Interclusters EFT with RGM

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1 Equation

Starting point

$$(\hat{H}_0 + \hat{U}) \mid \Psi >= E \mid \Psi > \qquad \hat{U} = \hat{V} + \hat{W}$$

where we split the local and non-local part of the potential $U = V + W$.

In configuration space, we aim to solve the scattering solutions of the Schrodinger equation having the form

$$(H_0 - E)\ \Psi(\vec{R}) + V(\vec{R})\ \Psi(\vec{R}) + \int d\vec{R}'\ W(\vec{R},\vec{R}';E)\ \Psi(\vec{R}') = 0 \tag{1}$$

where

$$H_0 = -\frac{\hbar^2}{2\mu}\Delta_{\vec{R}}$$

the local potential

$$V(\vec{R}) = \sum_{n=1}^{3} \eta_n e^{-\kappa_n R^2} \tag{2}$$

and a non-local and E-dependent term that we will write in the form

$$W(\vec{R},\vec{R}';E) = -\sum_{i=1}^{4} c_i\ W_i(R,R',\vec{R}\cdot\vec{R}';E)\ e^{-\left(\alpha_i R^2 + \beta_i \vec{R}\cdot\vec{R}' + \gamma_i R'^2\right)} \tag{3}$$

In detail

$$\begin{aligned}
W(\vec{R},\vec{R}';E) &= c_1 \left[\frac{\hbar^2}{2\mu}\left(4\alpha_1^2 R^2 + \beta_1^2 R'^2 + 4\alpha_1\beta_1 \vec{R}\cdot\vec{R}' - 2\alpha_1\right) + E\right]\ e^{-\left(\alpha_1 R^2 + \beta_1 \vec{R}\cdot\vec{R}' + \gamma_i R'^2\right)} && (4)\\
&- c_2 \qquad e^{-\left(\alpha_2 R^2 + \beta_2 R'^2 + \gamma_2 \vec{R}\cdot\vec{R}'\right)} && (5)\\
&- c_3 \qquad e^{-\left(\alpha_3 R^2 + \beta_3 R'^2 + \gamma_3 \vec{R}\cdot\vec{R}'\right)} && (6)\\
&- c_4 \qquad e^{-\left(\alpha_4 R^2 + \beta_4 R'^2 + \gamma_4 \vec{R}\cdot\vec{R}'\right)} && (7)
\end{aligned}$$

That is having a radial dependence $W(\vec{R},\vec{R}';E) \equiv f(R,R',\vec{R}\cdot\vec{R}';E)$

1. It depends on $3\times 2 + 4\times 4 = 20$ constants and the effective mass μ
2. Usually the RGM equation have the form

   $$E\int dr'\ N(r,r')\chi(r') = \int dr' H(r,r')\chi(r')$$

   that is with a "norm term" $N(r,r')$. Is it absent in your case ?

2 Partial wave solution

After projecting, the **reduced radial equation** takes the form

$$-\frac{\hbar^2}{2\mu}u_L''(R) - Eu_L(R) + \left[V(R) + \frac{\hbar^2}{2\mu}\frac{L(L+1)}{R^2}\right] u_L(R) + \int dR' W_L(R,R';E)u_L(R') = 0 \tag{8}$$

with the local potential

$$V(R) = \sum_{n=1}^{3} \eta_n e^{-\kappa_n R^2} \tag{9}$$

and the non-local E-dependent one

$$W_L(R,R';E) = F_L(R,R') + \sum_{n=1}^{4} 4\pi\, i^L\, c_n\, \left\{E\delta_{1n} + \bar{\delta}_{1n}\right\}\, j_L(i\beta_n RR')e^{-(\alpha_n R^2+\gamma_n R'^2)}\, RR' \tag{10}$$

where

$$\bar{\delta}_{1n} \equiv 1 - \delta_{1n}$$

$$\begin{aligned}
F_L(R,R') &= A(R,R')\,[B_L(R,R') + C_L(R,R') + D_L(R,R')] \\
A(R,R') &= -\frac{\hbar^2}{2\mu}4\pi c_1 e^{-(\alpha_1 R^2+\gamma_1 R'^2)} RR' \\
B_L(R,R') &= \left[-4\alpha_1^2 R^2 - \beta_1^2 R'^2 + 2\alpha_1 + \frac{L(L+1)}{R^2}\right] i^L j_L(i\beta_1 RR') \\
C_L(R,R') &= \bar{\delta}_{L0}\; 4\alpha_1\beta_1\; i^{L-1} j_{L-1}(i\beta_1 RR')(2L-3)\begin{pmatrix} 1 & L-1 & L \\ 0 & 0 & 0 \end{pmatrix}^2 RR' \\
D_L(R,R') &= 4\alpha_1\beta_1\; i^{L+1} j_{L+1}(i\beta_1 RR')(2L-1)\begin{pmatrix} 1 & L+1 & L \\ 0 & 0 & 0 \end{pmatrix}^2 RR'
\end{aligned}$$

1. Although not explicit, i think that W_L must be real
2. Since $j_L(z) \approx z^L$, W_L vanishes when $R, R \to 0$ and when $R, R' \to \infty$
3. Same remark concerning the absence of "norm term"
4. In practical solutions I prefer multiply equation (8) by $(2\mu/\hbar^2)$, introduce the wave number q driving the assymptotics, and write it in the form

$$\boxed{u_L''(R) + \left[q^2 - v(R) - \frac{L(L+1)}{R^2}\right] u_L(R) - \int dR'\; w_L(R,R';E)\; u_L(R') = 0} \tag{11}$$

where

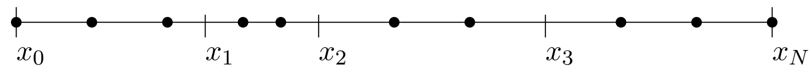
$$v = \frac{2\mu}{\hbar^2}V \qquad w = \frac{2\mu}{\hbar^2}W \qquad q^2 = \frac{2\mu}{\hbar^2}E$$

2.1 Solution using splines

We aim to solve

$$\varphi''(x) + [q^2 - v(x)]\varphi(x) - \int_0^\infty w(x,x')\varphi(x')dx' = 0 \tag{12}$$

on a given grid with of N+1 points $G = \{x_0, x_1, \ldots, x_N\}$ not necessarily equidistants.



We search the solution of (12) in the form

$$\varphi(x) = \sum_{j=0}^{2N+1} c_j S_j(x) \tag{13}$$

where S_j is a set of 2(N+1) given functions, depending on G, and c_j 2(N+1) coefficients to determine.

By inserting this expression in (12) we obtain

$$\sum_j [\hat{L}S_j](x)\ c_j \equiv 0 \tag{14}$$

where $\hat{L}$ denote some integro-differential operator acting on S_i

In order to transform (14) in a linear system for c_i, we "validate" this expression – that is we assume its validity – in a set of 2(N+1) "well chosen" points $\bar{x}_{i=0,1,\ldots,2N+1}$. One usually chose two inside each of the N intervals, eventually supplemented with the two extremes of the grid G.
Each collocation point $\bar{x}_i$ gives rise to a linear equation and this gives the $(2N+2)\times(2N+2)$ square linear system:

$$\sum_{i,j=0}^{2N+2} A_{ij} c_j = 0 \tag{15}$$

where

$$\begin{aligned} A_{ij} &= S_j''(\bar{x}_i) + [q^2 - v(\bar{x}_i)]S_j(\bar{x}_i) - w_{ij} \\ w_{ij} &= \int_0^\infty dx'\ w(\bar{x}_i, x')\ S_j(x') \end{aligned}$$

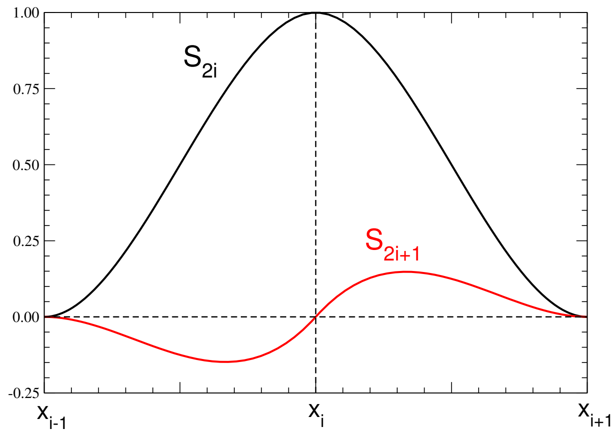
The linear system (15) will be still modified when introducing the appropriate boundary conditions.

2.1.1 Cubic "splines"

The essentials about "splines"[1]

1. There are two "spline" functions associated to each grid point x_i, S_{2i} and S_{2i+1}.
2. Their "support" consists in two consecutive intervals surrounding x_i : $D_i = [x_{i-1}, x_{i+1}]$ (vanish outside)
3. They are piece-wise cubic polynomials on each interval $[x_i, x_{i-1}]$ with C^1 matching conditions among them

[1] Although everybody call them "splines" they are in fact Cubic Hermite Interpolation Polynomials and hence "spline".
(See for instance Few-Body Syst. (2011) 49: 205-222)



4. Interesting properties are

$$\begin{array}{rcl} S_j(x_i) & = & \delta_{j,2i} \\ S'_j(x_i) & = & \delta_{j,2i+1} \end{array}$$

Because of that, the coeficients of an spline expansion of a function f on a grid $G = \{x_0, x_1, ..., x_N\}$

$$f(x) = \sum_{i=0}^{2N+1} c_i S_i(x)$$

have a simple interpretation in terms of the grid values:

$$\begin{array}{rcl} f(x_i) & = & c_{2i} \\ f'(x_i) & = & c_{2i+1} \end{array}$$

5. Their analytic expresions are:

$$\begin{array}{rcl} S_{2i}(x) & = & \left\{ \begin{array}{ll} 3\left(\frac{x-x_{i-1}}{x_i-x_{i-1}}\right)^2 - 2\left(\frac{x-x_{i-1}}{x_i-x_{i-1}}\right)^3 & \text{if } x \in [x_{i-1}, x_i] \\ 3\left(\frac{x_{i+1}-x}{x_{i+1}-x_i}\right)^2 - 2\left(\frac{x_{i+1}-x}{x_{i+1}-x_i}\right)^3 & \text{if } x \in [x_i, x_{i+1}] \end{array} \right. \\ S_{2i+1}(x) & = & \left\{ \begin{array}{ll} \left[-\left(\frac{x-x_{i-1}}{x_i-x_{i-1}}\right)^2 + \left(\frac{x-x_{i-1}}{x_i-x_{i-1}}\right)^3\right](x_i - x_{i-1}) & \text{if } x \in [x_{i-1}, x_i] \\ \left[+\left(\frac{x_{i+1}-x}{x_{i+1}-x_i}\right)^2 - \left(\frac{x_{i+1}-x}{x_{i+1}-x_i}\right)^3\right](x_{i+1} - x_i) & \text{if } x \in [x_i, x_{i+1}] \end{array} \right. \end{array}$$

and simalr expressiuon exist for their first and second derivatives.

