

LECTURE 3

Coherence

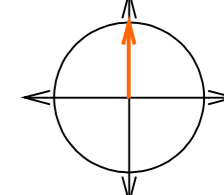
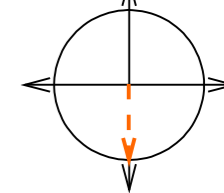
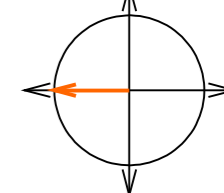
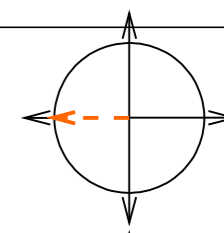
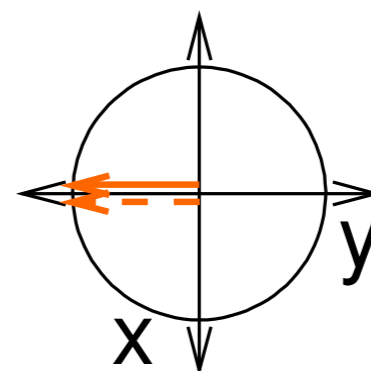
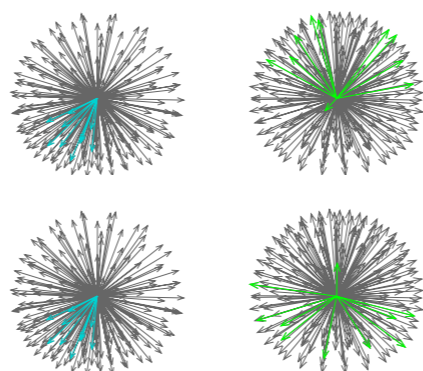
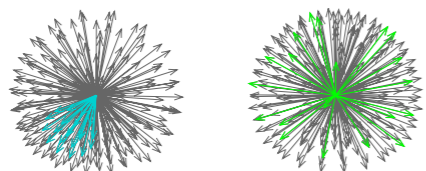
depicted as distributions
molecules with $\vec{\mu}$ of ^1H
closest to $-y$ selected

decomposed distributions
based on $\vec{\mu}$ of $^{13}\text{C}/^{15}\text{N}$
being closer to $+z$ vs. to $-z$
in the selected molecules

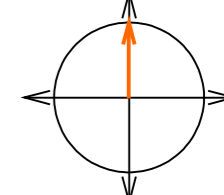
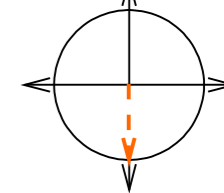
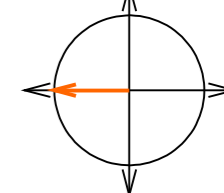
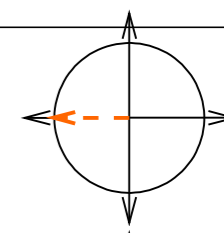
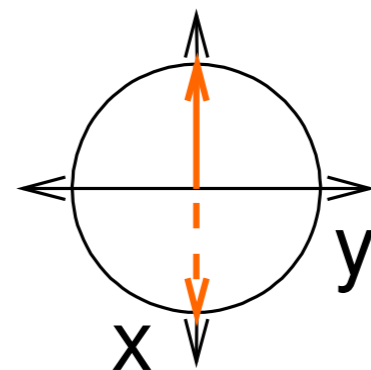
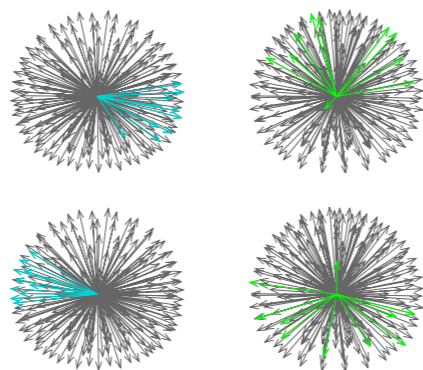
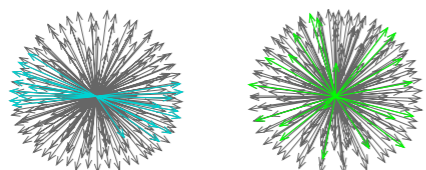
depicted as arrows

