```
In[ ]:= SetDirectory[NotebookDirectory[]]
Quantum`Notation`AutoLoadPalette = False;
Needs["Quantum`Notation`"]
SetQuantumAliases[];
```

Out[ ]=

```
/home/alessandro/Dropbox/0-Potential/Mathematica
```

Out[ ]=

```
Quantum`Notation`
A Mathematica package for Quantum calculations in Dirac bra-ket notation
by José Luis Gómez-Muñoz

This add-on does NOT work properly with the debugger turned on. Therefore the
  debugger must NOT be checked in the Evaluation menu of Mathematica.
Execute SetQuantumAliases[] in order to use
  the keyboard to enter quantum objects in Dirac's notation
SetQuantumAliases[] must be executed again in each
  new notebook that is created, only one time per notebook.

MATHEMATICA 13.1.0 for Linux x86 (64-bit) (June 16, 2022)

QUANTUM version EN CONSTRUCCION

TODAY IS Mon 26 May 2025 13:52:58
```

Useful definitions

In[∘]:=

```
SX[1] = 1/√2 ∑_{i=-1}^{1} ∑_{j=-1}^{1} If[i ≠ j && i + j ≠ 0, |1_Ŝ, i_Ŝz⟩·⟨1_Ŝ, j_Ŝz|, 0];
SY[1] = ⅈ/√2 ∑_{i=-1}^{1} ∑_{j=-1}^{1} If[i ≠ j && i + j ≠ 0, If[i > j, -1, 1] |1_Ŝ, i_Ŝz⟩·⟨1_Ŝ, j_Ŝz|, 0];
SZ[1] = ∑_{i=-1}^{1} i |1_Ŝ, i_Ŝz⟩·⟨1_Ŝ, i_Ŝz|;
Sv[1] = {SX[1], SY[1], SZ[1]};

SS[S_, i_] := Sv[S]〚i〛

Sbra[s_, sz_] := ⟨s_Ŝ, sz_Ŝz|
Sket[s_, sz_] := |s_Ŝ, sz_Ŝz⟩

TX[1] = 1/√2 ∑_{i=-1}^{1} ∑_{j=-1}^{1} If[i ≠ j && i + j ≠ 0, |1_T̂, i_T̂z⟩·⟨1_T̂, j_T̂z|, 0];
TY[1] = ⅈ/√2 ∑_{i=-1}^{1} ∑_{j=-1}^{1} If[i ≠ j && i + j ≠ 0, If[i > j, -1, 1] |1_T̂, i_T̂z⟩·⟨1_T̂, j_T̂z|, 0];
TZ[1] = ∑_{i=-1}^{1} i |1_T̂, i_T̂z⟩·⟨1_T̂, i_T̂z|;
Tv[1] = {TX[1], TY[1], TZ[1]};
TT[T_, i_] := Tv[T]〚i〛
Tbra[t_, tz_] := ⟨t_T̂, tz_T̂z|
Tket[t_, tz_] := |t_T̂, tz_T̂z⟩
```

We know that $\sigma_1 \cdot \sigma_2 = 2\,S(S-1) - 3$, so

In[∘]:=

```
σ1σ2 = Sum[(2 s (s + 1) - 3) |s_Ŝ⟩·⟨s_Ŝ|, {s, 0, 1}]
τ1τ2 = Sum[(2 t (t + 1) - 3) |t_T̂⟩·⟨t_T̂|, {t, 0, 1}]
```

Out[∘]=

```
-3 |0_Ŝ⟩·⟨0_Ŝ| + |1_Ŝ⟩·⟨1_Ŝ|
```

Out[∘]=

```
-3 |0_T̂⟩·⟨0_T̂| + |1_T̂⟩·⟨1_T̂|
```

Projectors

In[∘]:=

```
Pσ[s_] := {(1 - σ1σ2)/4, (3 + σ1σ2)/4}〚s + 1〛
Pτ[t_] := {(1 - τ1τ2)/4, (3 + τ1τ2)/4}〚t + 1〛
```

