Quantum Algorithms for Computational Nuclear Physics – Supplementary Information[1]

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Abstract. While quantum algorithms have been studied as an efficient tool for the stationary state energy determination in the case of molecular quantum systems, no similar study for analogical problems in computational nuclear physics (computation of energy levels of nuclei from empirical nucleon-nucleon or quark-quark potentials) have been realized yet. Although the difference between the above mentioned studies might seem negligible, it will be examined and first steps towards a particular simulation (on classical computer) of the Iterative Phase Estimation Algorithm for deuterium and tritium nuclei energy level computation will be carried out with the aim to prove algorithm feasibility (and extensibility to heavier nuclei) for its possible practical realization on a real quantum computer.

Let us denote spin ladder operators as

$$\hat{s}_{\pm} = \frac{1}{2}\left(\hat{\sigma}_x \pm i\hat{\sigma}_y\right) = \hat{s}_x \pm i\,\hat{s}_y\,, \tag{SI1}$$

fulfilling

$$\hat{s}_{\pm}\left|s = 1/2, m_s = \mp 1/2\right\rangle = \left|s = 1/2, m_s = \pm 1/2\right\rangle, \tag{SI2}$$

$$\hat{s}_{\pm}\left|s = 1/2, m_s = \pm 1/2\right\rangle = 0\,. \tag{SI3}$$

[1] The main article can be found in EPJ Web of Conferences, TESNAT 2015 Proceedings.

Using identity

$$\left(\vec{\sigma}_1 \cdot \vec{\sigma}_2\right) = \frac{1}{2}\left\{\left(\vec{\sigma}_1 + \vec{\sigma}_2\right)^2 - \vec{\sigma}_1^2 - \vec{\sigma}_2^2\right\} = 2\left\{\left(\vec{s}_1 + \vec{s}_2\right)^2 - \vec{s}_1^2 - \vec{s}_2^2\right\}, \tag{SI4}$$

we will provide the matrix elements between $\left|s, m_s\right\rangle$ states coupled from spinors (implying $s \in \{0,1\}$, $m_s \in \{-s,0,+s\}$). Only diagonal elements are non-zero and doesn't depend on m_S,

$$\left\langle 1, m_S \left|\left(\vec{\sigma}_1 \cdot \vec{\sigma}_2\right)\right| 1, m_S\right\rangle = 2\left\{1\cdot(1+1) - 2\cdot\frac{1}{2}\left(1+\frac{1}{2}\right)\right\} = 1, \tag{SI5}$$

$$\left\langle 0, m_S \left|\left(\vec{\sigma}_1 \cdot \vec{\sigma}_2\right)\right| 0, m_S\right\rangle = 2\left\{0 - 2\cdot\frac{1}{2}\left(1+\frac{1}{2}\right)\right\} = -3. \tag{SI6}$$

The latter should be used too to evaluate the matrix element of $\left(\vec{\tau}_1 \cdot \vec{\tau}_2\right)$ between isospin singlet states. The unit position vector will be denoted as $\vec{n}$ in all text (see (SI7) for its cartezian components in spherical coordinates, $\theta \in \langle 0;\pi\rangle$, $\phi \in \langle 0; 2\pi)$) and n_+, n_- (SI8) and nz should be its irreducible components. Therefore, for scalar products we can write (SI9) and (SI10).

$$\vec{n} = \left(\sin\theta\cos\phi, \quad \sin\theta\sin\phi, \quad \cos\theta\right), \tag{SI7}$$

$$n_\pm = n_x \pm i\, n_y = e^{\pm i\phi}\sin\theta, \tag{SI8}$$

$$\left(\vec{\sigma}_1 \cdot \vec{n}\right) = s_{1+}n_- + s_{1-}n_+ + \sigma_z n_z, \tag{SI9}$$

$$\begin{aligned}\left(\vec{\sigma}_1 \cdot \vec{n}\right)\left(\vec{\sigma}_2 \cdot \vec{n}\right) = {} & \left(s_{1+}s_{2-} + s_{1-}s_{2+}\right)n_+ n_- + \\ & \left(s_{1+}\sigma_{2z} + \sigma_{1z}s_{2+}\right)n_z n_- + \left(s_{1-}\sigma_{2z} + \sigma_{1z}s_{2-}\right)n_z n_+ +, \\ & s_{1+}s_{2+}n_-^2 + s_{1-}s_{2-}n_+^2 + \sigma_{1z}\sigma_{2z}n_z^2\end{aligned} \tag{SI10}$$

