

Radical Pair Model for Magnetic Field Effects on NMDA Receptor Activity

Supplementary Information

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A. Magnesium Isotope Effect

We performed calculations of FSF for the RPs with the spinful and spinless isotopes taken separately to understand the potential effects of the spin on the behaviour of the system.

Ser Pathway

Fig.I shows the quantity S for the radical pair with the serine oxyradical plotted against the reaction rate, k , and relaxation rate, r . Both calculations consider the contribution from the nucleus of Serine oxyradical that has the highest HFCC, . Fig.Ia shows the behaviour when the calculations consider the spinless isotopes, ^{24}Mg and ^{26}Mg . Fig.Ib shows the case where the HFI contribution from the spinful isotope, ^{25}Mg , is considered. We find that higher values of S are found when only the spinful isotope is considered for the calculation.

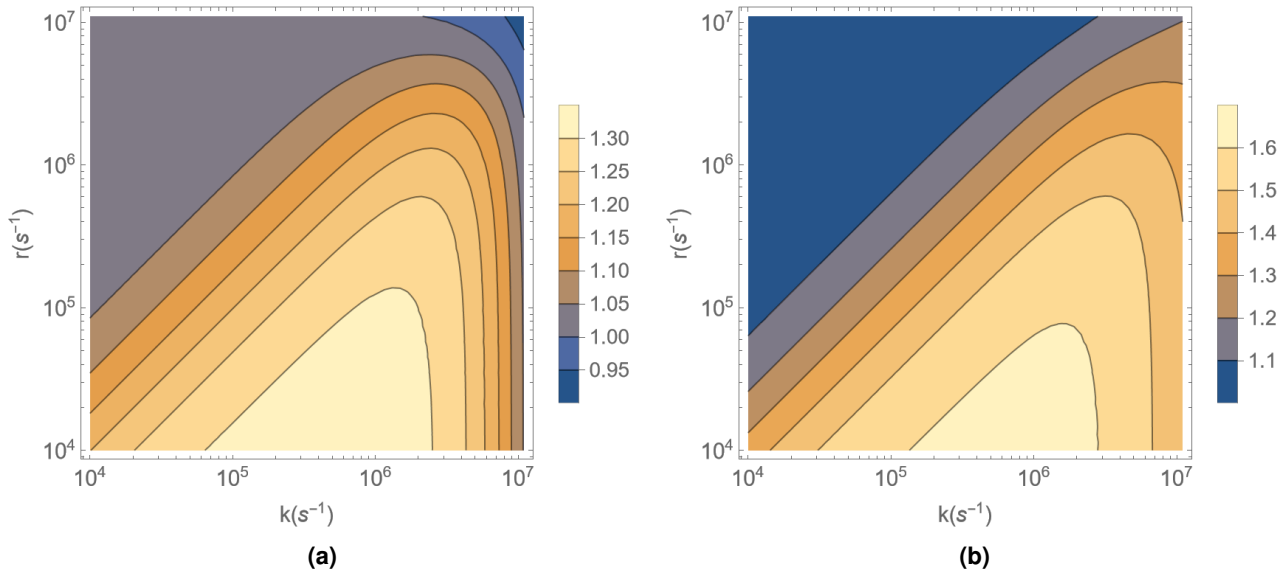


Figure I. Ratio of the fractional singlet yield percentages, S plotted against $k(\text{s}^{-1})$ and $r(\text{s}^{-1})$ for Ser radical case: (a) System containing only ^{24}Mg and ^{26}Mg isotopes is considered; (b) System containing ^{25}Mg isotope with the HFCC, $a_B = -11.22$ mT has been considered.

An example of the variation of fractional singlet yield percentage with magnetic field strength from 0.15 mT to 100 mT for a choice of k and r from the feasible region is given in Figs. IIa and IIb. We choose $k = 2 \times 10^6 \text{ s}^{-1}$ and $r = 3 \times 10^5 \text{ s}^{-1}$ for the

same. We find that the behaviour of the system is significantly different between the spinless and spinful cases. The singlet yield at low field are substantially lower for the spinful case. There are sudden spikes in the value at certain MF strengths, as well, which can be associated with the eigenenergies of certain states crossing over.