$S_{12} = 3\,(\sigma_1 \cdot \hat{r})\,(\sigma_2 \cdot \hat{r}) - \sigma_1 \cdot \sigma_2$

We know that $(\sigma_1 \cdot \hat{r})(\sigma_2 \cdot \hat{r}) = 2\left(\hat{S} \cdot \hat{r}\right)^2 - 1$ and therefore

$$S_{12} = 6\left(\hat{S} \cdot \hat{r}\right)^2 - 2\,S(S+1)$$

and also $S_{12} \mid 00\rangle = 0$

$$S_{12} \left| 1\, S_z \right\rangle = \left(6\left(\hat{S} \cdot \hat{r}\right)^2 - 4\right) \left| 1\, S_z \right\rangle$$

buuuuut for simplicity we use

$$\left\langle L = J-1,\ S = 1 \,\middle|\, S_{12} \,\middle|\, L = J-1,\ S = 1 \right\rangle = -2\,(J-1)\Big/\left(2\,J+1\right)$$

$$\left\langle L = J-1,\ S = 1 \,\middle|\, S_{12} \,\middle|\, L = J+1,\ S = 1 \right\rangle = 6\,\sqrt{J(J+1)}\Big/\left(2\,J+1\right)$$

$$\left\langle L = J+1,\ S = 1 \,\middle|\, S_{12} \,\middle|\, L = J-1,\ S = 1 \right\rangle = 6\,\sqrt{J(J+1)}\Big/\left(2\,J+1\right)$$

$$\left\langle L = J+1,\ S = 1 \,\middle|\, S_{12} \,\middle|\, L = J+1,\ S = 1 \right\rangle = -2\,(J+2)\Big/\left(2\,J+1\right)$$

In[∘]:=
$$\texttt{S12[l\_, lp\_, s\_, j\_]} = \left(-\frac{2\,(j-1)}{2\,j+1}\,\texttt{KroneckerDelta[l, j-1] KroneckerDelta[lp, j-1]} + \frac{6\,\sqrt{j\,(j+1)}}{2\,j+1}\,\big(\texttt{KroneckerDelta[lp, j+1] KroneckerDelta[l, j-1]} + \texttt{KroneckerDelta[lp, j-1] KroneckerDelta[l, j+1]}\big) \left| \texttt{lp}_{\hat{L}} \right\rangle \cdot \left\langle \texttt{l}_{\hat{L}} \right| - \frac{2\,(j+2)}{2\,j+1}\,\texttt{KroneckerDelta[l, j+1] KroneckerDelta[lp, j+1]} + 2\,\texttt{KroneckerDelta[lp, l] KroneckerDelta[l, j]}\right) \cdot \left| 1_{\hat{S}} \right\rangle \cdot \left\langle 1_{\hat{S}} \right| \ \texttt{// Expand;}$$

$$T_{12} = 3\,\tau_{1\,z}\,\tau_{2\,z} - \tau_1 \cdot \tau_2$$

We can write $\tau_{1\,z}\,\tau_{2\,z} = 2\,T_z^2 - 1$ and therefore

$$T_{12} = 6\,T_z^2 - 2\,T(T+1)$$

and since $T_{12} \mid 00\rangle = 0$

$$T_{12} \left| 1\, T_z \right\rangle = \left(6\,T_z^2 - 4\right) \left| 1\, T_z \right\rangle$$

In[∘]:=
$$\texttt{T12} = \texttt{Sum}\left[\left(6\,\texttt{tz}^2 - 4\right) \left| 1_{\hat{T}}, \texttt{tz}_{\hat{Tz}} \right\rangle \cdot \left\langle 1_{\hat{T}}, \texttt{tz}_{\hat{Tz}} \right|, \{\texttt{tz}, -1, 1\}\right]$$