With formulae above, we can easily derive the matrix elements between all terms in Hamada-Johnson or Agronne potentials. As for Hamada-Johnson potential:

$$\hat{V} = \hat{V}_C + \hat{V}_T \hat{S}_{12} + V_{LS}(r)\left(\hat{\vec{L}} \cdot \hat{\vec{s}}\right) + V_{LL}(r)\hat{L}_{12}, \qquad \text{(SI11)}$$

the terms in (SI11) are reffered by indices $i \in \{C, T, LS, LL\}$ and represents central, tensor, linear LS and quadratic LS potentials, V_i are allowed to be spin-parity dependent and are given by

$$\hat{S}_{12} = 3(\vec{\sigma}_1 \cdot \vec{n})(\vec{\sigma}_2 \cdot \vec{n}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2), \qquad \text{(SI11')}$$

$$\begin{aligned} \hat{L}_{12} &= (\vec{\sigma}_1 \cdot \vec{\sigma}_2)\hat{L}^2 - \frac{1}{2}\left\{(\vec{\sigma}_1 \cdot \vec{L})(\vec{\sigma}_2 \cdot \vec{L}) + (\vec{\sigma}_2 \cdot \vec{L})(\vec{\sigma}_1 \cdot \vec{L})\right\} \\ \hat{L}_{12} &= \left\{\delta_{LJ} + (\vec{\sigma}_1 \cdot \vec{\sigma}_2)\right\}\hat{L}^2 - \left(\vec{L} \cdot \vec{s}\right)^2 \end{aligned}, \qquad \text{(SI11'')}$$

$$\hat{V}_C = \frac{1}{3}(\vec{\tau}_1 \cdot \vec{\tau}_2)(\vec{\sigma}_1 \cdot \vec{\sigma}_2)V_C(r), \qquad \text{(SI12)}$$

$$\hat{V}_T = \frac{1}{3}(\vec{\tau}_1 \cdot \vec{\tau}_2)V_T(r), \qquad \text{(SI13)}$$

$$V_C(r) = 0.08\,\mu_\pi\, Y(x) \cdot \left[1 + a_C\, Y(x) + b_C\, Y^2(x)\right], \qquad \text{(SI14)}$$

$$V_T(r) = 0.08\,\mu_\pi\, Z(x) \cdot \left[1 + a_T\, Y(x) + b_T\, Y^2(x)\right], \qquad \text{(SI15)}$$

$$V_{LS}(r) = \mu_\pi\, G_{LS}\, Y^2(x) \cdot \left[1 + b_{LS}\, Y(x)\right], \qquad \text{(SI16)}$$

$$V_{LL}(r) = \mu_\pi\, G_{LL}\, x^{-2} Z(x) \cdot \left[1 + a_{LL}\, Y(x) + b_{LL} Y^2(x)\right], \qquad \text{(SI17)}$$

$$Y(x) = e^{-x}/x\ , \qquad \text{(SI18)}$$

$$Z(x) = \left(1 + 3x^{-1} + 3x^{-2}\right)Y(x), \qquad \text{(SI19)}$$

Where $x = r / r_\mu$, $r_\mu = 1.415$ fm, ratio of nucleon mass (M) and pion mass (μ_π) is $M / \mu_\pi = 6.73$. The hard-core radius $x_0 = 0.343$ is considered equal for all states (potential under $x < x_0$ is considered infinite and as a result the wave-function for such distances should drop to zero (while staying continuos, in the best case with its first derivative as well)).

I will add the centrifugal (effective) potential (SI20) (μ being reduced mass) resulting as angular part of kinetical energy operator to the central part of the interaction potential for the deuterium case and evaluate its matrix elements as (SI21) and (SI22)

$$\hat{V}_{cent} = \frac{\hat{L}^2}{2\,\mu\, r^2}, \tag{SI20}$$

$$\langle S_a | \hat{V}_{cent} + \hat{V}_C | S_b \rangle = -\int_0^\infty R_{S,a}(r) V_C(r)\, R_{S,b}(r)\, dr, \tag{SI21}$$

$$\langle D_a | \hat{V}_{cent} + \hat{V}_C | D_b \rangle = \frac{3\hbar^2}{\mu} \int_0^\infty R_{D,a}(r) \frac{1}{r^2} R_{D,b}(r)\, dr - \int_0^\infty R_{D,a}(r) V_C(r)\, R_{D,b}(r)\, dr, \tag{SI22}$$