decomposed arrows

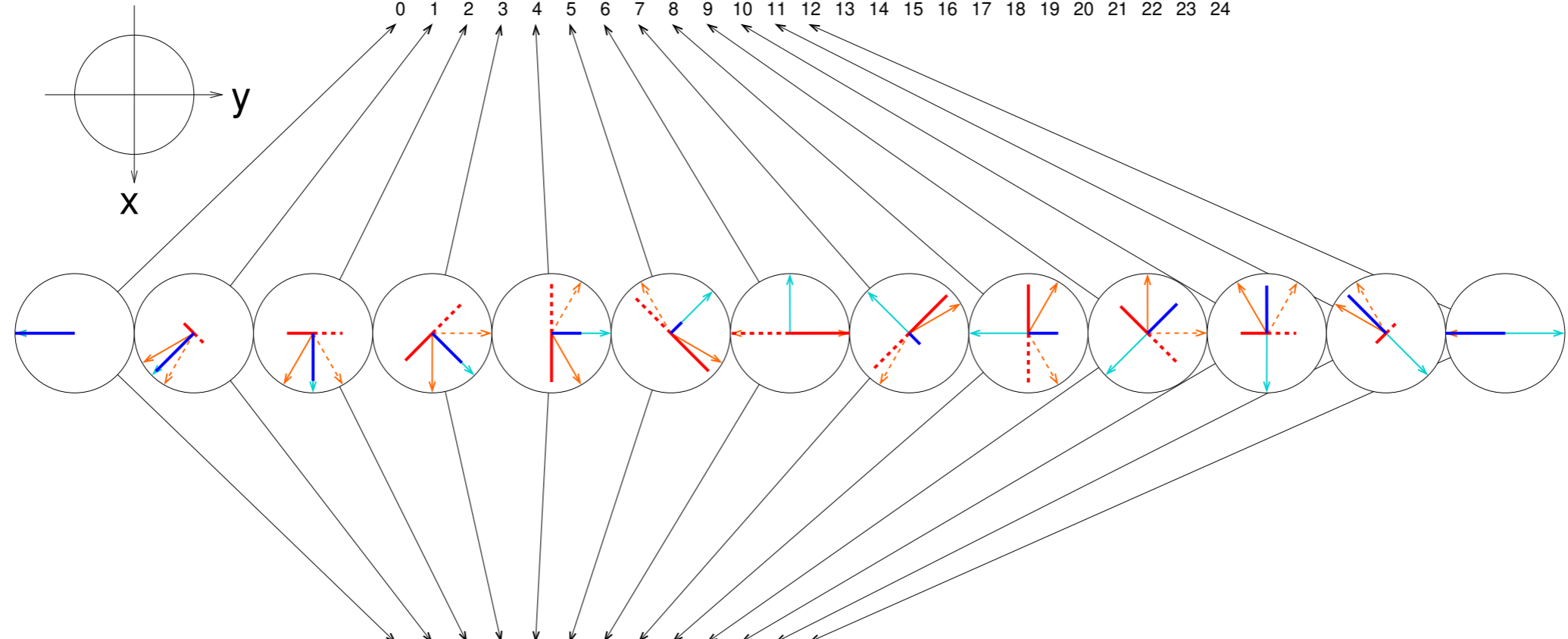
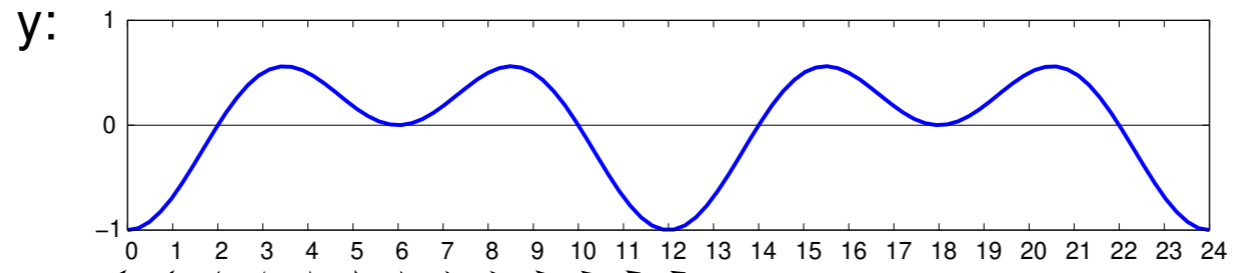
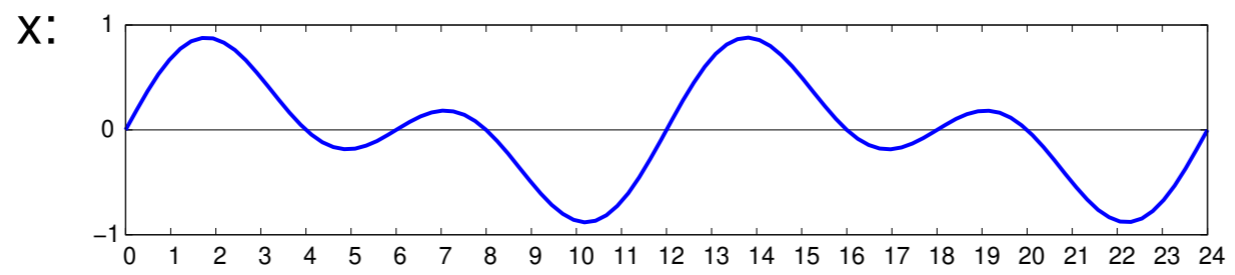
In-phase



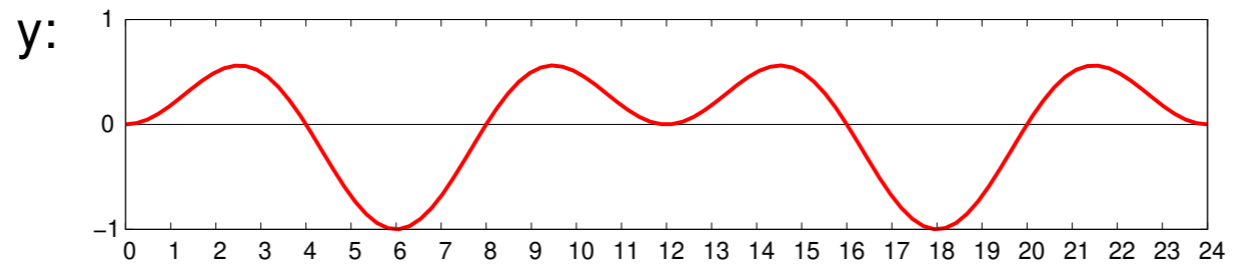
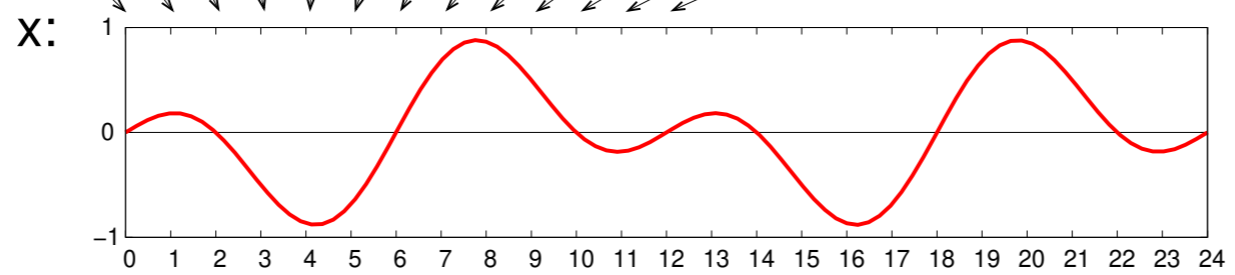
Anti-phase



