Spin: (2, 2)  $\rightarrow$  1, 1  $\rightarrow$  0,  $\vec{r}_{12} = [0.0, 0.0, 1.92]$ . Exc. frac: 0.97 0.3 data | fit ptl1, e ptl1, f1 0.2 ptl1, f0 ptl1, g  $Tr(\rho)$ Analytic 0.1 0.0 12 12 3 6 9 3 6 9 0 tΓı tΓı  $2.0 \times 10^{-5}$ data - fit  $1.0 \times 10^{-5}$ ef1 + f1eef1 - f1e f1f0 + f0f1f1f0 - f0f1 f0g + gf0• f0g - gf0  $-1.0 \times 10^{-5}$   $-2.0 \times 10^{-5}$ ge + eg ge - eg 12 6 9 12 3 6 9 0

1.00

0.75

0.50

0.25

0.00

0.20

0.15

0.10

0.05

0.00

0

3

 $+\Gamma$ 

0