They are represented in the figure above

2.1.2 Boundary conditions

We will see that the boundary conditions fixe two coefficients in expansion (13) and the number of unknown coefficients is in fact 2N

1. At the origin: since we are using the reduced radial equation one must fulfil

$$\phi(0) = 0 \quad \Longleftrightarrow \quad c_0 = 0$$

This means that c_0 is absent in the expansion (13) as well as the equation corresponding to $\bar{x}_0$

2. Asymptotic ($r \to \infty$) for scattering problem: **we impose at** $x = x_N$

$$
\begin{aligned}
\varphi(x) &= \varepsilon F_1(z) + C F_2(z) \qquad\qquad z = qx && (16)\\
\varphi'(x) &= \varepsilon q F_1'(z) + C q F_2'(z) && (17)
\end{aligned}
$$

with

- F_i two **known solutions** of the free equation (e.g. $\hat{j}_L, \hat{n}_L, \hat{h}_L^+, ...$) linearly independent
- ε=0,1 to cover all possibilities, including purely outgoing waves (e.g. resonances)

By eliminating C from (16) et (17) one gets a relation between the solution and its derivative at $x = x_N$

$$
\varphi' = q\frac{F_2'}{F_2}\,\varphi - \varepsilon q F_1 \left[\frac{F_2'}{F_2} - \frac{F_1'}{F_1}\right]
$$

We will write this in the generic form

$$
\varphi'(x_N) = \Delta_N\ \varphi(x_N) - \Delta_N' \tag{18}
$$

$$
\begin{aligned}
\Delta_N &= q\frac{F_2'}{F_2} && (19)\\
\Delta_N' &= \varepsilon q F_1 \left[\frac{F_2'}{F_2} - \frac{F_1'}{F_1}\right] && (20)
\end{aligned}
$$

In terms of spline coefficients (18) reads:

$$
\boxed{c_{2N+1} = \Delta_N\ c_{2N} - \Delta_N'} \tag{21}
$$

This relation allows us to eliminate c_{2N+1} in the expansion (13), eliminates the equation corresponding to $\bar{x}_{2N+1}$ in (15) and introduces two wain differences in the remaining $2N \times 2N$ linear system:

$$
\sum_{i,j=0}^{2N} A_{ij} c_j = 0 \tag{22}
$$

- Change the matrix elements involving $A_{*,2N+1}$

$$
\begin{aligned}
A_{2N-1,2N} &\to \hat{A}_{2N-1,2N} = A_{2N-1,2N} + A_{2N-1,2N+1}\Delta_N && (23)\\
A_{2N,2N} &\to \hat{A}_{2N,2N} = A_{2N,2N} + A_{2N,2N+1}\ \Delta_N && (24)
\end{aligned}
$$

- **Introduces an inhomogeneus term** in , which becomes

$$
Ac = b \qquad b = \begin{pmatrix} 0 \\ 0 \\ .. \\ y_{2N} \\ y_{2N+1} \end{pmatrix}
$$

with

$$
\begin{aligned}
y_{2N-1} &= \Delta_N'\ A_{2N-1,2N+1} && (25)\\
y_{2N} &= \Delta_N'\ A_{2N,2N+1} && (26)
\end{aligned}
$$

2.2 Solution using Finite Differences

We aim to solve

$$u''(x) + \frac{2\mu}{\hbar^2}\left[E - V(x)\right]u(x) = 0$$

that will be written in the form

$$u''(x) + \left[q^2 - v(x)\right]u(x) = 0 \tag{27}$$

with the usual notations

$$q^2 = \frac{2\mu}{\hbar^2}E \qquad v(x) = \frac{2\mu}{\hbar^2}V \tag{28}$$

In case of a non local terms it becomms

$$\boxed{u''(x) + \left[q^2 - v(x)\right]u(x) - \int dx' w(x,x')u(x') = 0 \qquad w = \frac{2\mu}{\hbar^2}W} \tag{29}$$

We search the unknown fonction $u(x)$ on an equidistant grid G=$\{x_0, x_1, \ldots, x_N\}$ with spacing h, i.e. $x_i = i.h$. This means that we want to determine u=$\{u_0, u_1, ..u_N\}$ where $u_i \equiv u(i.h)$

2.2.1 Recurrence Algorithm

Using the **symmetric discretisation** of the second derivative

$$h^2u''(x) = u(x-h) - 2u(x) + u(x+h) + h^2o(h^2)$$

equation (27) results into the **recurrence relation**

$$F_{i-1}u_{i-1} + D_iu_i + F_{i+1}u_{i+1} = 0 \qquad i = 1, \ldots N$$

with[2]

$$\begin{aligned} F_i &= 1 & (30)\\ D_i &= -2 + h^2(q^2 - v_i) & (31)\end{aligned}$$

Since $u_0 = 0$ there are N unknowns $u_1, ...u_N$. By developing the recurrence relation one obtains:

$$\begin{array}{ll} i=1 & D_1u_1 + F_2u_2 \qquad\quad = 0 \\ i=2 & F_1u_1 + D_2u_2 + F_1u_3 = 0 \\ i=3 & F_2u_2 + D_3u_3 + F_4u_4 = 0 \\ \ldots & \ldots \\ i=N & F_{N-1}u_{N-1} + D_Nu_N = -F_{N+1}u_{N+1} \end{array}$$

This can be written in the matrix form

$$Au = b \qquad \Longleftrightarrow \qquad \begin{pmatrix} D_1 & F_2 & & 0 & 0 & 0 \\ F_1 & D_2 & F_3 & 0 & 0 & 0 \\ 0 & F_2 & D_3 & F_4 & 0 & 0 \\ 0 & 0 & F_3 & D_4 & F_5 & 0 \\ 0 & 0 & 0 & F_4 & D_5 & F_6 \\ 0 & 0 & 0 & 0 & F_5 & D_6 \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ \ldots \\ u_N \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \ldots \\ -F_{N+1}u_{N+1} \end{pmatrix} \tag{32}$$

The term involving u_{N+1}, that we have placed in the right hand side, is mandatory to "close the system" and will incorporate the boundary conditions

[2]Althoug F_i is here trivial, we prefer to keep this form, which extend to more elaborate discretisation schemes

In case of a non local interaction the matrix A is changed into

$$A \to A = \begin{pmatrix} D_1 & F_2 & & 0 & 0 & 0 \\ F_1 & D_2 & F_3 & 0 & 0 & 0 \\ 0 & F_2 & D_3 & F_4 & 0 & 0 \\ 0 & 0 & F_3 & D_4 & F_5 & 0 \\ 0 & 0 & 0 & F_4 & D_5 & F_6 \\ 0 & 0 & 0 & 0 & F_{N-1} & D_N \end{pmatrix} - \begin{pmatrix} \bar{w}_{11} & \bar{w}_{12} & \bar{w}_{13} & \bar{w}_{14} & \bar{w}_{15} & \bar{w}_{1N} \\ \bar{w}_{21} & \bar{w}_{12} & \bar{w}_{13} & \bar{w}_{14} & \bar{w}_{15} & \bar{w}_{2N} \\ \bar{w}_{31} & \bar{w}_{12} & \bar{w}_{13} & \bar{w}_{14} & \bar{w}_{15} & \bar{w}_{3N} \\ \bar{w}_{41} & \bar{w}_{12} & \bar{w}_{13} & \bar{w}_{14} & \bar{w}_{15} & \bar{w}_{4N} \\ \bar{w}_{N-1,1} & \bar{w}_{12} & \bar{w}_{13} & \bar{w}_{14} & \bar{w}_{15} & \bar{w}_{N-1N} \\ \bar{w}_{N1} & \bar{w}_{12} & \bar{w}_{13} & \bar{w}_{14} & \bar{w}_{15} & \bar{w}_{NN} \end{pmatrix} \tag{33}$$

Where we used the discretisation

$$\int dx' w(x,x')u(x') \approx \sum_{i=1}^{N} h w_{ij} u_j \qquad \bar{w}_{ij} = h^3 w_{ij}$$

We can write the matrix elements using a compact notation

$$\boxed{A_{ij} = F_i\ \delta_{i-1,j} + D_i\ \delta_{i,j} + F_i\ \delta_{i+1,j} - \bar{w}_{ij}} \tag{34}$$

2.2.2 Scattering problem

The boundary condition for the scattering problem can be generically written as a linear relation between u_{N+1} and u_N in the form

$$u_{N+1} = \Delta_N u_N - \Delta'_N$$

which modifis the last equation of the linear system (32) and unables us to "close it" in a consisent way. The last equation change into

$$F_{N-1}u_{N-1} + D_N u_N = -F_{N+1}u_{N+1} \quad \longrightarrow \quad F_{N-1}u_{N-1} + (D_N + \Delta_N F_{N+1})\, u_N = F_{N+1}\Delta'_N$$

which introduces a change in the last diagonal matrix element and in the inhomogeneous term

$$D_N + \hat{w}_{NN} \ \to\ D_N + \hat{w}_{NN} + \Delta_N\ F_{N+1} \tag{35}$$

$$-F_{N+1}u_{N+1} \ \to\ \Delta'_N\ F_{N+1} \tag{36}$$

We will determine below the coefficients Δ_N and Δ'_N in the case of zero and non zero energy

1. **Zero energy** (compute the S-wave scattering length a_0)