The off-diagonal elements

$$\langle S_a | \hat{V}_{cent} | D_b \rangle = \langle S_a | \hat{V}_C | D_b \rangle = 0, \tag{SI23}$$

are zero due to angular-momentum eigenfunction orthonormality (similary for the LS potential parts, but in contrast with the tensor part). For the tensor potential part we will exploit the expression (SI10) and use the (18)-(22) formulae from the main article. Wile for deriving the action of (SI10) on $| S_a \rangle$ one can easily write

$$(\vec{\sigma}_1 \cdot \vec{n})(\vec{\sigma}_2 \cdot \vec{n}) | S_a \rangle = \frac{R_{S,a}(r)}{r} | T = 0 \rangle_{isospin} Y_{0,0} \left\{ \left(n_+ n_- - n_z^2 \right) |1,0\rangle_{spin} + \sqrt{2}\, n_z \left(n_- |\uparrow\uparrow\rangle - n_+ |\downarrow\downarrow\rangle \right) \right\}, \tag{SI24}$$

$$\begin{aligned} \hat{S}_{12} | S_a \rangle &= \frac{R_{S,a}(r)}{r} | T = 0 \rangle_{isospin} Y_{0,0} \times \\ &\times \left\{ \left(3 n_+ n_- - 3 n_z^2 - 1 \right) |1,0\rangle_{spin} + 3\sqrt{2}\, n_z \left(n_- |\uparrow\uparrow\rangle - n_+ |\downarrow\downarrow\rangle \right) \right\}, \end{aligned} \tag{SI24‘}$$

$$\left\langle S_b \left| \hat{V}_T \hat{S}_{12} \right| S_a \right\rangle \;=\; -A_{T,S,b,a} \int_0^\infty R_{S,a}(r) V_T(r) R_{S,b}(r)\, dr\,, \tag{SI25}$$

$$A_{T,S,b,a} \;=\; \left\langle Y_{0,0} \left| \left(3\, n_+ n_- - 3n_z^2 - 1\right) \right| Y_{0,0} \right\rangle \;=\; 3\left\langle Y_{0,0} \left| n_+ n_- - n_z^2 \right| Y_{0,0} \right\rangle - 1 = \; -1/2\,, \tag{SI26}$$

$$3\left\langle Y_{0,0} \left| n_+ n_- - n_z^2 \right| Y_{0,0} \right\rangle = (3/2) \int_{-1}^{1} \left(2t^2 - 1\right) dt \;=\; 1/2\,, \tag{SI27}$$

$$\left\langle S_b \left| \hat{V}_T \hat{S}_{12} \right| S_a \right\rangle \;=\; \frac{1}{2} \int_0^\infty R_{S,a}(r) V_T(r) R_{S,b}(r)\, dr\,, \tag{SI28}$$

and for the off-diagonal element, the coupling between S- and D-states, will be derived from (SI24‘) also relative easily

$$\left\langle D_b \left| \hat{V}_T \hat{S}_{12} \right| S_a \right\rangle \;=\; -A_{T,DS,b,a} \int_0^\infty R_{D,a}(r) V_T(r) R_{S,b}(r)\, dr\,, \tag{SI29}$$

$$A_{T,DS,b,a} \;=\; -\sqrt{\frac{2}{5}} \left\langle Y_{2,0} \left| \left(3n_+ n_- - 3n_z^2 - 1\right) \right| Y_{0,0} \right\rangle + 3\sqrt{\frac{3}{5}} \left(\left\langle Y_{2,-1} \left| n_z n_- \right| Y_{0,0} \right\rangle - \left\langle Y_{2,1} \left| n_z n_+ \right| Y_{0,0} \right\rangle \right), \tag{SI30}$$

$$\left\langle Y_{2,0}\left|\left(3n_+n_- - 3n_z^2 - 1\right)\right|Y_{0,0}\right\rangle = 3\left\langle Y_{2,0}\left|n_+n_- - n_z^2\right|Y_{0,0}\right\rangle = \frac{3\sqrt{5}}{4}\int_{-1}^{1}\left(2t^2-1\right)\left(3t^2-1\right)dt = \frac{4}{\sqrt{5}}, \qquad \text{(SI31)}^2$$

$$\left\langle Y_{2,-1}\left|n_z n_-\right|Y_{0,0}\right\rangle = -\left\langle Y_{2,1}\left|n_z n_+\right|Y_{0,0}\right\rangle^* = -\frac{1}{2}\sqrt{\frac{15}{2}}\int_{-1}^{1}(1-t^2)t^2\,dt = -\sqrt{\frac{2}{15}}, \qquad \text{(SI32)}$$

$$A_{T,DS,b,a} = -2\sqrt{2}, \qquad \text{(SI33)}$$

Slightly more complicated algebra will be needed for deriving the action of $\hat{S}_{12}$ on $\left|D_a\right\rangle$ state in oreder to derive the expression for the matrix element of the tensor part operator between two D-states. A table of action of different terms in (SI10) on different terms in D-state expansion with respect to the spinor components would be helpful.