In-phase:

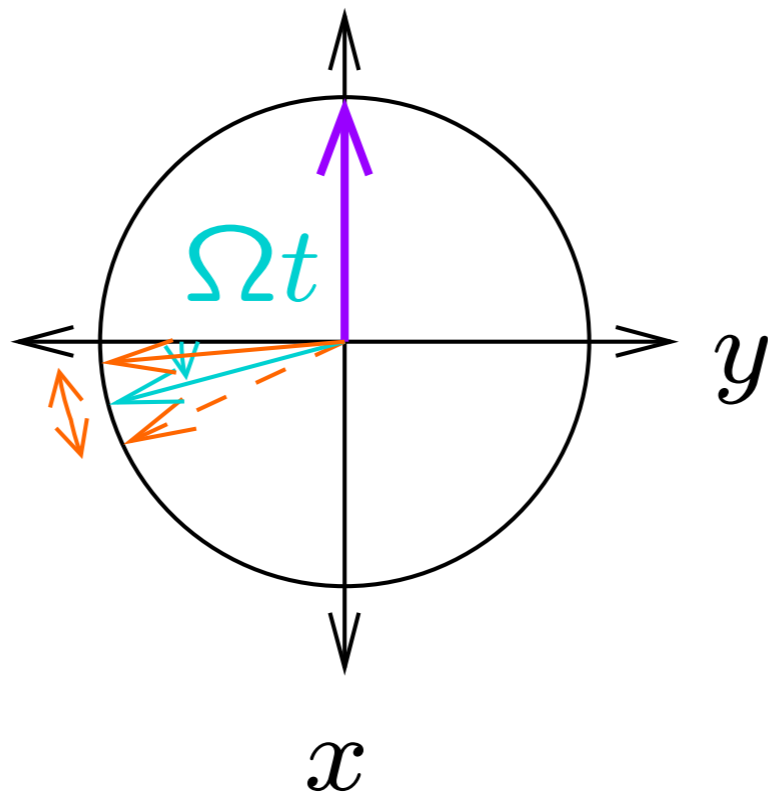


Anti-phase:

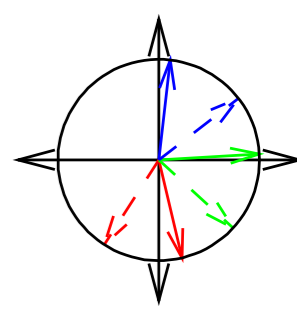
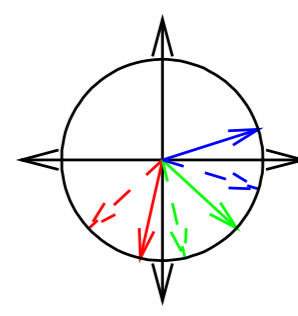
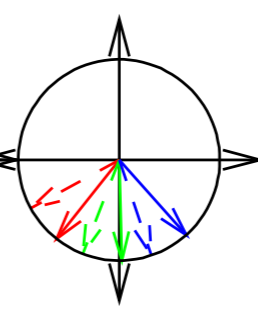
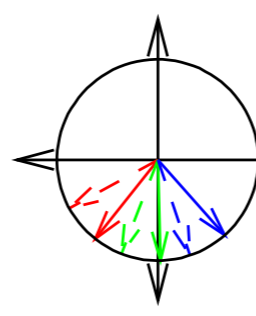
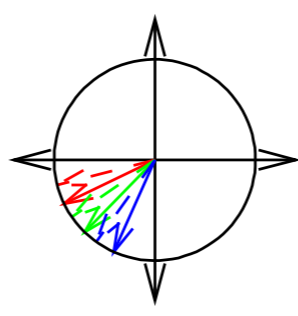
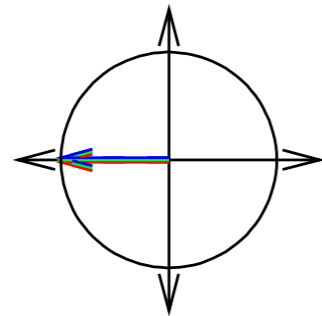
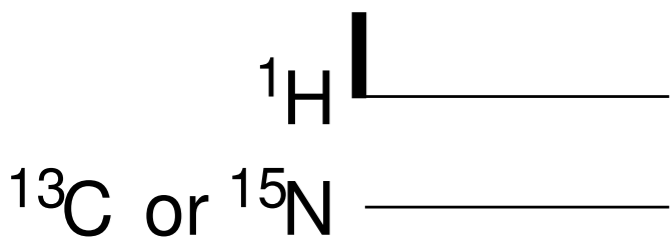