   We search a solution which behaves asymptotically as

   $$u = x - a \tag{37}$$

   This means fulfilling the condition $u'_N = 1$

   Using the discretized derivative, this is equivalent to impose

   $$u_{N+1} = u_N + h \tag{38}$$

   that is

   $$\boxed{\Delta_N = 1 \qquad \Delta'_N = -h}$$

   Once u_i is determined, the scattering length is given by

   $$a_0 = x_N - u_N$$

2. **Non zero energy** : we search a solution (S-wave) which behaves asymptotically as

$$u(x) = \sin(qx) + \tan\delta(q)\cos(qx)$$

and so

$$u'(x) = q[\cos(qx) - \tan\delta(q)\sin(qx)]$$

By eliminating $\tan\delta(q)$ from these two equations at $x = x_N$ we obtain a relation between u_{N+1} and u_N

$$u_{N+1} = (1 - hq\tan z_N)u_N + hq\,(\cos z_N + \sin z_N \tan z_N) \qquad z_N = qx_N \tag{39}$$

which is the counterpart of (38) and gives the coefficients

$$\boxed{\Delta_N = 1 - hq\tan z_N \qquad \Delta'_N = -hq\,(\cos z_N + \sin z_N \tan z_N)}$$

Once u_i is determined, $\tan\delta(q)$ can be determinded by

$$\tan\delta(q) = \frac{u_N - sinz_N}{\cos z_N}$$

and the effective range fonction

$$Z_0(q) = q\cot\delta(q) = \frac{q\cos z_N}{u_N - sinz_N}$$

```
W=-150*exp(-R*R-RP*RP)
q=0   (Exact 2.06053...)     Z
0050x0.100   2.069883
0100x0.050   2.062785
0250x0.020   2.060817
0500x0.010   2.060536
1000x0.005   2.060466
2500x0.002   2.060447    -0.485332
q=0.01
N  x h        Z
0050x0.100  -0.479332
0100x0.050  -0.480490
0250x0.020  -0.480647
0500x0.010  -0.480611
1000x0.005  -0.480577
2500x0.002  -0.480551
5000x0.001  -0.480541
```

3 Model 2+2 (dimer-dimer)

Eq. (11) with L=0 gives :

Local term:

$$V(R) = \sum_{n=2}^{nL} \eta_n \; e^{-\left(\frac{R}{\rho_n}\right)^2} \qquad \rho_n = \frac{1}{\sqrt{w_n}} \tag{40}$$

which depends on parameters η_n, w_n

Non-Local term:

$$W(R,R') = 4\pi RR' \; \left\{ \xi_1 \; e^{-a_1 R^2 - c_1 R'^2} \left[(4a_1^2 R^2 - 2a_1) + q^2 \right] - \sum_{n=2}^{nNL} \xi_n \; j_0(ib_n RR') \; e^{-a_n R^2 - c_n R'^2} \right\} \tag{41}$$

which depends on parameters ξ_n, a_n, b_n, c_n

We introduce the ranges σ_n and σ'_n

$$\sigma_n = \frac{1}{\sqrt{a_n}} \qquad \sigma'_n = \frac{1}{\sqrt{c_n}}$$

and the real function

$$\chi(x) \equiv j_0(ix) = \frac{\sinh(x)}{x} = \frac{e^{+x} - e^{-x}}{2x} \tag{42}$$

W can be written in the form

$$W(R,R') = 4\pi RR' \left\{ \xi_1 \left[\frac{2}{\sigma_1^2} \left(2\left(\frac{R}{\sigma_1}\right)^2 - 1 \right) + q^2 \right] e^{-\left(\frac{R}{\sigma_1}\right)^2 - \left(\frac{R'}{\sigma'_1}\right)^2} - \sum_{n=2}^{nNL} \xi_n \, \chi(b_n RR') \, e^{-\left(\frac{R}{\sigma_n}\right)^2 - \left(\frac{R'}{\sigma'_n}\right)^2} \right\} \tag{43}$$

Still, this last expression can be cast into a more compact form

$$\boxed{W(R,R') = 4\pi RR' \sum_{n=1}^{nNL} \xi_n \, \chi_n(R,R') \, e^{-\left(\frac{R}{\sigma_n}\right)^2 - \left(\frac{R'}{\sigma'_n}\right)^2}} \tag{44}$$

with

$$\chi_n(R,R) = \begin{cases} \left[\left(\frac{2}{\sigma_1}\right)^2 \left(2\left(\frac{R}{\sigma_1}\right)^2 - 1 \right) - q^2 \right] & \text{if} \quad n = 1 \\ -\chi(b_n RR') & \text{if} \quad n > 1 \end{cases} \tag{45}$$

All model parameters $\{\eta_n, w_n, \xi_n, a_n, b_n, c_n\}$ depend only on $\{\lambda, \alpha, C(\lambda), D(\lambda)\}$ according to the following tables:

1. Model (ab)-(ab)

$nL = 2$	V	
n	η_n	w_n
2	$2C\left(\frac{2\alpha}{2\alpha+\lambda}\right)^{3/2}$	$\frac{2\alpha\lambda}{2\alpha+\lambda}$

$nNL = 2$	W			
n	ξ_n	a_n	b_n	c_n
1	$8\alpha^{3/2}\frac{\hbar^2}{2\mu}$	α	0	α
2	$-16\alpha^{3/2}C\left(\frac{2\alpha}{2\alpha+\lambda}\right)^{3/2}$	$\frac{\alpha(2\alpha+3\lambda)}{2\alpha+\lambda}$	0	α

2. Model (ab)-(ac) [3]

	V $(nL\!=\!4)$	
n	η_n	w_n
2	$3C\left(\frac{2\alpha}{2\alpha+\lambda}\right)^{3/2}$	$\frac{2\alpha\lambda}{2\alpha+\lambda}$
3	$D\left(\frac{2\alpha}{2\alpha+\lambda}\right)^{3}$	$\frac{4\alpha\lambda}{2\alpha+\lambda}$
4	$D\left[\frac{2\alpha}{\sqrt{(2\alpha+\lambda)^2+2\alpha\lambda}}\right]^3$	$\frac{4\alpha\lambda(\alpha+\lambda)}{4\alpha^2+6\alpha\lambda+\lambda^2}$

	W $(nNL\!=\!5)$			
n	ξ_n	a_n	b_n	c_n
1	$8\alpha^{3/2}\frac{\hbar^2}{2\mu}$	α	0	α
2	$-8\alpha^{3/2}C$	$\alpha+\lambda$	2λ	$\alpha+\lambda$
3	$-16\alpha^{3/2}C\left(\frac{2\alpha}{2\alpha+\lambda}\right)^{3/2}$	$\frac{\alpha(2\alpha+3\lambda)}{2\alpha+\lambda}$	0	α
4	$-8\alpha^{3/2}D\left(\frac{\alpha}{\alpha+\lambda}\right)^{3/2}$	$\frac{2\alpha^2+4\alpha\lambda+\lambda^2}{2(\alpha+\lambda)}$	$\frac{\lambda^2}{\alpha+\lambda}$	$\frac{2\alpha^2+4\alpha\lambda+\lambda^2}{2(\alpha+\lambda)}$
5	$-8\alpha^{3/2}D\left(\frac{2\alpha(\alpha+\lambda)}{2\alpha^2+3\alpha\lambda+\lambda^2}\right)^{3/2}$	$\frac{2\alpha^2+5\alpha\lambda+\lambda^2}{2\alpha+\lambda}$	2λ	$\alpha+\lambda$

In the non local term it can happen that the product

$$\chi(b_n RR')\; e^{-\left(\frac{R}{\sigma_n}\right)^2-\left(\frac{R'}{\sigma'_n}\right)^2} = \frac{1}{2b_nRR'}\left[e^{b_nRR'-a_nR^2-c_nR'^2} - e^{-b_nRR'-a_nR^2-c_nR'^2}\right] \tag{46}$$

is divergent in some regions of the (R,R') plane due to the first term in the above expression, which has an incresingly positive argument

$$Arg = b_nRR' - a_nR^2 - c_nR'^2 > 0$$

Strictly speaking, the calculations are meaningless, although I obtain some stable results limiting the divergent exponent to 100. For instance this happens in model *ab-ac* for n=5.

To analyze this behaviour let us write:

$$Arg = b_nRR' - a_nR^2 - c_nR'^2 = g_nxx' - x^2 - x'^2 \qquad g_n \equiv b_n\sigma_n\sigma'_n = \frac{b_n}{\sqrt{a_nc_n}} \quad x = \frac{R}{\sigma} \quad x = \frac{R'}{\sigma'}$$

- For a fixed x, the argument becomes always < 0 at large enough x'.

  $$Arg = g_nxx' - x^2 - x'^2 < 0 \quad\Leftrightarrow\quad x'^2 - g_nxx' + x^2 > 0$$

  Roots are

  $$x' = \frac{g_nx \pm \sqrt{g_n^2x^2 - 4x^2}}{2} = \frac{g_nx}{2}\left[1 \pm \sqrt{1-\frac{4}{g_n^2}}\right]$$

  If $g_n < 2$, $\frac{4}{g_n^2} > 1$ and so no roots : sign of Arg is constant and < 0
  If $g_n > 2$, the condition for sign of Arg < 0 is

  $$x' > \frac{g_nx}{2}\left[1 + \sqrt{1-\frac{4}{g_n^2}}\right]$$

- If $x' = \lambda x$

  $$g_nxx' - x^2 - x'^2 = (g_n\lambda - 1 - \lambda^2)x^2 < 0 \qquad\Leftrightarrow\qquad g_n < \frac{1+\lambda^2}{\lambda}$$

  In the diagonal, $\lambda = 1$, il faut $g_n < 2$

[3] $a(5)$ has been corrected from the initial value $\frac{2\alpha^2+5\alpha\lambda+\lambda^2}{2(\alpha+\lambda)}$