prefactor	spinor	n_+n_-	n_+n_-	n_zn_-	n_zn_-	n_zn_+	n_zn_+	n_-^2	n_+^2	n_z^2

$$Y_{2,\pm2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\exp(\pm 2i\phi)$$

$$Y_{2,\pm1}(\theta,\phi) = \mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\exp(\pm i\phi)$$

[2] $$Y_{2,0}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3\cos^2\theta-1\right)$$

$$Y_{1,\pm1}(\theta,\phi) = \mp\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\exp(\pm i\phi)$$

$$Y_{1,0}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$$

		$s_{1+}s_{2-}$	$s_{1-}s_{2+}$	$s_{1+}\sigma_{2z}$	$\sigma_{1z}s_{2+}$	$s_{1-}\sigma_{2z}$	$\sigma_{1z}s_{2-}$	$s_{1+}s_{2+}$	$s_{1-}s_{2-}$	$\sigma_{1z}\ \sigma_{2z}$
$-\sqrt{\frac{2}{5}}Y_{2,0}$	$2^{-1/2}\lvert\uparrow\downarrow\rangle$		$2^{-1/2}\lvert\downarrow\uparrow\rangle$		$2^{-1/2}\lvert\uparrow\uparrow\rangle$	$-2^{-1/2}\lvert\downarrow\downarrow\rangle$				$-2^{-1/2}\lvert\downarrow\uparrow\rangle$
$-\sqrt{\frac{2}{5}}Y_{2,0}$	$2^{-1/2}\lvert\downarrow\uparrow\rangle$	$2^{-1/2}\lvert\uparrow\downarrow\rangle$		$2^{-1/2}\lvert\uparrow\uparrow\rangle$			$-2^{-1/2}\lvert\downarrow\downarrow\rangle$			$-2^{-1/2}\lvert\downarrow\uparrow\rangle$
$\sqrt{\frac{3}{10}}Y_{2,-1}$	$\lvert\uparrow\uparrow\rangle$					$\sqrt{2}\left(2^{-1/2}\lvert\downarrow\uparrow\rangle\right)$	$\sqrt{2}\left(2^{-1/2}\lvert\uparrow\downarrow\rangle\right)$		$\lvert\downarrow\downarrow\rangle$	$\lvert\uparrow\uparrow\rangle$
$\sqrt{\frac{3}{10}}Y_{2,+1}$	$\lvert\downarrow\downarrow\rangle$			$-\sqrt{2}\left(2^{-1/2}\lvert\uparrow\downarrow\rangle\right)$	$-\sqrt{2}\left(2^{-1/2}\lvert\downarrow\uparrow\rangle\right)$			$\lvert\uparrow\uparrow\rangle$		$\lvert\downarrow\downarrow\rangle$

Table S1: Action of different terms in the $(\vec{\sigma}_1\cdot\vec{n})(\vec{\sigma}_2\cdot\vec{n})$ expansion (SI10) on different terms in D-state expansion into spinors.

By summing all terms in the table S1 above we will get

$$(\vec{\sigma}_1\cdot\vec{n})(\vec{\sigma}_2\cdot\vec{n})\lvert D_a\rangle = \frac{R_{D,a}(r)}{r}\lvert T=0\rangle_{isospin}\cdot\left\{\left\{-\sqrt{\frac{2}{5}}Y_{2,0}\left(n_+n_- - n_z^2\right)+\sqrt{\frac{3}{5}}n_z\left(n_+Y_{2,-1}-n_-Y_{2,+1}\right)\right\}\lvert 1,0\rangle_{spin}+\frac{2}{\sqrt{5}}Y_{2,0}n_z\left(n_+\lvert\downarrow\downarrow\rangle - n_-\lvert\uparrow\uparrow\rangle\right)+\cdots\right\}$$
$$\cdots = \sqrt{\frac{3}{10}}\left\{\left(n_+^2Y_{2,-1}+n_z^2\,Y_{2,1}\right)\lvert\downarrow\downarrow\rangle+\left(n_-^2Y_{2,1}+n_z^2\,Y_{2,-1}\right)\lvert\uparrow\uparrow\rangle\right\} \quad ,\text{(SI34)}$$