$t > 0$

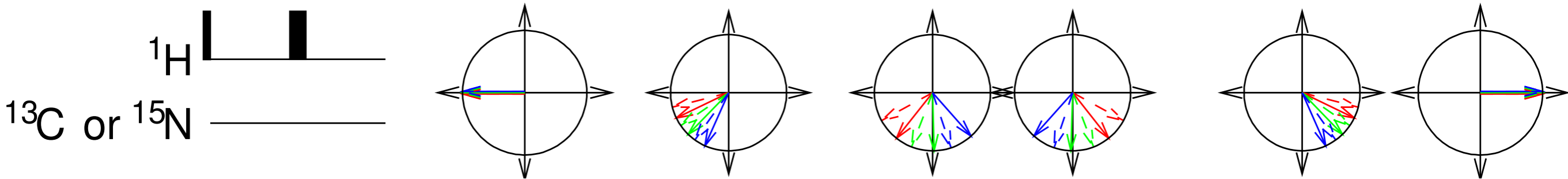
$\pm \pi J t$



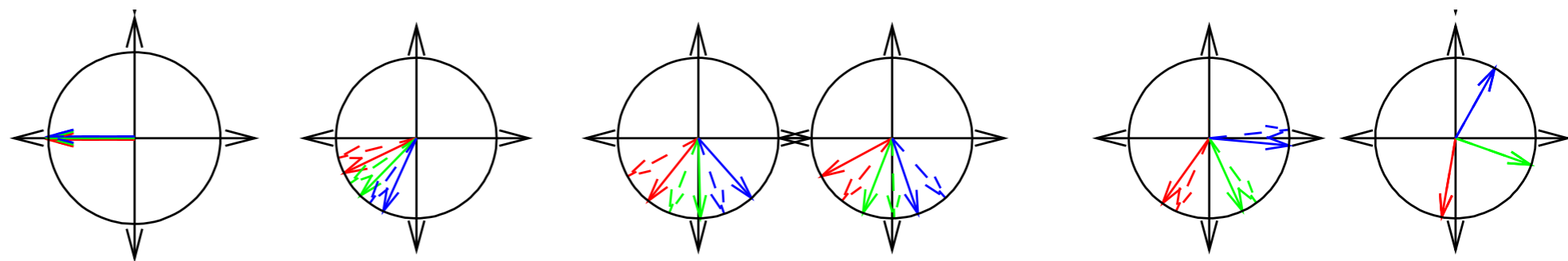
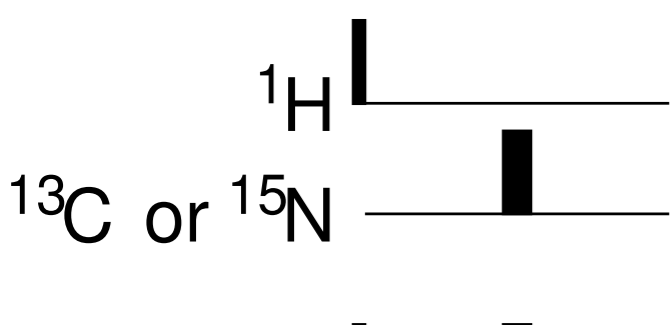
Free coherence evolution



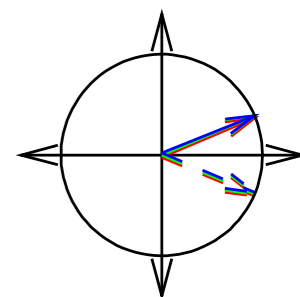
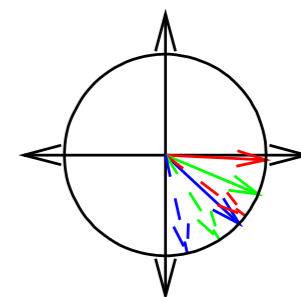
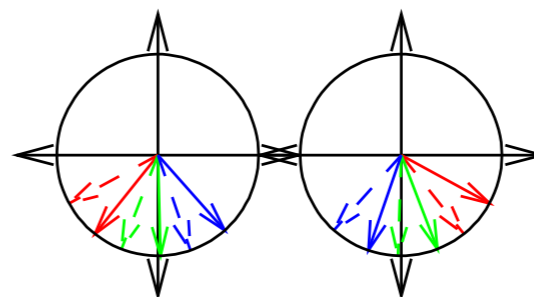
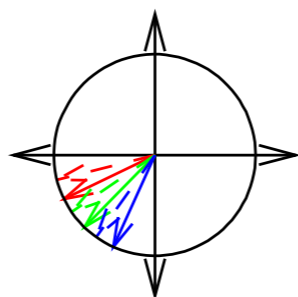
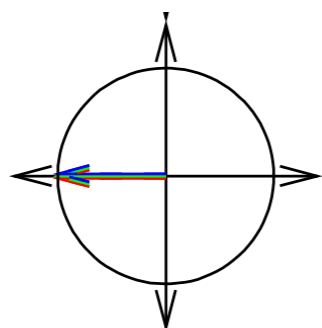
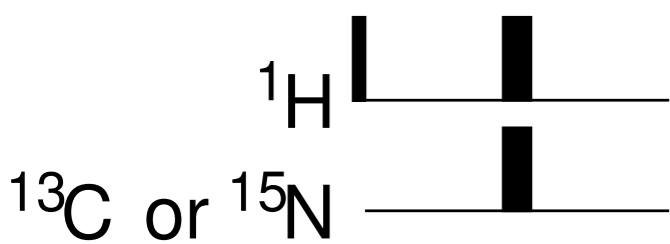
Refocusing spin echo