3.1 Results model (ab)-(ab)

i	lambda	alpha	C0	D0	rho	sigma		sigmap	
1	0.0025	0.01085409	-1.10605700	-1.15933300	21.12	9.60	8.74	9.60	9.60
2	0.0900	0.01085514	-13.49359000	2.15038800	7.56	9.60	5.94	9.60	9.60
3	0.3025	0.01085640	-39.79732700	24.96554500	7.03	9.60	5.67	9.60	9.60
4	0.6400	0.01085554	-80.01355400	81.33634000	6.90	9.60	5.60	9.60	9.60
5	1.1025	0.01085210	-134.14148400	191.49126400	6.85	9.60	5.58	9.60	9.60
6	1.6900	0.01085481	-202.18538700	379.17501000	6.83	9.60	5.57	9.60	9.60
7	2.4025	0.01085130	-284.13810300	683.99962100	6.82	9.60	5.56	9.60	9.60
8	3.2400	0.01086136	-380.01517000	1143.33290000	6.81	9.60	5.55	9.60	9.60
9	4.2025	0.01085691	-489.79280800	1884.50607900	6.80	9.60	5.55	9.60	9.60
10	5.2900	0.01085517	-613.48535700	2977.88400300	6.80	9.60	5.55	9.60	9.60
11	6.5025	0.01084950	-751.08549900	4589.00460800	6.80	9.60	5.55	9.60	9.60
12	7.8400	0.01084884	-902.60416400	7067.64588100	6.80	9.60	5.55	9.60	9.60
13	9.3025	0.01084997	-1068.03834400	10667.30447600	6.80	9.60	5.55	9.60	9.60
14	10.8900	0.01085217	-1247.38743100	16133.94159100	6.79	9.60	5.55	9.60	9.60
15	12.6025	0.01085409	-1440.65012300	24382.00819500	6.79	9.60	5.54	9.60	9.60
16	14.4400	0.01084667	-1647.80803700	36688.65838000	6.79	9.60	5.55	9.60	9.60
17	16.4025	0.01085322	-1868.90565500	52963.12362700	6.79	9.60	5.54	9.60	9.60
18	18.4900	0.01087420	-2103.94832300	80952.12957300	6.78	9.59	5.54	9.59	9.59
19	20.7025	0.01085536	-2352.81914300	119013.69526900	6.79	9.60	5.54	9.60	9.60
20	23.0400	0.01085344	-2615.63825000	190732.88917600	6.79	9.60	5.54	9.60	9.60

xN=50 n=100 ng=16

# i	lambda	alpha	C0	D_0	a_0	
1	0.0025	0.01085409	-1.10605700	-1.15933300	0.112039D+04	0.000000D+00
2	0.0900	0.01085514	-13.49359000	2.15038800	0.315831D+01	0.000000D+00
3	0.3025	0.01085640	-39.79732700	24.96554500	0.312835D+02	0.000000D+00
4	0.6400	0.01085554	-80.01355400	81.33634000	0.200716D+02	0.000000D+00
5	1.1025	0.01085210	-134.14148400	191.49126400	0.182151D+02	0.000000D+00
6	1.6900	0.01085481	-202.18538700	379.17501000	0.174587D+02	0.000000D+00
7	2.4025	0.01085130	-284.13810300	683.99962100	0.170538D+02	0.000000D+00
8	3.2400	0.01086136	-380.01517000	1143.33290000	0.167924D+02	0.000000D+00
9	4.2025	0.01085691	-489.79280800	1884.50607900	0.166218D+02	0.000000D+00
10	5.2900	0.01085517	-613.48535700	2977.88400300	0.164969D+02	0.000000D+00
11	6.5025	0.01084950	-751.08549900	4589.00460800	0.164053D+02	0.000000D+00
12	7.8400	0.01084884	-902.60416400	7067.64588100	0.163307D+02	0.000000D+00
13	9.3025	0.01084997	-1068.03834400	10667.30447600	0.162694D+02	0.000000D+00
14	10.8900	0.01085217	-1247.38743100	16133.94159100	0.162181D+02	0.000000D+00
15	12.6025	0.01085409	-1440.65012300	24382.00819500	0.161751D+02	0.000000D+00
16	14.4400	0.01084667	-1647.80803700	36688.65838000	0.161451D+02	0.000000D+00
17	16.4025	0.01085322	-1868.90565500	52963.12362700	0.161100D+02	0.000000D+00
18	18.4900	0.01087420	-2103.94832300	80952.12957300	0.160685D+02	0.000000D+00
19	20.7025	0.01085536	-2352.81914300	119013.69526900	0.160590D+02	0.000000D+00
20	23.0400	0.01085344	-2615.63825000	190732.88917600	0.160399D+02	0.000000D+00

xN=100 n=200 ng=16

# i	lambda	alpha	C0	D_0	a_0	
1	0.0025	0.01085409	-1.10605700	-1.15933300	0.485982D+03	0.000000D+00
2	0.0900	0.01085514	-13.49359000	2.15038800	0.315831D+01	0.000000D+00
3	0.3025	0.01085640	-39.79732700	24.96554500	0.312835D+02	0.000000D+00
4	0.6400	0.01085554	-80.01355400	81.33634000	0.200716D+02	0.000000D+00
5	1.1025	0.01085210	-134.14148400	191.49126400	0.182151D+02	0.000000D+00
6	1.6900	0.01085481	-202.18538700	379.17501000	0.174587D+02	0.000000D+00
7	2.4025	0.01085130	-284.13810300	683.99962100	0.170538D+02	0.000000D+00
8	3.2400	0.01086136	-380.01517000	1143.33290000	0.167924D+02	0.000000D+00
9	4.2025	0.01085691	-489.79280800	1884.50607900	0.166218D+02	0.000000D+00
10	5.2900	0.01085517	-613.48535700	2977.88400300	0.164969D+02	0.000000D+00
11	6.5025	0.01084950	-751.08549900	4589.00460800	0.164053D+02	0.000000D+00
12	7.8400	0.01084884	-902.60416400	7067.64588100	0.163307D+02	0.000000D+00
13	9.3025	0.01084997	-1068.03834400	10667.30447600	0.162694D+02	0.000000D+00
14	10.8900	0.01085217	-1247.38743100	16133.94159100	0.162181D+02	0.000000D+00
15	12.6025	0.01085409	-1440.65012300	24382.00819500	0.161751D+02	0.000000D+00
16	14.4400	0.01084667	-1647.80803700	36688.65838000	0.161451D+02	0.000000D+00
17	16.4025	0.01085322	-1868.90565500	52963.12362700	0.161100D+02	0.000000D+00
18	18.4900	0.01087420	-2103.94832300	80952.12957300	0.160685D+02	0.000000D+00
19	20.7025	0.01085536	-2352.81914300	119013.69526900	0.160590D+02	0.000000D+00
20	23.0400	0.01085344	-2615.63825000	190732.88917600	0.160399D+02	0.000000D+00