or after regrouping

$$(\vec{\sigma}_1\cdot\vec{n})(\vec{\sigma}_2\cdot\vec{n})\lvert D_a\rangle = \frac{R_{D,a}(r)}{r}\lvert T=0\rangle_{isospin}\cdot\left\{\left\{-\sqrt{\frac{2}{5}}Y_{2,0}\left(n_+n_- - n_z^2\right)+\sqrt{\frac{3}{5}}n_z\left(n_+Y_{2,-1}-n_-Y_{2,+1}\right)\right\}\lvert 1,0\rangle_{spin}+\cdots\right\}$$
$$\cdots = \left\{\left\{\frac{2}{\sqrt{5}}Y_{2,0}n_zn_+ + \sqrt{\frac{3}{10}}\left(n_+^2Y_{2,-1}+n_z^2\,Y_{2,1}\right)\right\}\lvert\downarrow\downarrow\rangle+\left\{-\frac{2}{\sqrt{5}}Y_{2,0}n_zn_- + \sqrt{\frac{3}{10}}\left(n_-^2Y_{2,1}+n_z^2\,Y_{2,-1}\right)\right\}\lvert\uparrow\uparrow\rangle\right\} \quad , \qquad \text{(SI35)}$$

and therefore

$$\left\langle D_b \middle| \hat{V}_T \hat{S}_{12} \middle| D_a \right\rangle = -A_{T,D,b,a} \int_0^\infty R_{D,b}(r) V_T(r) R_{D,a}(r)\, dr \,, \tag{SI36}$$

$$\begin{aligned} A_{T,D,b,a}+1 &= 3\left\{ \frac{2}{5}\left\langle Y_{2,0} \middle| \left(n_+ n_- - n_z^2\right) \middle| Y_{2,0} \right\rangle + \frac{\sqrt{6}}{5}\left\{ \left\langle Y_{2,0} \middle| n_z n_- \middle| Y_{2,+1} \right\rangle - \left\langle Y_{2,0} \middle| n_z n_+ \middle| Y_{2,-1} \right\rangle \right\} + 2\cdot\{\cdots\} \right\}, \\ \cdots &= \frac{\sqrt{6}}{5}\left\langle Y_{2,+1} \middle| n_z n_+ \middle| Y_{2,0} \right\rangle + \frac{3}{10}\left(\left\langle Y_{2,1} \middle| n_+^2 \middle| Y_{2,-1} \right\rangle + \left\langle Y_{2,1} \middle| n_z^2 \middle| Y_{2,1} \right\rangle \right) \end{aligned} \tag{SI37}$$

$$\left\langle Y_{2,0} \middle| \left(n_+ n_- - n_z^2\right) \middle| Y_{2,0} \right\rangle = \frac{5}{8}\int_{-1}^{1} \left(3t^2-1\right)^2 (2t^2-1)\, dt = \frac{1}{21}\,, \tag{SI38}$$

$$\left\langle Y_{2,0} \middle| n_z n_- \middle| Y_{2,+1} \right\rangle = \left\langle Y_{2,+1} \middle| n_z n_+ \middle| Y_{2,0} \right\rangle = -\left\langle Y_{2,0} \middle| n_z n_- \middle| Y_{2,+1} \right\rangle^* = \frac{5}{4}\sqrt{\frac{3}{2}}\int_{-1}^{1} \left(3t^2-1\right) t^2 (1-t^2)\, dt = \frac{1}{7}\sqrt{\frac{2}{3}}\,, \tag{SI39}$$

$$\left\langle Y_{2,1} \middle| n_+^2 \middle| Y_{2,-1} \right\rangle = \frac{15}{4}\int_{-1}^{1} t^2 (1-t^2)^2\, dt = \frac{4}{7}\,, \tag{SI40}$$

$$\left\langle Y_{2,1} \middle| n_z^2 \middle| Y_{2,1} \right\rangle = \frac{15}{4}\int_{-1}^{1} t^4 (1-t^2)\, dt = \frac{3}{7}\,, \tag{SI41}$$

$$A_{T,D,b,a} = \frac{54}{35}\,, \tag{SI42}$$

For *LS* and *LL* parts :