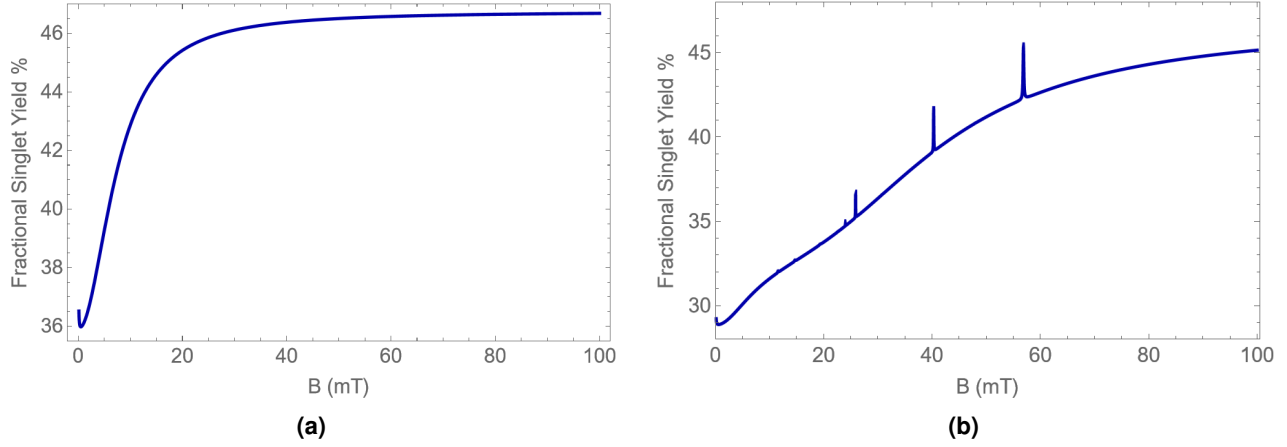


Figure II. Variation of the fractional singlet yield percentage with magnetic field strength ranging from 0.15 mT to 100 mT for the Tyr Pathway. The figure is plotted for the choice of $k = 2 \times 10^6 \text{ s}^{-1}$ and $r = 3 \times 10^5 \text{ s}^{-1}$: (a) System containing only ^{24}Mg and ^{26}Mg isotopes is considered; (b) System containing ^{25}Mg isotope with the HFCC, $a_B = -11.22 \text{ mT}$ has been considered.

Tyr Pathway

Similar plots of the quantity S as in the previous section were plotted for the radical pair involving the tyrosine oxyradical in Fig. III. We consider the HFCC contribution from the hydrogen nucleus of the Tyrosine radical having the highest HFCC, $a_A = 1.86 \text{ mT}$, for all the plots.