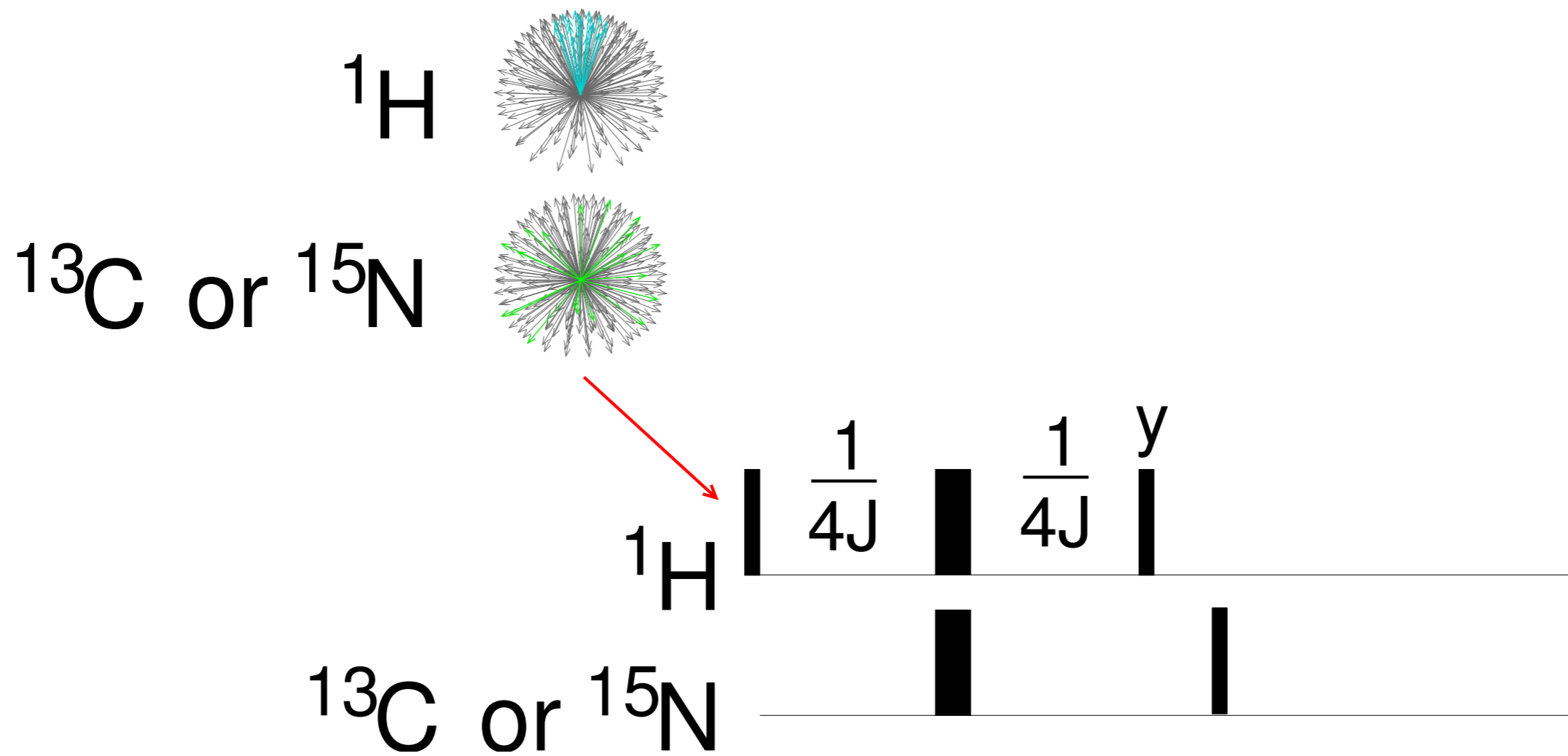
Decoupling spin echo



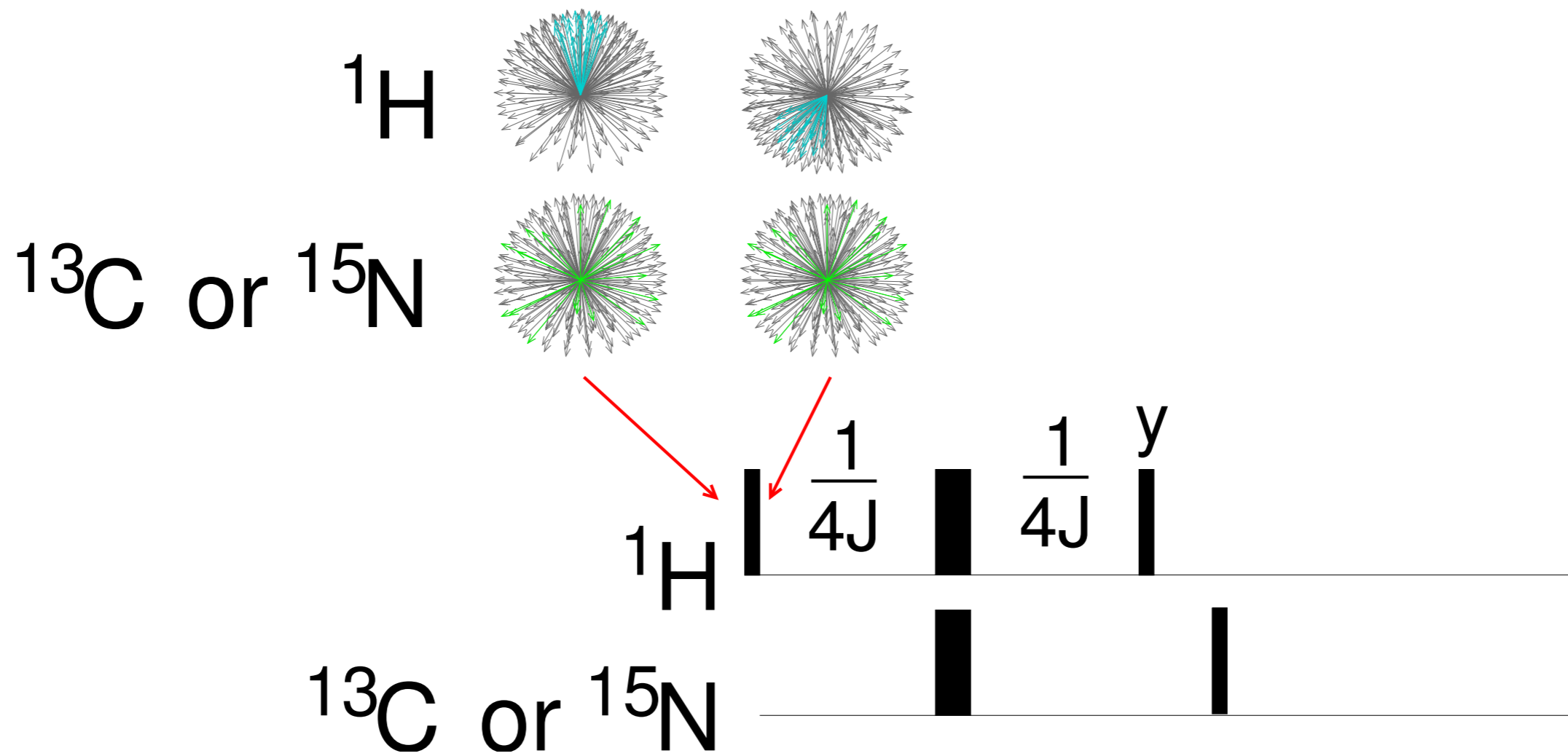