3.2 Results model (ab)-(ac)

i	lambda	alpha	C0	D0	rho			sigma					sigmap				
1	0.0025	0.01085409	-1.10605700	-1.15933300	21.12	14.93	21.02	9.60	8.65	8.74	8.73	8.01	9.60	8.65	9.60	8.73	8.65
2	0.0900	0.01085514	-13.49359000	2.15038800	7.56	5.35	6.05	9.60	3.15	5.94	4.06	2.91	9.60	3.15	9.60	4.06	3.15
3	0.3025	0.01085640	-39.79732700	24.96554500	7.03	4.97	5.21	9.60	1.79	5.67	2.44	1.73	9.60	1.79	9.60	2.44	1.79
4	0.6400	0.01085554	-80.01355400	81.33634000	6.90	4.88	5.00	9.60	1.24	5.60	1.72	1.22	9.60	1.24	9.60	1.72	1.24
5	1.1025	0.01085210	-134.14148400	191.49126400	6.85	4.85	4.92	9.60	0.95	5.58	1.33	0.94	9.60	0.95	9.60	1.33	0.95
6	1.6900	0.01085481	-202.18538700	379.17501000	6.83	4.83	4.88	9.60	0.77	5.57	1.08	0.76	9.60	0.77	9.60	1.08	0.77
7	2.4025	0.01085130	-284.13810300	683.99962100	6.82	4.82	4.85	9.60	0.64	5.56	0.91	0.64	9.60	0.64	9.60	0.91	0.64
8	3.2400	0.01086136	-380.01517000	1143.33290000	6.81	4.81	4.84	9.60	0.55	5.55	0.78	0.55	9.60	0.55	9.60	0.78	0.55
9	4.2025	0.01085691	-489.79280800	1884.50607900	6.80	4.81	4.83	9.60	0.49	5.55	0.69	0.49	9.60	0.49	9.60	0.69	0.49
10	5.2900	0.01085517	-613.48535700	2977.88400300	6.80	4.81	4.82	9.60	0.43	5.55	0.61	0.43	9.60	0.43	9.60	0.61	0.43
11	6.5025	0.01084950	-751.08549900	4589.00460800	6.80	4.81	4.82	9.60	0.39	5.55	0.55	0.39	9.60	0.39	9.60	0.55	0.39
12	7.8400	0.01084884	-902.60416400	7067.64588100	6.80	4.81	4.82	9.60	0.36	5.55	0.50	0.36	9.60	0.36	9.60	0.50	0.36
13	9.3025	0.01084997	-1068.03834400	10667.30447600	6.80	4.81	4.81	9.60	0.33	5.55	0.46	0.33	9.60	0.33	9.60	0.46	0.33
14	10.8900	0.01085217	-1247.38743100	16133.94159100	6.79	4.80	4.81	9.60	0.30	5.55	0.43	0.30	9.60	0.30	9.60	0.43	0.30
15	12.6025	0.01085409	-1440.65012300	24382.00819500	6.79	4.80	4.81	9.60	0.28	5.54	0.40	0.28	9.60	0.28	9.60	0.40	0.28
16	14.4400	0.01084667	-1647.80803700	36688.65838000	6.79	4.80	4.81	9.60	0.26	5.55	0.37	0.26	9.60	0.26	9.60	0.37	0.26
17	16.4025	0.01085322	-1868.90565500	52963.12362700	6.79	4.80	4.81	9.60	0.25	5.54	0.35	0.25	9.60	0.25	9.60	0.35	0.25
18	18.4900	0.01087420	-2103.94832300	80952.12957300	6.78	4.80	4.80	9.59	0.23	5.54	0.33	0.23	9.59	0.23	9.59	0.33	0.23
19	20.7025	0.01085536	-2352.81914300	119013.69526900	6.79	4.80	4.81	9.60	0.22	5.54	0.31	0.22	9.60	0.22	9.60	0.31	0.22
20	23.0400	0.01085344	-2615.63825000	190732.88917600	6.79	4.80	4.81	9.60	0.21	5.54	0.29	0.21	9.60	0.21	9.60	0.29	0.21

```
state= 1    g=0.0000  0.3744  0.0000  0.0357  0.3465
state= 2    g=0.0000  1.7847  0.0000  1.3231  1.6476
state= 3    g=0.0000  1.9307  0.0000  1.7450  1.8712
state= 4    g=0.0000  1.9666  0.0000  1.8719  1.9357
state= 5    g=0.0000  1.9805  0.0000  1.9239  1.9618
state= 6    g=0.0000  1.9872  0.0000  1.9497  1.9748
state= 7    g=0.0000  1.9910  0.0000  1.9644  1.9822
state= 8    g=0.0000  1.9933  0.0000  1.9735  1.9867
state= 9    g=0.0000  1.9948  0.0000  1.9795  1.9898
state=10    g=0.0000  1.9959  0.0000  1.9837  1.9918
state=11    g=0.0000  1.9967  0.0000  1.9867  1.9934
state=12    g=0.0000  1.9972  0.0000  1.9890  1.9945
state=13    g=0.0000  1.9977  0.0000  1.9907  1.9954
state=14    g=0.0000  1.9980  0.0000  1.9921  1.9960
state=15    g=0.0000  1.9983  0.0000  1.9931  1.9966
state=16    g=0.0000  1.9985  0.0000  1.9940  1.9970
state=17    g=0.0000  1.9987  0.0000  1.9947  1.9974
state=18    g=0.0000  1.9988  0.0000  1.9953  1.9977
state=19    g=0.0000  1.9990  0.0000  1.9958  1.9979
state=20    g=0.0000  1.9991  0.0000  1.9962  1.9981
```

```
#   xN=50 n=100 ng=16
#   i    lambda    alpha          C0             D_0           a_0
    1    0.0025    0.01085409     -1.10605700    -1.15933300   -.474675D+04 -.000000D+00
    2    0.0900    0.01085514    -13.49359000     2.15038800   0.141817D+02 0.000000D+00
    3    0.3025    0.01085640    -39.79732700    24.96554500   0.147946D+02 0.000000D+00
    4    0.6400    0.01085554    -80.01355400    81.33634000   0.145599D+02 0.000000D+00
    5    1.1025    0.01085210   -134.14148400   191.49126400   0.142771D+02 0.000000D+00
    6    1.6900    0.01085481   -202.18538700   379.17501000   0.138019D+02 0.000000D+00
    7    2.4025    0.01085130   -284.13810300   683.99962100   0.128473D+02 0.000000D+00
    8    3.2400    0.01086136   -380.01517000  1143.33290000   0.994015D+01 0.000000D+00
    9    4.2025    0.01085691   -489.79280800  1884.50607900   0.255087D+03 0.000000D+00
   10    5.2900    0.01085517   -613.48535700  2977.88400300   0.211923D+02 0.000000D+00
   11    6.5025    0.01084950   -751.08549900  4589.00460800   0.184801D+02 0.000000D+00
   12    7.8400    0.01084884   -902.60416400  7067.64588100   0.175633D+02 0.000000D+00
   13    9.3025    0.01084997  -1068.03834400 10667.30447600   0.171015D+02 0.000000D+00
   14   10.8900    0.01085217  -1247.38743100 16133.94159100   0.168224D+02 0.000000D+00
   15   12.6025    0.01085409  -1440.65012300 24382.00819500   0.166357D+02 0.000000D+00
   16   14.4400    0.01084667  -1647.80803700 36688.65838000   0.165081D+02 0.000000D+00
   17   16.4025    0.01085322  -1868.90565500 52963.12362700   0.164042D+02 0.000000D+00
   18   18.4900    0.01087420  -2103.94832300 80952.12957300   0.163121D+02 0.000000D+00
   19   20.7025    0.01085536  -2352.81914300 119013.69526900 0.162632D+02 0.000000D+00
   20   23.0400    0.01085344  -2615.63825000 190732.88917600 0.162137D+02 0.000000D+00
```

```
#   xN=100 n=200 ng=16
#   i    lambda    alpha          C0             D_0           a_0
    1    0.0025    0.01085409     -1.10605700    -1.15933300   0.478442D+03 0.000000D+00
    2    0.0900    0.01085514    -13.49359000     2.15038800   0.141817D+02 0.000000D+00
    3    0.3025    0.01085640    -39.79732700    24.96554500   0.147946D+02 0.000000D+00
    4    0.6400    0.01085554    -80.01355400    81.33634000   0.145599D+02 0.000000D+00
    5    1.1025    0.01085210   -134.14148400   191.49126400   0.142771D+02 0.000000D+00
    6    1.6900    0.01085481   -202.18538700   379.17501000   0.138019D+02 0.000000D+00
    7    2.4025    0.01085130   -284.13810300   683.99962100   0.128473D+02 0.000000D+00
    8    3.2400    0.01086136   -380.01517000  1143.33290000   0.994015D+01 0.000000D+00
    9    4.2025    0.01085691   -489.79280800  1884.50607900   0.255087D+03 0.000000D+00
   10    5.2900    0.01085517   -613.48535700  2977.88400300   0.211923D+02 0.000000D+00
   11    6.5025    0.01084950   -751.08549900  4589.00460800   0.184801D+02 0.000000D+00
   12    7.8400    0.01084884   -902.60416400  7067.64588100   0.175633D+02 0.000000D+00
   13    9.3025    0.01084997  -1068.03834400 10667.30447600   0.171015D+02 0.000000D+00
   14   10.8900    0.01085217  -1247.38743100 16133.94159100   0.168224D+02 0.000000D+00
   15   12.6025    0.01085409  -1440.65012300 24382.00819500   0.166357D+02 0.000000D+00
   16   14.4400    0.01084667  -1647.80803700 36688.65838000   0.165081D+02 0.000000D+00
   17   16.4025    0.01085322  -1868.90565500 52963.12362700   0.164042D+02 0.000000D+00
   18   18.4900    0.01087420  -2103.94832300 80952.12957300   0.163121D+02 0.000000D+00
   19   20.7025    0.01085536  -2352.81914300 119013.69526900 0.162632D+02 0.000000D+00
   20   23.0400    0.01085344  -2615.63825000 190732.88917600 0.162137D+02 0.000000D+00
```

3.3 Dimer-Dimer Toy Model (JK)

Two parameters α, λ (in fm^{-2}) and the reduced mass $\mu = 938.92$ MeV, which determine a numerical function $C_0(\lambda)$ (in MeV) given below,

- A local term
$$V(R) = C_0(\lambda)\ \frac{1}{(b\sqrt{\lambda})^3}\ \ e^{-\left(\frac{R}{b}\right)^2} \tag{47}$$
driven by a range parameter
$$\frac{1}{b^2} = \frac{2\alpha\lambda}{2\alpha+\lambda} \quad \Leftrightarrow \quad b^2 = \frac{1}{\lambda} + \frac{1}{2\alpha} \tag{48}$$
and having MeV dimension given by C_0 (notice that $b\sqrt{\lambda}$ dimensionless)

```
TEST VALUES V(R)
i      lambda      alpha          C0           V(2)           V(10)          V(20)
010   1.48320000  0.00119019     -1.828446   -0.116166D-03  -0.924686D-04  -0.453269D-04
100   4.49440000  0.00130720   -357.319483   -0.495666D-02  -0.385702D-02  -0.176126D-02
198   6.30870000  0.00136145  -1382.322273   -0.122529D-01  -0.943546D-02  -0.417017D-02
```

- A non local term[4]
$$W(R,R') = 32\pi\alpha^{3/2}RR'\ e^{-\left(\frac{R'}{b_1}\right)^2} \left\{ \left[\frac{\hbar^2}{2\mu}(4\alpha^2R^2 - 2\alpha) + E\right] e^{-\left(\frac{R}{b_1}\right)^2} - \frac{2C_0(\lambda)}{(b\sqrt{\lambda})^3} e^{-\left(\frac{R}{b_2}\right)^2} \right\} \tag{49}$$
with the two range parameters [5]
$$\frac{1}{b_1^2} = \alpha \quad \Leftrightarrow \quad b_1^2 = \frac{1}{\alpha} \qquad\qquad \frac{1}{b_2^2} = \frac{\alpha(2\alpha+3\lambda)}{2\alpha+\lambda} \quad \Leftrightarrow \quad b_2^2 = \frac{1}{\alpha}\frac{2\alpha+\lambda}{2\alpha+3\lambda} = b_1^2\frac{2\alpha+\lambda}{2\alpha+3\lambda}$$

```
TEST VALUES W(R,R')
i      lambda      alpha          C0           W(2,30)        W(20,30)       W(40,20)
010   1.48320000  0.00119019     -1.828446   -0.410905D-02  -0.119713D-02   0.423542D-01
100   4.49440000  0.00130720   -357.319483   -0.382420D-02   0.312843D-02   0.480615D-01
198   6.30870000  0.00136145  -1382.322273   -0.277361D-02   0.690361D-02   0.503769D-01
```

  - Notice that $V(R,R')$ is not symmetric
  - The ranges b, b_1, b_2 are unusually large for a Nuclear Physics problem
  - The variation on R' is trivial $\sim x\exp(-x^2)$
  - The variation on R can have a structure (zero) depending on α and E. For $E=0$ it is at $R \approx \sqrt{\frac{1}{2\alpha}}$

---

[4] A factor $4\pi RR'$ is introduced here in W to be compatible with equation (8) and (11)

[5] We used
$$\frac{32\sqrt{2}\alpha^3}{(2\alpha+\lambda)^{3/2}} = \frac{16\alpha^{3/2}}{b^3\lambda^{3/2}}$$