Out[∘]=
$$2 \left| 1_{\hat{T}}, -1_{\hat{Tz}} \right\rangle \cdot \left\langle 1_{\hat{T}}, -1_{\hat{Tz}} \right| - 4 \left| 1_{\hat{T}}, 0_{\hat{Tz}} \right\rangle \cdot \left\langle 1_{\hat{T}}, 0_{\hat{Tz}} \right| + 2 \left| 1_{\hat{T}}, 1_{\hat{Tz}} \right\rangle \cdot \left\langle 1_{\hat{T}}, 1_{\hat{Tz}} \right|$$

Operator needed

In[∘]:=
```
Clear[Op]
Op[1][l_, lp_, s_, j_] = 1;
Op[2][l_, lp_, s_, j_] = τ1τ2;
Op[3][l_, lp_, s_, j_] = σ1σ2;
Op[4][l_, lp_, s_, j_] = σ1σ2 · τ1τ2 // Expand;
Op[5][l_, lp_, s_, j_] = S12[l, lp, s, j];
Op[6][l_, lp_, s_, j_] = S12[l, lp, s, j] · τ1τ2 // Expand;
Op[7][l_, lp_, s_, j_] = 1/2 (j (j + 1) - s (s + 1) - l (l + 1));
Op[8][l_, lp_, s_, j_] = 1/2 (j (j + 1) - s (s + 1) - l (l + 1)) τ1τ2 // Expand;
Op[9][l_, lp_, s_, j_] = 1/4 (j (j + 1) - s (s + 1) - l (l + 1))^2;
Op[10][l_, lp_, s_, j_] = l (l + 1);
Op[11][l_, lp_, s_, j_] = l (l + 1) σ1σ2 // Expand;

Op[12][l_, lp_, s_, j_] = T12;
Op[13][l_, lp_, s_, j_] = σ1σ2 · T12 // Expand;
Op[14][l_, lp_, s_, j_] = S12[l, lp, s, j] · T12 // Expand;
Op[15][l_, lp_, s_, j_] = 1/2 (j (j + 1) - s (s + 1) - l (l + 1)) T12 // Expand;
```

In[∘]:= $C\alpha[\alpha\_][r\_] := \frac{1}{\pi^{3/2}\, R[\alpha]^3}\, e^{-r^2/R[\alpha]^2}$

In[∘]:=
```
CC[r_] := Cα[0][r] × Pτ[0] + Cα[1][r] × Pτ[1]
```

Nuclear potential at LO

In[ ]:=
```
Clear[vc, vτ]
vc[0][r_] = 3/16 (C01 Cα[1][r] + C10 Cα[0][r]);
vτ[0][r_] = 1/16 (C01 Cα[1][r] - 3 C10 Cα[0][r]);
vσ[0][r_] = 1/16 (-3 C01 Cα[1][r] + C10 Cα[0][r]);
vστ[0][r_] = -1/16 (C01 Cα[1][r] + C10 Cα[0][r]);
vt[0][r_] = 0;
vtτ[0][r_] = 0;
vb[0][r_] = 0;
vbτ[0][r_] = 0;
vbb[0][r_] = 0;
vq[0][r_] = 0;
vqσ[0][r_] = 0;

vT[0][r_] = 0;
vσT[0][r_] = 0;
vtT[0][r_] = 0;
vbT[0][r_] = 0;
```

