l,l`,m,m`,0) \quad (13)$$

$$A_{nl} = [\Gamma(n+1)/\Gamma(n+l+3/2)]^{1/2} = 2^{n+\ell}\sqrt{2}/\pi^{1/4}\sqrt{n}!(n+l)!/(2^\star(n+l)+1)!$$
$$= (-1)^m \qquad for \quad m=n \quad (14)$$

$$B_{nlm} = (-1)^m[\Gamma(n+l+3/2)/(\Gamma(n-m+1)\Gamma(m+l+3/2)\Gamma(m+1))]$$
$$= (-1)^m(2^\star(n+l)+1)!(m+l)!/(2^\star(m+l)+1)!/(n+l)!2^{(2^\star(m-n))} \quad (15)$$

$$I(l,l`,m,m`,k) = \int_0^\infty u^{l+l`+k+2m+2m'} exp(-u^2)du \quad (16)$$

In tables (1,2) some values of A_{nl} and B_{nlm} are given. The matrix element for SW central part (neutrons) is

Table 1 . The coefficients A_{nl}(nl=00 etc.)

nl=00	**01**	**02**	**10**	**03**
$\sqrt{2}/\pi^{1/4}$	$2\sqrt{3}/\pi^{1/4}$	$2\sqrt{(2/15)}/\pi^{1/4}$	$2\sqrt{3}/\pi^{1/4}$	$4/\sqrt{105}/\pi^{1/4}$
nl=11	**04**	**12**	**20**	**05**
$2\sqrt{(2/15)}/\pi^{1/4}$	$4\sqrt{(2/105)}/\pi^{1/4}$	$41\sqrt{105}/\pi^{1/4}$	$4\sqrt{15}/\pi^{1/4}$	$8/3/\sqrt{1155}/\pi^{1/4}$
nl=13	**21**	**06**	**14**	**22**
$4/3\sqrt{(2/105)}/\pi^{1/4}$	$4\sqrt{(2/105)}/\pi^{1/4}$	$8/3\sqrt{(2/15015)}$	$8/3\sqrt{1155}/\pi^{1/4}$	$8/3/\sqrt{105}/\pi^{1/4}$
		$/\pi^{1/4}$		

$$\int R_{n`l`}(r)V_c(r)R_{nl}(r)R^2dr = 2^\star A_{nl}A_{n`l`}\sum_{m=0}^{n} B_{nlm}\sum_{m'=0}^{n'} B^\star_{n`l`m`}$$
$$^\star\alpha^{(\ell+\ell`+3)/2+m+m`} \star \int_0^\infty u^{\ell+\ell`+2+2\star m+2\star m`} V_c(r)^\star exp(-\alpha^\star u^2)du \quad (17)$$

and for the spin-orbit part we have:

$$\int_0^\infty R_{n`l`}(r)(-\aleph^\star(\mathbf{l}^\star\mathbf{s})/r^\star(dV/dr)R_{nl}(r)r^2dr = -\aleph^\star(\mathbf{l}^\star\mathbf{s})^\star 2^\star A^\star_{nl}A^\star_{n`l`} \tag{18}$$

$$^\star\sum_{m=0}^{n} B_{nlm}\sum_{m`=0}^{n`} B_{n`l`m`}\alpha^{(\ell+\ell`+3)/2+m+m`}$$

$$\star\int_0^\infty u^{\ell+\ell`+1+2^\star m`}(dV(u)/du)^\star exp(-\alpha^\star u^2)du. \tag{19}$$

The integrals from eq. (18,19) can be evaluated analytically by residue theorem with Padé approximants for SW and unified potentials. The method is potential and type particle free. The rational functions approximations of the potential have only complex poles in the right half plane. A circle sector (C) with $\pi/4$ angle for integration contour [9] was choosed. From relations (18,19) we note that the integrants are of the following type:

Table 2 . The coefficients B_{nlm}(nlm=000 etc.)