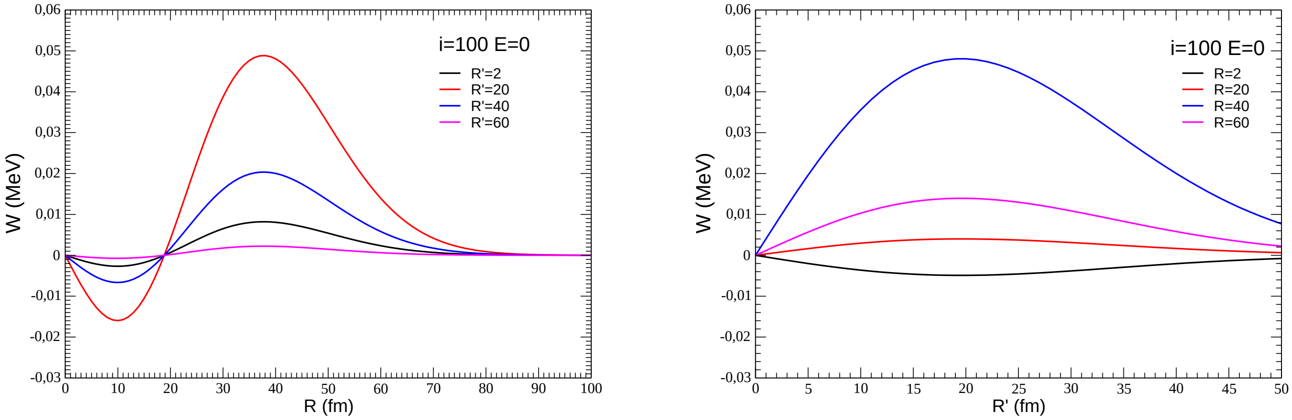


TABLE FOR C_0 (corresponding to mu=938 MeV)

i	lambda [fm^-1]	alpha [fm^-2]	C0[MeV]	b	b1	b2
1	0.63250000	0.00077171	0.83382111	25.485149	35.997549	20.800079
2	0.77460000	0.00105652	0.90776882	21.784003	30.765299	17.778483
3	0.89440000	0.00110491	0.91369538	21.298911	30.084067	17.383331
4	1.00000000	0.00109934	0.83396922	21.349903	30.160184	17.425738
5	1.09540000	0.00122357	1.37935968	20.237421	28.588120	16.517636
6	1.18320000	0.00116872	0.37470813	20.704194	29.251272	16.899340
7	1.26490000	0.00115710	0.00273375	20.806378	29.397781	16.983158
8	1.34160000	0.00120176	-0.50265132	20.415725	28.846367	16.664395
9	1.41420000	0.00125485	-1.12940812	19.979017	28.229559	16.307976
10	1.48320000	0.00119019	-1.82844597	20.512806	28.986238	16.744158
11	1.54920000	0.00126792	-2.72133438	19.874409	28.083684	16.222962
12	1.61250000	0.00121848	-3.68073733	20.272333	28.647768	16.548123
13	1.67330000	0.00126717	-4.83339523	19.879076	28.091993	16.227102
14	1.73210000	0.00130049	-6.12301834	19.622635	27.729784	16.017806
15	1.78890000	0.00123366	-7.48372394	20.145894	28.470970	16.445274
16	1.84390000	0.00127897	-9.08293304	19.785902	27.962102	16.151387
17	1.89740000	0.00127640	-10.79866171	19.805397	27.990239	16.167414
18	1.94940000	0.00132586	-12.72678747	19.432620	27.463202	15.863071
19	2.00000000	0.00123879	-14.67527162	20.102728	28.411957	16.410421
20	2.04940000	0.00122735	-16.87450660	20.195784	28.544063	16.486498
21	2.09760000	0.00131155	-14.92686728	19.537273	27.612617	15.948793
22	2.14480000	0.00124551	-21.84398418	20.047649	28.335207	16.365669
23	2.19090000	0.00122351	-24.55846572	20.226635	28.588821	16.511905
24	2.23610000	0.00134849	-27.69202731	19.267390	27.231787	15.728596
25	2.28040000	0.00122853	-30.62982902	20.184870	28.530351	16.477919
26	2.32380000	0.00125436	-34.00330272	19.975985	28.235072	16.307390
27	2.36640000	0.00134601	-37.71568075	19.284472	27.256862	15.742721
28	2.40830000	0.00123155	-41.21067985	20.159556	28.495349	16.457403
29	2.44950000	0.00123523	-45.19861754	20.129361	28.452870	16.432792
30	2.49000000	0.00125159	-49.41210919	19.997336	28.266300	16.325022
31	2.52980000	0.00130885	-53.95787299	19.555307	27.641083	15.964088
32	2.56900000	0.00135703	-58.72700386	19.205232	27.145964	15.678246
33	2.60770000	0.00123411	-63.26698013	20.137869	28.465778	16.439908
34	2.64580000	0.00123557	-68.38264994	20.125841	28.448955	16.430123
35	2.68330000	0.00126348	-73.83190969	19.902389	28.132985	16.247683
36	2.72030000	0.00127965	-79.49354643	19.776234	27.954672	16.144696
37	2.75680000	0.00130418	-85.46884687	19.589421	27.690528	15.992173
38	2.79280000	0.00124058	-91.37906356	20.084704	28.391453	16.396665
39	2.82840000	0.00133743	-98.17811347	19.344376	27.344153	15.792128
40	2.86360000	0.00124230	-104.48231212	20.070588	28.371791	16.385197
41	2.89830000	0.00128009	-111.63742606	19.772268	27.949867	16.141613
42	2.93260000	0.00126966	-118.86583963	19.853141	28.064434	16.207683
43	2.96650000	0.00133031	-126.61959764	19.395601	27.417230	15.834075
44	3.00000000	0.00130310	-134.41282198	19.596779	27.702000	15.998387
45	3.03320000	0.00129846	-142.67347449	19.631639	27.751452	16.026879
46	3.06590000	0.00131786	-151.31892909	19.486640	27.546432	15.908496
47	3.09840000	0.00124216	-159.72002777	20.071058	28.373390	16.385761
48	3.13050000	0.00132586	-169.42925062	19.427639	27.463202	15.860362
49	3.16230000	0.00132720	-179.00345407	19.417755	27.449334	15.852313
50	3.19370000	0.00129809	-188.69826687	19.634012	27.755407	16.028932
51	3.22490000	0.00125184	-198.61382760	19.993053	28.263477	16.322147
52	3.25580000	0.00124683	-209.18057966	20.033076	28.320204	16.354850
53	3.28630000	0.00125499	-220.21678061	19.967820	28.227984	16.301582
54	3.31660000	0.00135532	-232.33938473	19.215048	27.163084	15.686885
55	3.34660000	0.00129957	-243.38866953	19.622473	27.739598	16.019609
56	3.37640000	0.00125706	-255.60187410	19.951182	28.204733	16.288051
57	3.40590000	0.00135898	-269.21706892	19.188971	27.126482	15.665646
58	3.43510000	0.00127936	-281.32840182	19.776540	27.957840	16.145473
59	3.46410000	0.00124728	-294.61729807	20.029003	28.315095	16.351650
60	3.49280000	0.00124707	-308.52111851	20.030629	28.317479	16.352994
61	3.52140000	0.00128045	-323.30449766	19.767946	27.945938	16.138505
62	3.54960000	0.00124327	-337.69784067	20.061081	28.360721	16.377892
63	3.57770000	0.00125755	-352.84952774	19.946880	28.199238	16.284651
64	3.60560000	0.00127134	-369.23069817	19.838427	28.045885	16.196104