In[ ]:=
```
vLO[r_] = C01 Pσ[0] · Pτ[1] · CC[r] + C10 Pσ[1] · Pτ[0] · CC[r];
```

Nuclear potential at NLO

In[∘]:=
```
vc[1][r_] = vc[0][r] + C1 (-CC''[r] - 2/r CC'[r]) // Expand;
vτ[1][r_] = vτ[0][r] + C2 (-CC''[r] - 2/r CC'[r]) // Expand;
vσ[1][r_] = vσ[0][r] + C3 (-CC''[r] - 2/r CC'[r]) // Expand;
vστ[1][r_] = vστ[0][r] + C4 (-CC''[r] - 2/r CC'[r]) // Expand;
vt[1][r_] = -C5 (CC''[r] - 1/r CC'[r]) // Expand;
vtτ[1][r_] = -C6 (CC''[r] - 1/r CC'[r]) // Expand;
vb[1][r_] = -C7 1/r CC'[r] // Expand;
vbτ[1][r_] = 0;
vbb[1][r_] = 0;
vq[1][r_] = 0;
vqσ[1][r_] = 0;

vT[1][r_] = C0IT CC[r] // Expand;
vσT[1][r_] = 0;
vtT[1][r_] = 0;
vbT[1][r_] = 0;
```

Nuclear potential at N3LO

In[∘]:=

$$vc[3][r\_] = vc[1][r] + D1\left(CC''''[r] + \frac{4}{r}\,CC'''[r]\right) \,//\, Expand;$$

$$v\tau[3][r\_] = v\tau[1][r] + D2\left(CC''''[r] + \frac{4}{r}\,CC'''[r]\right) \,//\, Expand;$$

$$v\sigma[3][r\_] = v\sigma[1][r] + D3\left(CC''''[r] + \frac{4}{r}\,CC'''[r]\right) \,//\, Expand;$$

$$v\sigma\tau[3][r\_] = v\sigma\tau[1][r] + D4\left(CC''''[r] + \frac{4}{r}\,CC'''[r]\right) \,//\, Expand;$$

$$vt[3][r\_] = vt[1][r] + D5\left(CC''''[r] + \frac{1}{r}\,CC'''[r] - \frac{6}{r^2}\,CC''[r] + \frac{6}{r^3}\,CC'[r]\right) \,//\, Expand;$$

$$vt\tau[3][r\_] = vt\tau[1][r] + D6\left(CC''''[r] + \frac{1}{r}\,CC'''[r] - \frac{6}{r^2}\,CC''[r] + \frac{6}{r^3}\,CC'[r]\right) \,//\, Expand;$$

$$vb[3][r\_] = vb[1][r] + D7\left(\frac{1}{r}\,CC'''[r] + \frac{2}{r^2}\,CC''[r] - \frac{2}{r^3}\,CC'[r]\right) \,//\, Expand;$$

$$vb\tau[3][r\_] = D8\left(\frac{1}{r}\,CC'''[r] + \frac{2}{r^2}\,CC''[r] - \frac{2}{r^3}\,CC'[r]\right) \,//\, Expand;$$

$$vbb[3][r\_] = -D9\,\frac{1}{r^2}\left(CC''[r] - \frac{1}{r}\,CC'[r]\right) \,//\, Expand;$$

$$vq[3][r\_] = -D10\,\frac{1}{r^2}\left(CC''[r] - \frac{1}{r}\,CC'[r]\right) \,//\, Expand;$$

$$vq\sigma[3][r\_] = -D11\,\frac{1}{r^2}\left(CC''[r] - \frac{1}{r}\,CC'[r]\right) \,//\, Expand;$$

$$vT[3][r\_] = vT[1][r] + C1IT\left(-CC''[r] - \frac{2}{r}\,CC'[r]\right) \,//\, Expand;$$

$$v\sigma T[3][r\_] = C2IT\left(-CC''[r] - \frac{2}{r}\,CC'[r]\right) \,//\, Expand;$$

$$vtT[3][r\_] = -C3IT\left(CC''[r] - \frac{1}{r}\,CC'[r]\right) \,//\, Expand;$$

$$vbT[3][r\_] = -C4IT\,\frac{1}{r}\,CC'[r] \,//\, Expand;$$

Potential and tests

In[∘]:=

```
vrop[iop_][order_][r_] :=
  {vc, vτ, vσ, vστ, vt, vtτ, vb, vbτ, vbb, vq, vqσ, vT, vσT, vtT, vbT}[[iop]][order][r]
```