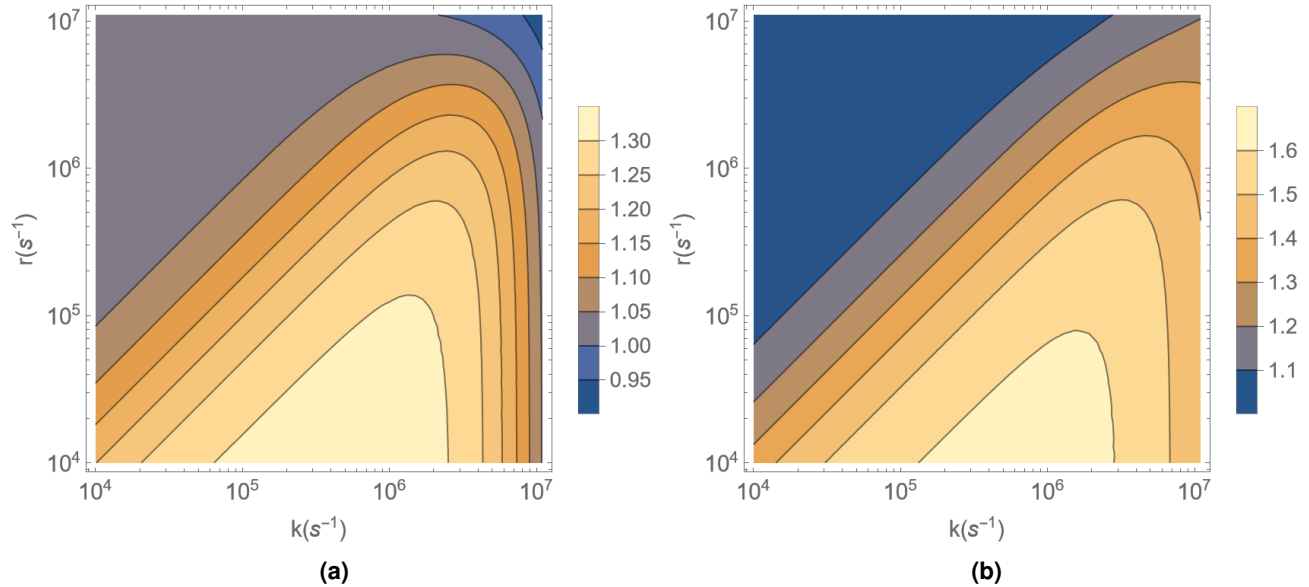


Figure III. Ratio of the fractional singlet yield percentages, S plotted against $k(\text{s}^{-1})$ and $r(\text{s}^{-1})$ for Tyr radical case: (a) System containing only ^{24}Mg and ^{26}Mg isotopes is considered; (b) System containing ^{25}Mg isotope with the HFCC, $a_B = -11.22 \text{ mT}$ has been considered.

Figs. IVa and IVb show examples of the variation of fractional singlet yield percentage with magnetic field strength from 0.15 mT to 100 mT for the choice of $k = 2 \times 10^6 \text{ s}^{-1}$ and $r = 2 \times 10^5 \text{ s}^{-1}$ which fall in the range of possible values of k and r .

The differences that one observes between the spinful and spinless isotopes for this case are similar to those for the Ser pathway.

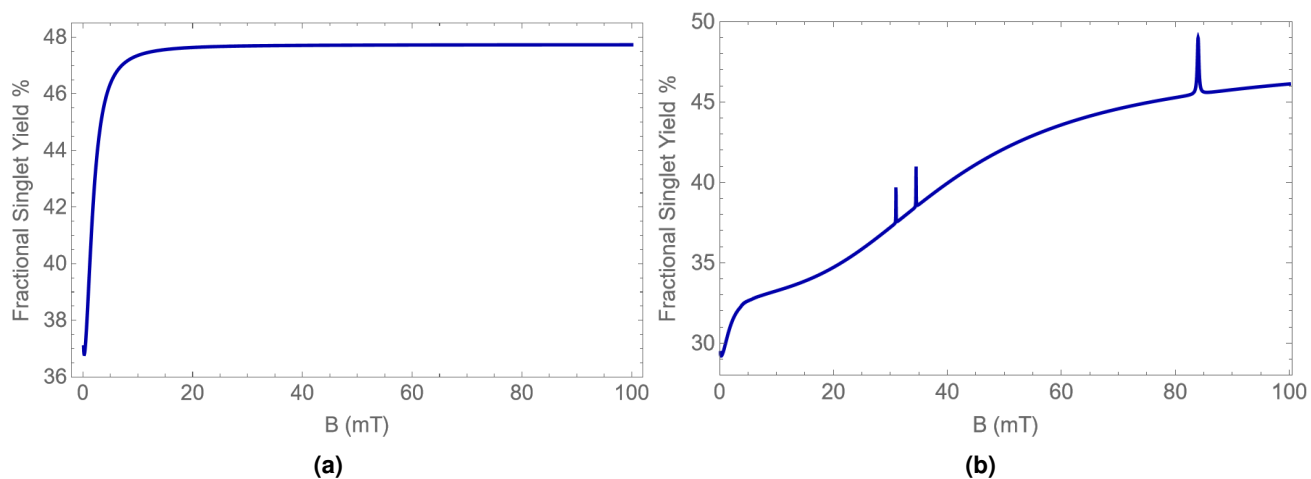


Figure IV. Variation of the fractional singlet yield percentage with magnetic field strength ranging from 0.15 mT to 100 mT for the Tyr Pathway. The figure is plotted for the choice of $k = 2 \times 10^6 \text{ s}^{-1}$ and $r = 2 \times 10^5 \text{ s}^{-1}$: (a) System containing only ^{24}Mg and ^{26}Mg isotopes is considered; (b) System containing ^{25}Mg isotope with the HFCC, $a_B = -11.22$ mT has been considered.

B. Isotope Contributions at Low Field

We plot examples in Fig.V from both the Ser and Tyr pathway by considering the contribution from the spinless and spinful isotopes separately to understand the contribution of the same to the drop in FSY at MF strength close to 0 mT. We find that the drop in FSY values occur with or without the contribution from the ^{25}Mg isotope.

C. HFCCs of Other Nuclei

For the calculations in this paper, we consider only the HFI contribution of the nuclei of the oxyradical with the highest HFCC. This is a common approximation that is used in such calculations for the sake of simplicity.

The next highest HFCC of a nucleus in the Serine oxyradical was 5.73 mT. Similarly, in the case of the Tyrosine oxyradical, the next highest HFCCs were -0.64 mT and -0.53 mT.