65	3.63320000	0.00124752	−384.49861566	20.026743	28.312371	16.349896
66	3.66060000	0.00125959	−402.24630720	19.930573	28.176393	16.271379
67	3.68780000	0.00129028	−420.04146205	19.692231	27.839281	16.076764
68	3.71480000	0.00126263	−437.62674167	19.906482	28.142453	16.251733
69	3.74170000	0.00129259	−456.55285556	19.674540	27.814394	16.062345
70	3.76830000	0.00132265	−476.26049725	19.449790	27.496507	15.878829
71	3.79470000	0.00125090	−489.80963130	19.999393	28.274094	16.327642
72	3.82100000	0.00132067	−511.06340871	19.464260	27.517112	15.890671
73	3.84710000	0.00126600	−536.04931445	19.879755	28.104971	16.229971
74	3.87300000	0.00125166	−556.53110139	19.993191	28.265509	16.322614
75	3.89870000	0.00132208	−580.69829068	19.453751	27.502434	15.882126
76	3.92430000	0.00126284	−602.43567723	19.904467	28.140113	16.250186
77	3.94970000	0.00127860	−626.37018189	19.781453	27.966148	16.149746
78	3.97490000	0.00124961	−649.55818837	20.009408	28.288685	16.335902
79	4.00000000	0.00127540	−675.34262765	19.806157	28.001210	16.169941
80	4.02490000	0.00127850	−700.73567828	19.782107	27.967242	16.150313
81	4.04970000	0.00132766	−726.46225750	19.412609	27.444578	15.848597
82	4.07430000	0.00128291	−753.53598652	19.748023	27.919132	16.122501
83	4.09880000	0.00133213	−784.26761927	19.379957	27.398494	15.821954
84	4.12310000	0.00126111	−810.38077531	19.917797	28.159408	16.261156
85	4.14730000	0.00128531	−820.92248864	19.729479	27.893053	16.107388
86	4.17130000	0.00127270	−870.95038122	19.826883	28.030896	16.186936
87	4.19520000	0.00135966	−905.81221403	19.182736	27.119697	15.660947
88	4.21900000	0.00128262	−935.46364051	19.750040	27.922288	16.124207
89	4.24260000	0.00128066	−968.53447565	19.765105	27.943646	16.136517
90	4.26610000	0.00126521	−1001.60340106	19.885314	28.113744	16.234686
91	4.28950000	0.00130101	−1037.60967247	19.609945	27.724242	16.009834
92	4.31280000	0.00125808	−1064.04792433	19.941486	28.193297	16.280572
93	4.33590000	0.00132037	−1110.90724835	19.465671	27.520237	15.892041
94	4.35890000	0.00128896	−1148.14944095	19.701245	27.853532	16.084414
95	4.38180000	0.00125677	−1187.10080987	19.951779	28.207987	16.289002
96	4.40450000	0.00127821	−1229.08288372	19.783808	27.970414	16.151849
97	4.42720000	0.00132778	−336.50534073	19.411190	27.443338	15.847586
98	4.44970000	0.00126514	−343.30802017	19.885621	28.114522	16.235003
99	4.47210000	0.00131461	−350.31272295	19.508064	27.580462	15.926707
100	4.49440000	0.00130720	−357.31948294	19.563216	27.658523	15.971751
101	4.51660000	0.00127027	−364.35955314	19.845365	28.057694	16.202154
102	4.53870000	0.00137967	−371.64725307	19.042737	26.922314	15.546754
103	4.56070000	0.00137118	−378.86211857	19.101536	27.005534	15.594776
104	4.58260000	0.00128684	−386.05191339	19.717173	27.876467	16.097498
105	4.60430000	0.00127684	−393.40225401	19.794164	27.985416	16.160374
106	4.62600000	0.00129657	−400.86010911	19.643040	27.771671	16.036977
107	4.64760000	0.00127031	−408.32850381	19.844895	28.057253	16.201813
108	4.66900000	0.00135220	−416.00610227	19.234915	27.194403	15.703727
109	4.69040000	0.00127774	−423.55099023	19.787095	27.975558	16.154628
110	4.71170000	0.00129683	−431.28707987	19.640972	27.768887	16.035315
111	4.73290000	0.00125240	−439.00787873	19.986114	28.257157	16.317155
112	4.75390000	0.00127077	−446.88246054	19.841184	28.052174	16.198816
113	4.77490000	0.00128922	−454.82704050	19.698752	27.850724	16.082516
114	4.79580000	0.00127511	−462.79665107	19.807361	28.004394	16.171209
115	4.81660000	0.00129325	−470.88044093	19.668006	27.807296	16.057423
116	4.83740000	0.00131159	−479.03422128	19.530064	27.612196	15.944790
117	4.85800000	0.00126273	−487.16330620	19.904103	28.141339	16.250224
118	4.87850000	0.00128038	−495.45545681	19.766488	27.946702	16.137858
119	4.89900000	0.00138470	−503.93998928	19.007713	26.873371	15.518271
120	4.91930000	0.00129849	−512.22479913	19.628192	27.751131	16.024942
121	4.93960000	0.00126408	−520.65055701	19.893392	28.126307	16.241501
122	4.95980000	0.00128114	−529.22095076	19.760542	27.938411	16.133026
123	4.98000000	0.00126298	−537.80902745	19.902007	28.138553	16.248547
124	5.00000000	0.00138795	−546.67788310	18.985350	26.841890	15.500039
125	5.02000000	0.00127864	−555.27094272	19.779780	27.965710	16.148751
126	5.03980000	0.00127731	−564.09248049	19.790050	27.980266	16.157143
127	5.05960000	0.00134908	−573.09452001	19.256702	27.225831	15.721634
128	5.07940000	0.00127371	−581.94280460	19.817944	28.019780	16.179931
129	5.09900000	0.00132728	−591.05776429	19.414077	27.448507	15.850152
130	5.11860000	0.00130630	−600.12774273	19.569257	27.668049	15.976873
131	5.13810000	0.00132273	−609.32512668	19.447383	27.495676	15.877360
132	5.15750000	0.00137792	−618.65259881	19.054125	26.939405	15.556242
133	5.17690000	0.00131714	−627.86867128	19.488549	27.553960	15.910984
134	5.19620000	0.00133332	−637.27497043	19.369982	27.386265	15.814171
135	5.21540000	0.00127156	−646.62542796	19.834554	28.043458	16.193529
136	5.23450000	0.00128695	−656.16974378	19.715642	27.875275	16.096435
137	5.25360000	0.00134218	−665.84873425	19.305922	27.295724	15.761877
138	5.27260000	0.00131801	−675.46814336	19.482029	27.544865	15.905685
139	5.29150000	0.00133367	−685.22222752	19.367352	27.382671	15.812048
140	5.31040000	0.00126849	−694.91103790	19.858443	28.077373	16.213060
141	5.32920000	0.00128331	−704.80304328	19.743483	27.914780	16.119193
142	5.34790000	0.00133941	−714.83448782	19.325778	27.323934	15.778114
143	5.36660000	0.00127213	−724.72627666	19.829976	28.037175	16.189828
144	5.38520000	0.00128670	−734.82702696	19.717420	27.877983	16.097924
145	5.40370000	0.00130139	−744.99768012	19.605857	27.720194	16.006830
146	5.42220000	0.00133735	−755.27497256	19.340583	27.344970	15.790221
147	5.44060000	0.00128841	−765.47421662	19.704290	27.859477	16.087215
148	5.45890000	0.00134582	−775.92905414	19.279624	27.258786	15.740453
149	5.47720000	0.00133898	−786.34106529	19.328765	27.328321	15.780584
150	5.49550000	0.00128849	−796.74442854	19.703632	27.858612	16.086691
151	5.51360000	0.00130261	−807.33243620	19.596584	27.707210	15.999284
152	5.53170000	0.00136109	−818.06992659	19.171161	27.105447	15.651904
153	5.54980000	0.00139845	−828.83907470	18.913458	26.740931	15.441477
154	5.56780000	0.00130075	−839.43410262	19.610539	27.727013	16.010691
155	5.58570000	0.00131468	−850.30060780	19.506402	27.579728	15.925661
156	5.60360000	0.00128368	−861.15318461	19.740406	27.910757	16.116743
157	5.62140000	0.00129727	−872.15838327	19.636768	27.764178	16.032121
158	5.63910000	0.00135691	−883.31941646	19.200563	27.147165	15.675937
159	5.65690000	0.00132464	−894.37840604	19.432906	27.475846	15.865663
160	5.67450000	0.00129215	−905.50509476	19.675574	27.819129	16.063820
161	5.69210000	0.00129395	−916.76638729	19.661876	27.799773	16.052638
162	5.70960000	0.00131904	−928.14216590	19.474052	27.534108	15.899273
163	5.72710000	0.00128546	−939.47405321	19.726643	27.891426	16.105531

164	5.74460000	0.00129853	-950.96614123	19.627146	27.750704	16.024290
165	5.76190000	0.00135982	-962.62178564	19.179919	27.118102	15.659106
166	5.77930000	0.00132502	-974.15990198	19.430024	27.471905	15.863336
167	5.79660000	0.00131412	-985.81359221	19.510389	27.585603	15.928962
168	5.81380000	0.00130295	-997.53599767	19.593789	27.703595	15.997067
169	5.83100000	0.00131593	−1009.37624157	19.496946	27.566625	15.917993
170	5.84810000	0.00136630	−1021.36090842	19.134337	27.053718	15.621904
171	5.86520000	0.00129263	−1033.16570282	19.671776	27.813964	16.060758
172	5.88220000	0.00138065	−1045.36698368	19.034660	26.912758	15.540519
173	5.89920000	0.00136868	−1057.43576482	19.117662	27.030186	15.608299
174	5.91610000	0.00138204	−1069.62528281	19.025064	26.899220	15.532690
175	5.93300000	0.00134398	−1081.77933205	19.292431	27.277439	15.751015
176	5.94980000	0.00136997	−1094.13399062	19.108626	27.017457	15.600930
177	5.96660000	0.00130567	−1106.37057147	19.573266	27.674723	15.980339
178	5.98330000	0.00133112	−1118.86401404	19.385321	27.408887	15.826875
179	6.00000000	0.00129204	−1131.29019953	19.676168	27.820314	16.064371
180	6.01660000	0.00130440	−1143.89516414	19.582753	27.688192	15.988095
181	6.03320000	0.00131684	−1156.56996350	19.490064	27.557099	15.912413
182	6.04980000	0.00138265	−1169.42846563	19.020771	26.893286	15.529211
183	6.06630000	0.00131529	−1182.07150714	19.501517	27.573331	15.921771
184	6.08280000	0.00132774	−1194.95518254	19.409898	27.443752	15.846963
185	6.09920000	0.00136731	−1207.96750535	19.127088	27.043725	15.616035
186	6.11560000	0.00129872	−1220.81312571	19.625442	27.748674	16.022972
187	6.13190000	0.00131088	−1233.90501943	19.534233	27.619673	15.948498
188	6.14820000	0.00133681	−1247.09710142	19.343924	27.350493	15.793103
189	6.16440000	0.00141896	−1260.48239849	18.775861	26.546968	15.329251
190	6.18060000	0.00132014	−1273.53762451	19.465598	27.522635	15.892463
191	6.19680000	0.00130470	−1286.84549133	19.580379	27.685009	15.986190
192	6.21290000	0.00131672	−1300.28519711	19.490829	27.558355	15.913071
193	6.22900000	0.00132885	−1313.79472065	19.401694	27.432287	15.840290
194	6.24500000	0.00136948	−1327.43870730	19.111834	27.022290	15.603607
195	6.26100000	0.00135334	−1341.02321947	19.225401	27.182947	15.696343
196	6.27690000	0.00139462	−1354.80817348	18.938847	26.777625	15.462358
197	6.29290000	0.00140725	−1368.59763797	18.853695	26.657190	15.392830
198	6.30870000	0.00136145	−1382.32227298	19.168047	27.101863	15.649519

3.3.1 Resultats numeriques (schro3)

```
VLOC      Rimas a_0=-0.8285 i=100
q       xN   N     a
0.0100  100  100  -.811921D+00
0.0010  100  100  -.828354D+00
0.0001  100  100  -.828521D+00
             200  -.828521D+00
              50  -.828521D+00

VLOC+VNONLOC      (i=100 WRONG b)   Rimas method =-22.9 (pas tres stable)
q       xN   N     a   (ng=16)
0.00000 200  100  0.452610D+02
0.00000 100  100  0.452577D+02
              50  0.452576D+02
              20  0.452576D+02

0.00001 100  100  0.452577D+02
0.0001  100  100  0.452580D+02
             200  0.452580D+02
              50  0.452579D+02
              20  0.452579D+02
              10  0.452574D+02
               5  0.452379D+02

0.0001  100  100  0.452580D+02
0.0001  200  200  0.452613D+02
0.0001  400  400  0.452613D+02

VLOC+VNONLOC    (i=100 RIGHT b)
q       xN   N     a   (ng=16)
0.00000 100  100  0.447843D+02
             200  0.447843D+02
0.00000 200  200  0.447875D+02

W=-150.D0*DEXP(-(R**2+RP**2))
q       xN   N     a   (ng=16)
0.0000  05 100  0.206053D+01    schro3p
            50  0.206054D+01
            20  0.206062D+01
            10  0.206201D+01
0.0000  10 100  0.206054D+01    schro3p
            50  0.206057D+01
            20  0.206201D+01
            10  0.208672D+01

0.0001  10  10  0.208672D+01
            20  0.206201D+01
            40  0.206062D+01
            50  0.206057D+01
            80  0.206054D+01
0.0001     100  0.206054D+01
0.00001    100  0.206054D+01
0.001      100  0.206054D+01
0.01       100  0.206074D+01
```