Simultaneous spin echo



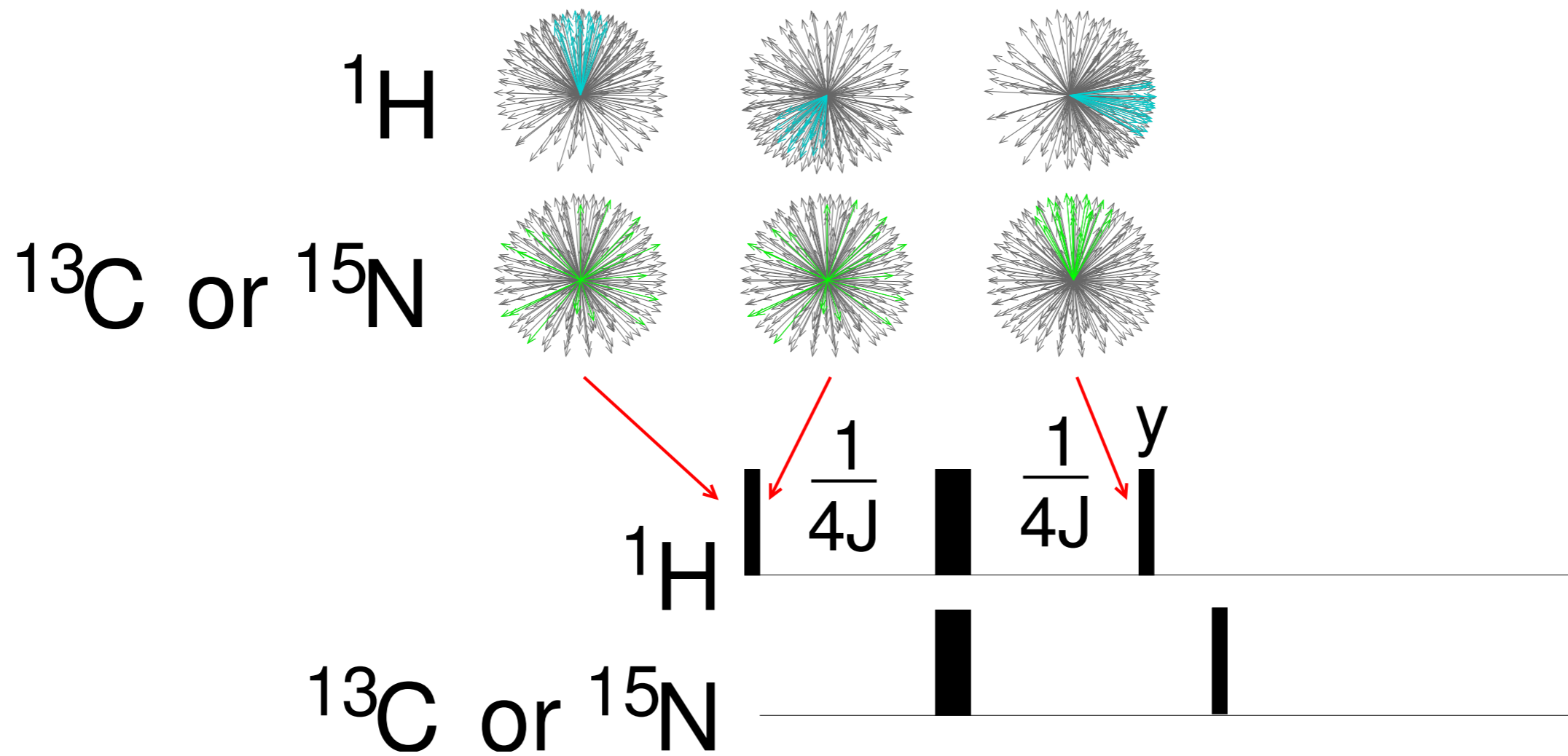
INEPT



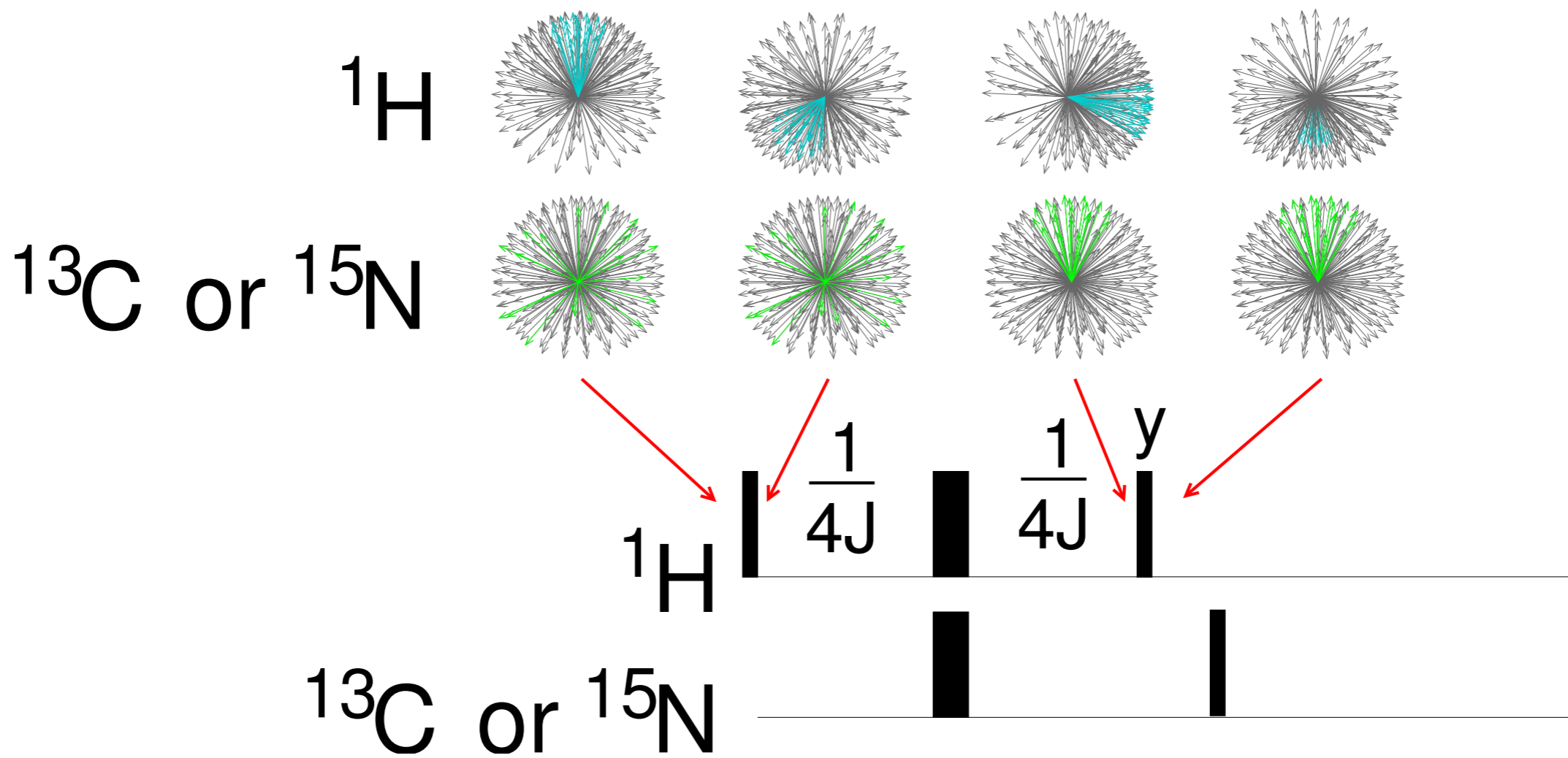