nlm=000	**010**	**020**	**100**	**101**	**030**	**110**	**111**
1	1	1	3	-1	1	5	-1
nlm=400	**120**	**121**	**200**	**201**	**202**	**050**	**130**
1	7	-1	15	-5	1	1	9
nlm=131	**210**	**211**	**212**	**060**	**140**	**141**	**220**
-1	35	-7	1	1	11	-1	63
nlm=221	**222**	**300**	**301**	**302**	**303**	**070**	**150**
-9	1	105	-35	7	-1	1	13
nlm=151	**230**	**231**	**232**	**310**	**311**	**312**	**313**
-1	99	-11	1	315	-63	9	-1
nlm=080	**160**	**161**	**240**	**241**	**242**	**320**	**321**
1	15	-1	143	-13	1	693	-99
nlm=322	**323**	**400**	**401**	**402**	**403**	**404**	**090**
11	-1	945	-315	63	-9	1	1
nlm=170	**171**	**250**	**251**	**252**	**330**	**331**	**332**
17	-1	195	-15	1	1287	-143	13
nlm=333	**410**	**411**	**412**	**413**	**414**	**0100**	**180**
-1	3465	-693	99	-11	1	1	19

$$f(z) = z^N \star (a_0 + a_1^\star z + a_2^\star z^2)/(b_0 + b_1^\star z + a_2^\star z^2 + b_3^\star z^3 + b_4^\star z^4 + b_5^\star z^5)exp(-\alpha^\star z^2), \tag{20}$$

where N is an integer. Then by residue theorem we have:

$$\int_c f(z)dz = 2\pi i^\star \sum_{k=1}^{P} R_k, \tag{21}$$

where $z_1, \cdots, z_5$ are f(z)'s poles, R_k residues respectively. It can be shown that $\int_C$ f(z) dz on real axis is $\int_0^\infty$ f(x)dx. Because the poles in (0,∞) are simple complex ones, the residues are computed by the formula :$R_k = lim[(z - z_k)^\star f(z)]$ for $z \to z_k$

We choose those poles $z_1, \cdots, z_5$ which belong to the interior of contour C. So we obtained analytical expressions. Taking into account relations (14, 15, 26) for the λ multipole reduced transition probability we have:

$$\int_0^\infty R_{n'l'}(r) r^\lambda R_{nl}(r) r^2 dr = 2^\star \alpha^{-\lambda/2} \star \sum_{N=0}^{N_{max}} a_{nl} A_{nl} \sum_{N'=0}^{N'_{max}} a_{n'l'} A_{n'l'}$$

$$^\star \sum_{m=0}^{n} B_{nlm} \sum_{m'=0}^{n'} B_{n'l'm'} I(l, l', m, m', \lambda + 2) \qquad (22)$$

where $a_{n,l}$, $a_{n'l'}$ are developments' coefficients for oscillator harmonic base and N_{max}, N'_{max} ($N_{max} = N'_{max}$) are the number of shells taken into account. The same procedure can be also applied to the following core Saxon-Woods potentials [10]:

$$V(r) = -V_o(r/r_c)^\star Heaviside(r_c - r) - V_0/(1 + exp(\alpha(r - R_0)))^\star Heaviside(r - r_c)$$

$$V(r) = -[r^2 r_c^2/(V_0 - V_d) + V_d]^\star Heaviside(r_c - r) - V_0/(1 + exp(a^\star r - r_c)) \star \qquad (23)$$

$$Heaviside(r - r_c), \qquad (24)$$

where r_c is in the region where the potential V(r) don't vary significantly and V_d is the neck potential at r=0

The paper presents the analytical matrix elements of the hamiltonian in the oscillator base. The Padé approximation of the potential part (Saxon - Woods and alike) was used. By residue calculus the potential matrix elements obtained are analytical. Also many parts of the expressions need only be computed once. The expressions was computed by Maple. The evaluation time can be reduced and the relations obtained are suited for parallel computation.

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