In[∘]:=

```
V[l_, lp_, s_, j_][order_][r_] := Sum[Op[i][l, lp, s, j]·vrop[i][order][r], {i, 15}] // Expand
```

Matrix element of the potential

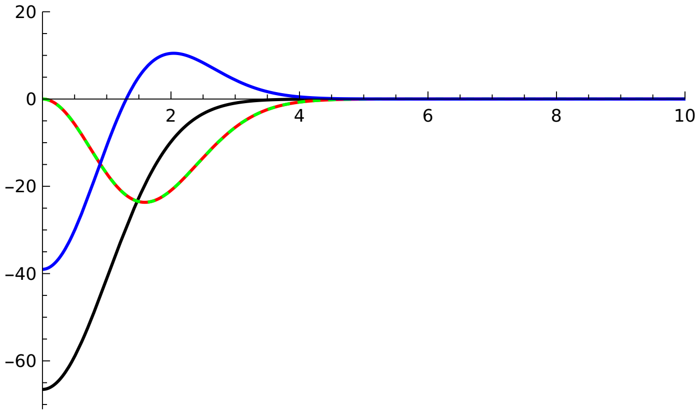
```
In[∘]:= BRAJ[j_, jz_, l_, s_, t_, tz_] := ⟨j_ĵ, jz_Ĵz| · ⟨l_L̂, s_Ŝ| · ⟨t_T̂, tz_T̂z|
        KETJ[j_, jz_, l_, s_, t_, tz_] := |j_ĵ, jz_Ĵz⟩ · |l_L̂, s_Ŝ⟩ · |t_T̂, tz_T̂z⟩

        VM[j_, jz_, lp_, l_, s_, t_, tz_][order_][r_] :=
         BRAJ[j, jz, lp, s, t, tz] · V[l, lp, s, j][order][r] · KETJ[j, jz, l, s, t, tz] // Simplify

In[∘]:= Op[5][l_, lp_, s_, j_] = S12[l, lp, s, j];
        Op[6][l_, lp_, s_, j_] = S12[l, lp, s, j] · τ1τ2 // Expand;
```

Deuteron potential

```
In[∘]:= V10[0, 0][r_] = ħc VM[1, 1, 0, 0, 1, 0, 0][3][r] /. R[0] → R // Simplify;
        V10[0, 2][r_] = ħc VM[1, 1, 0, 2, 1, 0, 0][3][r] /. R[0] → R // Simplify;
        V10[2, 0][r_] = ħc VM[1, 1, 2, 0, 1, 0, 0][3][r] /. R[0] → R // Simplify;
        V10[2, 2][r_] = ħc VM[1, 1, 2, 2, 1, 0, 0][3][r] /. R[0] → R // Simplify;
```

In[ ]:=
```
C01 = -0.512268575 × 10;
C10 = -0.569749961 × 10;
C1 = -0.953469705;
C2 = 0.475392426;
C3 = 0.399019793;
C4 = -0.535686282;
C5 = -0.324751963;
C6 = -0.648172781;
C7 = -0.134307736 × 10;
D1 = 0.376343898 × 10^-1;
D2 = 0.185768643 × 10^-1;
D3 = 0.208685298 × 10^-1;
D4 = 0.104907424 × 10^-1;
D5 = 0.782433560 × 10^-2;
D6 = 0.189873465 × 10^-1;
D7 = -0.222332010 × 10^-1;
D8 = -0.146786284 × 10^-1;
D9 = 0.226506657 × 10^-1;
D10 = 0.218482111 × 10^-1;
D11 = 0.936405658 × 10^-2;
C0IT = 0.713292586 × 10^-2;
C1IT = -0.113805789 × 10^-1;
C2IT = -0.126174063 × 10^-1;
C3IT = 0.374105167 × 10^-3;
C4IT = 0.298742271 × 10^-1;

R = 1.54592984;
ħc = 197.32697;

Plot[{V10[0, 0][r], V10[0, 2][r], V10[2, 0][r], V10[2, 2][r]}, {r, 0, 10},
 PlotRange → {{0, 10}, {All, 20}}, PlotStyle → {Black, Red, {Green, Dashed}, Blue}]

Export["Deuteron_nuclear_potential_generated_using_Dirac_notation.dat",
 Table[{r, V10[0, 0][r], V10[0, 2][r], V10[2, 0][r], V10[2, 2][r]}, {r, 0, 10, 0.01}]]

Clear[R, C01, C10, C1, C2, C3, C4, C5, C6, C7, D1, D2, D3,
 D4, D5, D6, D7, D8, D9, D10, D11, C0IT, C1IT, C2IT, C3IT, C4IT, ħc]
```