The operators acting on impuls momenta are diagonal within the $\left| J(l,s)m \right\rangle$ basis as can be seen from

$$\left(\vec{L}\cdot\vec{s}\right) = \frac{\hat{J}^2 - \hat{L}^2 - \hat{s}^2}{2}\,, \tag{SI43}$$

$$\left(\vec{L}\cdot\vec{s}\right)\left|J(l,s)m\right\rangle = \frac{j(j+1)-l(l+1)-s(s+1)}{2}\left|J(l,s)m\right\rangle, \quad \text{(SI44)}$$

$$\left\langle J'(l',s')m'\right|\left(\vec{L}\cdot\vec{s}\right)\left|J(l,s)m\right\rangle = \delta_{JJ'}\delta_{ll'}\delta_{ss'}\delta_{mm'}\frac{j(j+1)-l(l+1)-s(s+1)}{2}, \quad \text{(SI45)}$$

$$\begin{aligned}\left(\vec{L}\cdot\vec{s}\right)\left|1(0,1)0\right\rangle &= 0\\ \left(\vec{L}\cdot\vec{s}\right)\left|1(2,1)0\right\rangle &= -3\end{aligned}, \quad \text{(SI46)}$$

and

$$\hat{L}_{12}\left|J(l,s)m\right\rangle = \left\{\delta_{LJ}+\left(\vec{\sigma}_1\cdot\vec{\sigma}_2\right)\right\}\hat{L}^2\left|J(l,s)m\right\rangle-\left(\vec{L}\cdot\vec{s}\right)^2\left|J(l,s)m\right\rangle, \quad \text{(SI47)}$$

$$\hat{L}_{12}\left|J(l,s)m\right\rangle = \left\{\left\{\delta_{lJ}+\delta_{s,1}-3\delta_{s,0}\right\}l(l+1)-\frac{1}{4}\left(J(J+1)-l(l+1)-s(s+1)\right)^2\right\}\left|J(l,s)m\right\rangle, \quad \text{(SI48)}$$

particularly pro deuterium $s = 1$, $l = 0$ or 2 and therefore $\delta_{lJ} = 0$ and

$$\hat{L}_{12}\left|J(l,s)m\right\rangle = \left\{l(l+1)-\frac{1}{4}\left(J(J+1)-l(l+1)-s(s+1)\right)^2\right\}\left|J(l,s)m\right\rangle, \quad \text{(SI49)}$$

$$\begin{aligned}\hat{L}_{12}\left|1(0,1)0\right\rangle &= 0\\ \hat{L}_{12}\left|1(2,1)0\right\rangle &= -3\left|1(2,1)0\right\rangle\end{aligned}, \quad \text{(SI50)}$$

$$\left\langle S_a\right|V_{LS}(r)\left(\vec{L}\cdot\vec{s}\right)\left|S_b\right\rangle = \left\langle D_a\right|V_{LS}(r)\left(\vec{L}\cdot\vec{s}\right)\left|S_b\right\rangle = \left\langle S_a\right|V_{LS}(r)\left(\vec{L}\cdot\vec{s}\right)\left|D_b\right\rangle = 0, \quad \text{(SI51)}$$

$$\left\langle D_a\right|V_{LS}(r)\left(\vec{L}\cdot\vec{s}\right)\left|D_b\right\rangle = -3\int_0^\infty R_{D,a}(r)V_{LS}(r)R_{D,b}(r)dr, \quad \text{(SI52)}$$

$$\left\langle S_a \middle| V_{LL}(r)\hat{L}_{12} \middle| S_b \right\rangle = \left\langle D_a \middle| V_{LL}(r)\hat{L}_{12} \middle| S_b \right\rangle = \left\langle S_a \middle| V_{LL}(r)\hat{L}_{12} \middle| D_b \right\rangle = 0\,, \tag{SI53}$$

$$\left\langle D_a \middle| V_{LL}(r)\hat{L}_{12} \middle| D_b \right\rangle = -3\int_0^\infty R_{D,a}(r)V_{LL}(r)R_{D,b}(r)dr\,. \tag{SI54}$$

Now, for the variational energy and wave-function estimation (in order to obtain the initial eigenvector guess for the quantum algorithm simulation and for control energy eigenvalue estimation) two methods for dealing with the hard-core will be introduced. The first is to work with the radial (part of the) wave-function of the form

(...)