4 Model 1+3

Starting with equations (28) of Johannes notes, [6] we write the potential in the same form than for dimer-dimer, i.e. (40) and (41), to be inserted in eq. (11)

That mean identify the local term to

$$V_L(R) = \sum_{n=2}^{nL=3} \eta_n e^{-w_n R^2}$$

and the non local to

$$\boxed{W_L(R,R') = 4\pi RR' \sum_{n=1}^{nNL=3} \xi_n \; e^{-\left(\frac{R}{\sigma_n}\right)^2 - \left(\frac{R'}{\sigma'_n}\right)^2} \chi_{n,L}(R,R')} \tag{50}$$

where

$$\boxed{\chi_{n,L}(R,R') = \begin{cases} \left[4a_1^2R^2 - 2a_1 + q^2 \quad + b_1^2 R'^2 - \frac{L(L+1)}{r^2} + \right] \chi_L(x_1) - 4a_1b_1RR'\bar{\chi}_L(x_1) & \text{if} \quad n=1 \\ -\chi_L(x_n) & \text{if} \quad n>1 \end{cases}} \tag{51}$$

and

$$\begin{aligned} \chi_L(x) &= i^L j_L(ix) \\ \bar{\chi}_L(x) &= \mid 2L-1 \mid \begin{pmatrix} 1 & \mid L-1 \mid & L \\ 0 & 0 & 0 \end{pmatrix}^2 \chi_{\mid L-1 \mid}(x_1) + (2L+3) \begin{pmatrix} 1 & L+1 & L \\ 0 & 0 & 0 \end{pmatrix}^2 \chi_{L+1}(x_1) \quad (52) \\ x_n &= b_n RR' \quad (53) \end{aligned}$$

- As in the dimer-dimer case, we have introduced the ranges parameters σ_n and σ'_n

  $$\sigma_n = \frac{1}{\sqrt{a_n}} \qquad \sigma'_n = \frac{1}{\sqrt{c_n}}$$

  such that

  $$e^{-a_nR^2 - c_nR'^2} = e^{-\left(\frac{R}{\sigma_n}\right)^2 - \left(\frac{R'}{\sigma'_n}\right)^2}$$

  and the bracket (after absorving a global minus sign)

  $$\left[(4a_1^2R^2 - 2a_1 + q^2) \;\; + \;\; b_1^2R'^2 - \frac{L(L+1)}{r^2}\right] \qquad q^2 = \frac{2\mu}{\hbar^2}E$$

  Notice that the parts inside (..) is the same than for dimer-dimer

- The function $\chi_L(x)$ are listed below

  1. L=0 : using

     $$j_0(z) = \frac{\sin z}{z}$$

     we obtain

     $$\chi_0(x) = j_0(ix) = \frac{\sinh(x)}{x} = \frac{e^{+x} - e^{-x}}{2x} \tag{54}$$

[6]

$$0 = (\ldots)\phi + V\phi - \int dR' \; 4\pi RR'\xi_1 e^{A_1} \{...\}\phi - \int dR' \; \left[4\pi RR' \sum \xi_n e^{A_n} \chi_L(x_n)\right]\phi$$

$$0 = (-\ldots)\phi - V\phi - \int dR' \; 4\pi RR'\xi_1 e^{A_1} \{-\ldots\}\phi - \int dR' \; \left[4\pi RR' \sum \xi_n e^{A_n} (-\chi_L(x_n))\right]\phi$$

2. L=1 : using

$$j_1(z) = \frac{1}{z}\left[j_0(z) - \cos(z)\right]$$

we obtain

$$\chi_1(x) \equiv i j_1(ix) = \frac{1}{x}\left[\chi_0(x) - \frac{e^x + e^{-x}}{2}\right] = \frac{1}{x}\left[\frac{e^{+x} - e^{-x}}{2x} - \frac{e^x + e^{-x}}{2}\right] \tag{55}$$

3. L=2 : using recurrence relation

$$j_2(z) = \frac{3}{z} j_1(z) - j_0(z)$$

and so

$$\chi_2(x) = i^2 j_2(ix) = \frac{3}{x}\chi_1(x) + j_0(x)$$

- The relvant 3j symbols are given by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = \begin{cases} 0 & \text{if} \quad j_1 + j_2 + j_3 = \text{odd} \\ (-)^p \sqrt{\Delta(j_1 j_2 j_3)} \; \frac{p!}{(p-j_1)!(p-j_2)!(p-j_3)!} & \text{if} \quad j_1 + j_2 + j_3 = \text{even} = 2p \end{cases}$$

where

$$\Delta(abc) = \frac{(a+b-c)!(b+c-a)!(c+a-b)!}{(a+b+c+1)!}$$

- The parameters are

	V (nL=3)	
n	η_n	w_n
2	$2C\left(\frac{3\alpha}{3\alpha+\lambda}\right)^{3/2}$	$\frac{3\alpha\lambda}{3\alpha+\lambda}$
3	$8D\left[\frac{3\alpha^2}{12\alpha^2+16\alpha\lambda+\lambda^2}\right]^{3/2}$	$\frac{12\alpha\lambda(\alpha+\lambda)}{12\alpha^2+16\alpha\lambda+\lambda^2}$

	W (nNL=5)			
n	ξ_n	a_n	b_n	c_n
1	$\frac{27}{8}\left(\frac{3}{2}\alpha\right)^{3/2}\frac{\hbar^2}{2\mu}$	$\frac{15}{16}\alpha$	$\frac{18}{16}\alpha$	$\frac{15}{16}\alpha$
2	$-54\left(\frac{3}{2}\alpha\right)^{3/2} C\left(\frac{\alpha}{4\alpha+\lambda}\right)^{3/2}$	$\frac{3\alpha(5\alpha+8\lambda)}{4(4\alpha+\lambda)}$	$\frac{9\alpha(\alpha+\lambda)}{2(4\alpha+\lambda)}$	$\frac{3\alpha(5\alpha+2\lambda)}{4(4\alpha+\lambda)}$
3	$-27\left(\frac{3}{2}\alpha\right)^{3/2} D\left(\frac{\alpha}{4\alpha+5\lambda}\right)^{3/2}$	$\frac{3(20\alpha^2+52\alpha\lambda+27\lambda^2)}{16(4\alpha+5\lambda)}$	$\frac{9(4\alpha^2+8\alpha\lambda+3\lambda^2)}{8(4\alpha+5\lambda)}$	$\frac{3(20\alpha^2+28\alpha\lambda+3\lambda^2)}{16(4\alpha+5\lambda)}$

with

$$\mu = \frac{3}{4}m_N \qquad \frac{\hbar^2}{2\mu} = 27.647374 \qquad \frac{2\mu}{\hbar^2} = 0.0361698$$

4.1 Potential L=0

$$\chi_{n,0}(R,R') = \begin{cases} \left[4a_1^2R^2 - 2a_1 + q^2 \quad + b_1^2{R'}^2\right]\chi_0(x_1) - 4a_1b_1RR'\bar{\chi}_0(x_1) & \text{if} \quad n=1 \\ -\chi_0(x_n) & \text{if} \quad n>1 \end{cases} \tag{56}$$

with

- $\chi_0(x)$ given in (54)
- $\bar{\chi}_0(x)$ given by (52)

$$\bar{\chi}_0(x) = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}^2 \chi_1(x_1) + 3\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}^2 \chi_1(x_1) = \frac{4}{3}\chi_1(x_1)$$

Since

$$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = -\frac{1}{\sqrt{3}}$$

This is a strange result, since it involves χ_1 !!!

Does not fit with your remark on eq (28) that for $l=0$ it gives $j_0(x_n)$

4.2 Potential L=1

$$\chi_{n,1}(R,R') = \begin{cases} \left[4a_1^2R^2 - 2a_1 + q^2 \quad + b_1^2{R'}^2 - \frac{2}{r^2}\right]\chi_1(x_1) - 4a_1b_1RR'\bar{\chi}_1(x_1) & \text{if} \quad n=1 \\ -\chi_1(x_n) & \text{if} \quad n>1 \end{cases} \tag{57}$$

with

- $\chi_1(x)$ given in (55)
- $\bar{\chi}_1(x)$ given by (52)

$$\bar{\chi}_1(x) = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 \chi_0(x_1) + 5\begin{pmatrix} 1 & 2 & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 \chi_2(x_1) = \frac{1}{3}\,\chi_0(x_1) + \frac{2}{3}\begin{pmatrix} 1 & 2 & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 \chi_2(x_1)$$

Since

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = -\frac{1}{\sqrt{3}} \qquad \begin{pmatrix} 1 & 2 & 1 \\ 0 & 0 & 0 \end{pmatrix} = +\frac{2}{\sqrt{30}}$$

5 3d-solution

We use spherical coordinates $\vec{R} = (r, \theta, \varphi)$ and denote $u = \cos\theta$

$$\vec{R} = \begin{pmatrix} r\sin\theta\cos\varphi \\ r\sin\theta\sin\varphi \\ r\cos\theta \end{pmatrix} \qquad \vec{R'} = \begin{pmatrix} r'\sin\theta'\cos\varphi' \\ r'\sin\theta'\sin\varphi' \\ r'\cos\theta' \end{pmatrix}$$

$$\vec{R} \cdot \vec{R'} = RR'[\sin\theta\sin\theta'\cos(\varphi - \varphi') + \cos\theta\cos\theta']$$

$$\Psi(R) = \Psi(r, u, \varphi)$$

$$dR = r^2 dr du d\varphi$$

We restrict to a solution in the (r, θ) plane, that is with $\varphi = 0$

References

[1] V.I. Kukulin, V. M. Krasnopol'sky, J. Horacek, Theory of Resonances (1989)

[2] R.A. Malfliet, J. A. Tjon, Nucl. Phys. **A127** (1969) 161

[3] A. Spyrou et al, Physics Letters B 683 (2010) 129?133

[4] H. Al Falou et al., J. Phys.: Conf. Ser. **312** (2011) 092012

[5] Yuki Kubota, "Neutron-neutron correlation in Borromean nucleus ^{11}Li via the (p, pn) reaction", PhD Univ. Tokyo, (2016)

[6] Yu. Aksyutina et al, Phys. Lett. B 666 (2008) 430