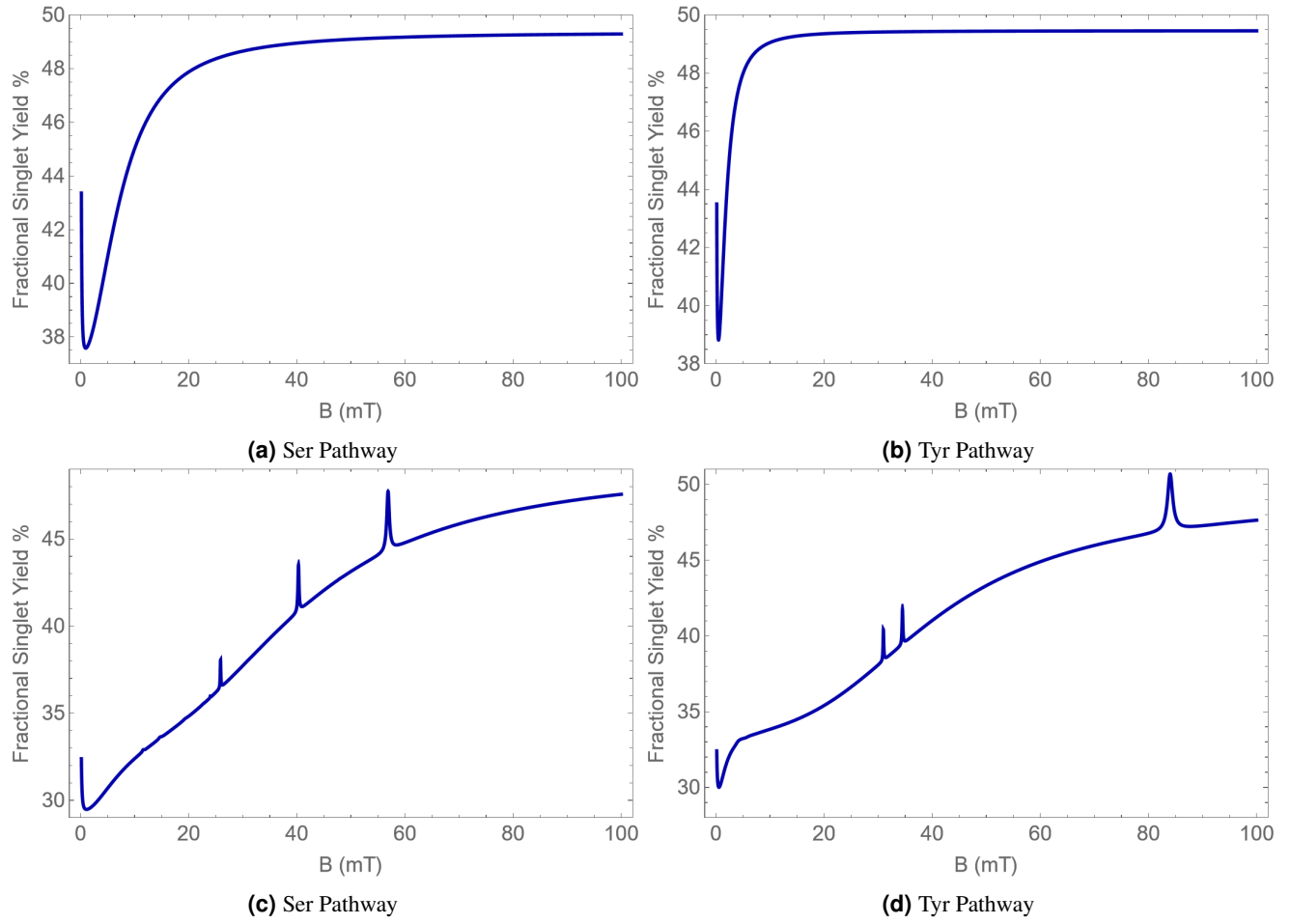


Figure V. Variation of the FSY percentage with magnetic field strength ranging from 0.15 mT to 100 mT plotted with $k = 7.5 \times 10^6 \text{ s}^{-1}$ and $r = 2 \times 10^5 \text{ s}^{-1}$. (a) and (b) are plotted considering a system with only ^{24}Mg and ^{26}Mg isotopes; (c) and (d) are plotted considering system with only ^{25}Mg isotope at its natural abundance of 10%. The HFI contribution from the same is $a_B = -11.22 \text{ mT}$.