Out[ ]=



Out[ ]=

```
Deuteron_nuclear_potential_generated_using_Dirac_notation.dat
```

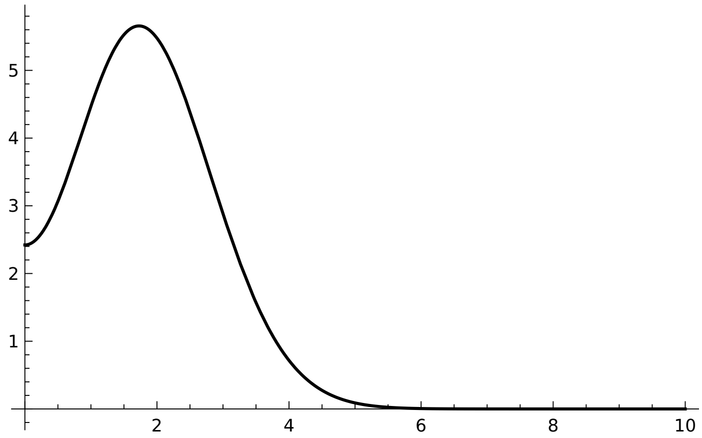
3P1 potential

In[ ]:=

```
V11[r_] = ħc VM[1, 1, 1, 1, 1, 1, 0][3][r] /. R[1] → R // Simplify;
```

In[ ]:=
```
C01 = -0.512268575 × 10;
C10 = -0.569749961 × 10;
C1 = -0.953469705;
C2 = 0.475392426;
C3 = 0.399019793;
C4 = -0.535686282;
C5 = -0.324751963;
C6 = -0.648172781;
C7 = -0.134307736 × 10;
D1 = 0.376343898 × 10^-1;
D2 = 0.185768643 × 10^-1;
D3 = 0.208685298 × 10^-1;
D4 = 0.104907424 × 10^-1;
D5 = 0.782433560 × 10^-2;
D6 = 0.189873465 × 10^-1;
D7 = -0.222332010 × 10^-1;
D8 = -0.146786284 × 10^-1;
D9 = 0.226506657 × 10^-1;
D10 = 0.218482111 × 10^-1;
D11 = 0.936405658 × 10^-2;
C0IT = 0.713292586 × 10^-2;
C1IT = -0.113805789 × 10^-1;
C2IT = -0.126174063 × 10^-1;
C3IT = 0.374105167 × 10^-3;
C4IT = 0.298742271 × 10^-1;

R = 1.83039397;
ℏc = 197.32697;

Plot[V11[r], {r, 0, 10}, PlotRange → All, PlotStyle → Black]

Export["3P1_nuclear_potential_generated_using_Dirac_notation.dat",
 Table[{r, V11[r]}, {r, 0, 10, 0.01}]]

Clear[R, C01, C10, C1, C2, C3, C4, C5, C6, C7, D1, D2, D3,
 D4, D5, D6, D7, D8, D9, D10, D11, C0IT, C1IT, C2IT, C3IT, C4IT, ℏc]
```

Out[ ]=



Out[ ]=

3P1_nuclear_potential_generated_using_Dirac_notation.dat