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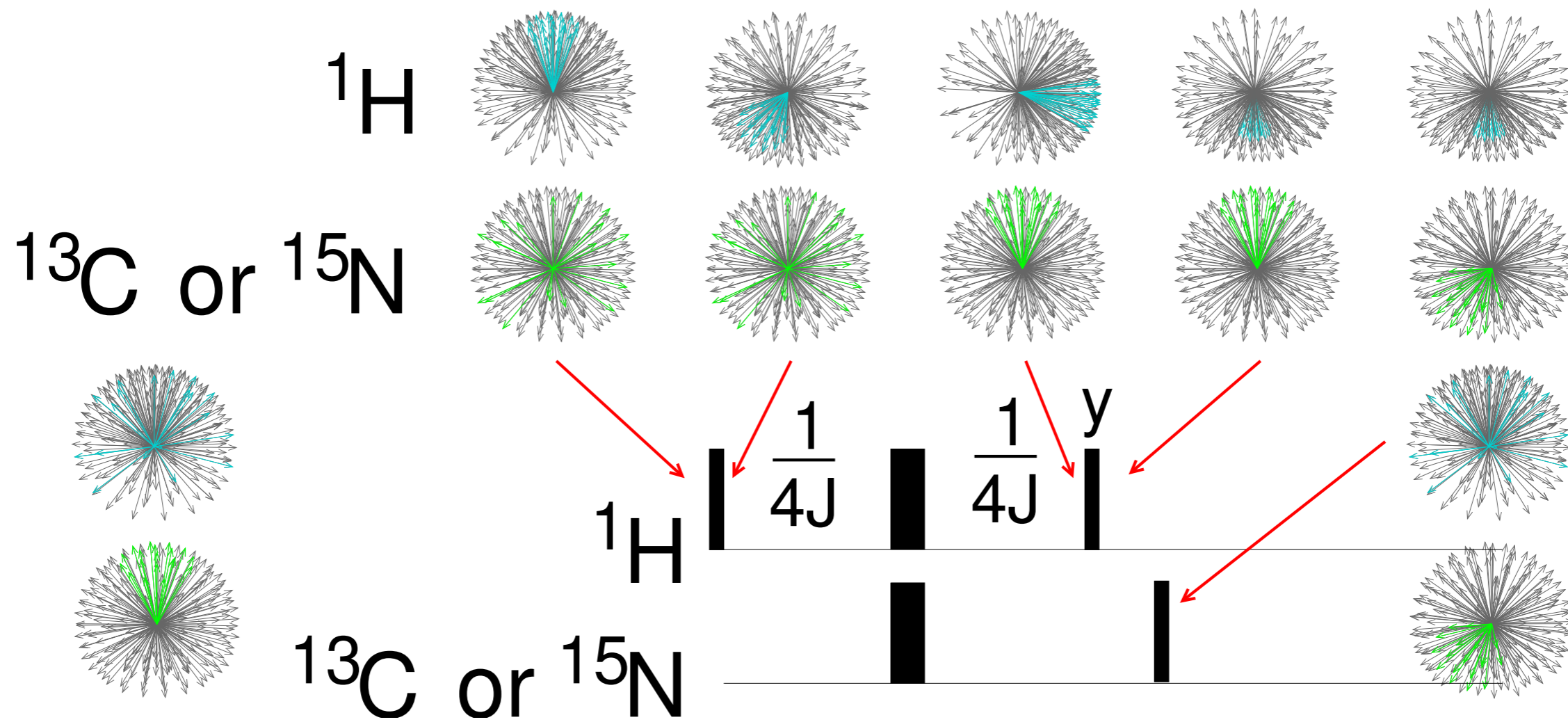
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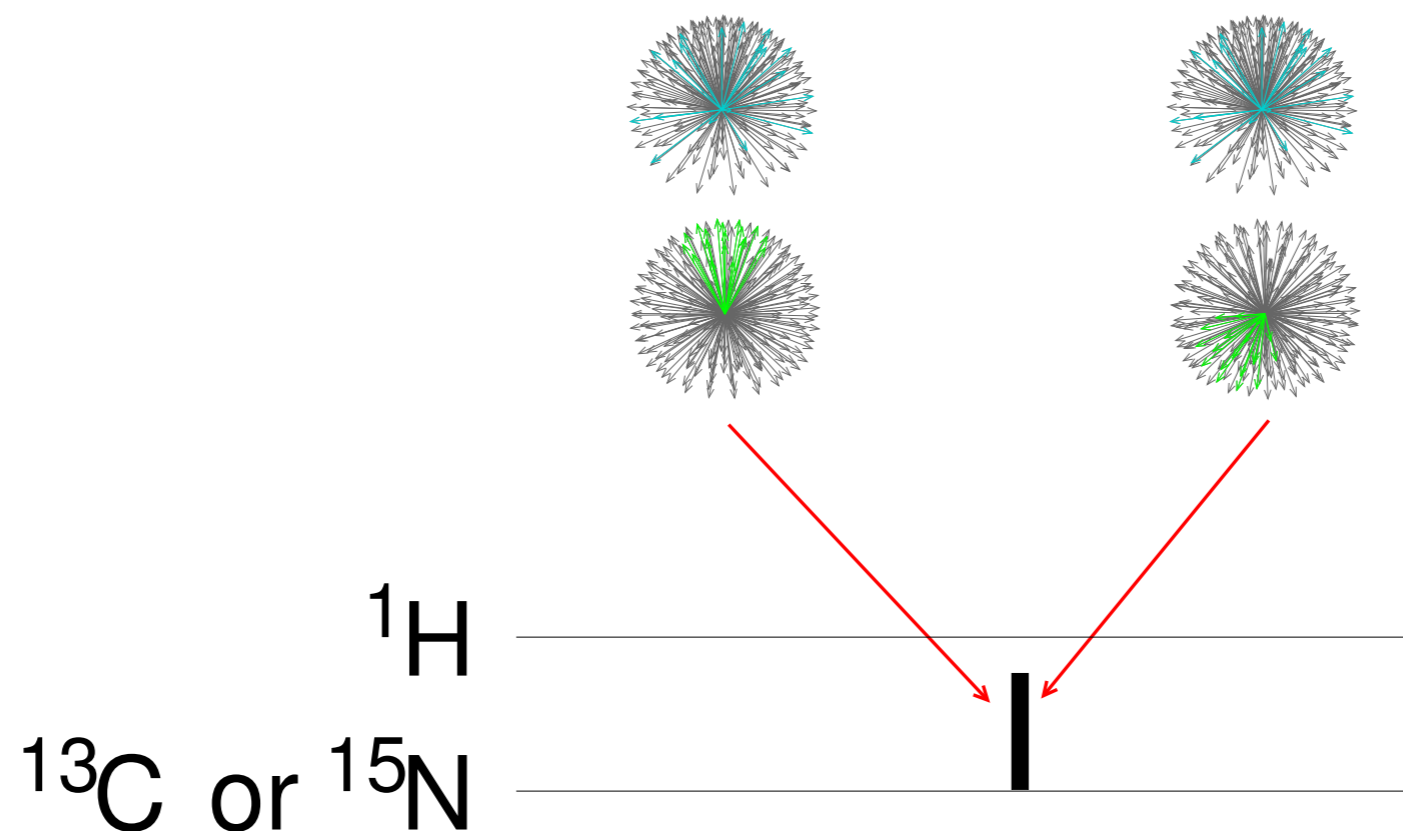
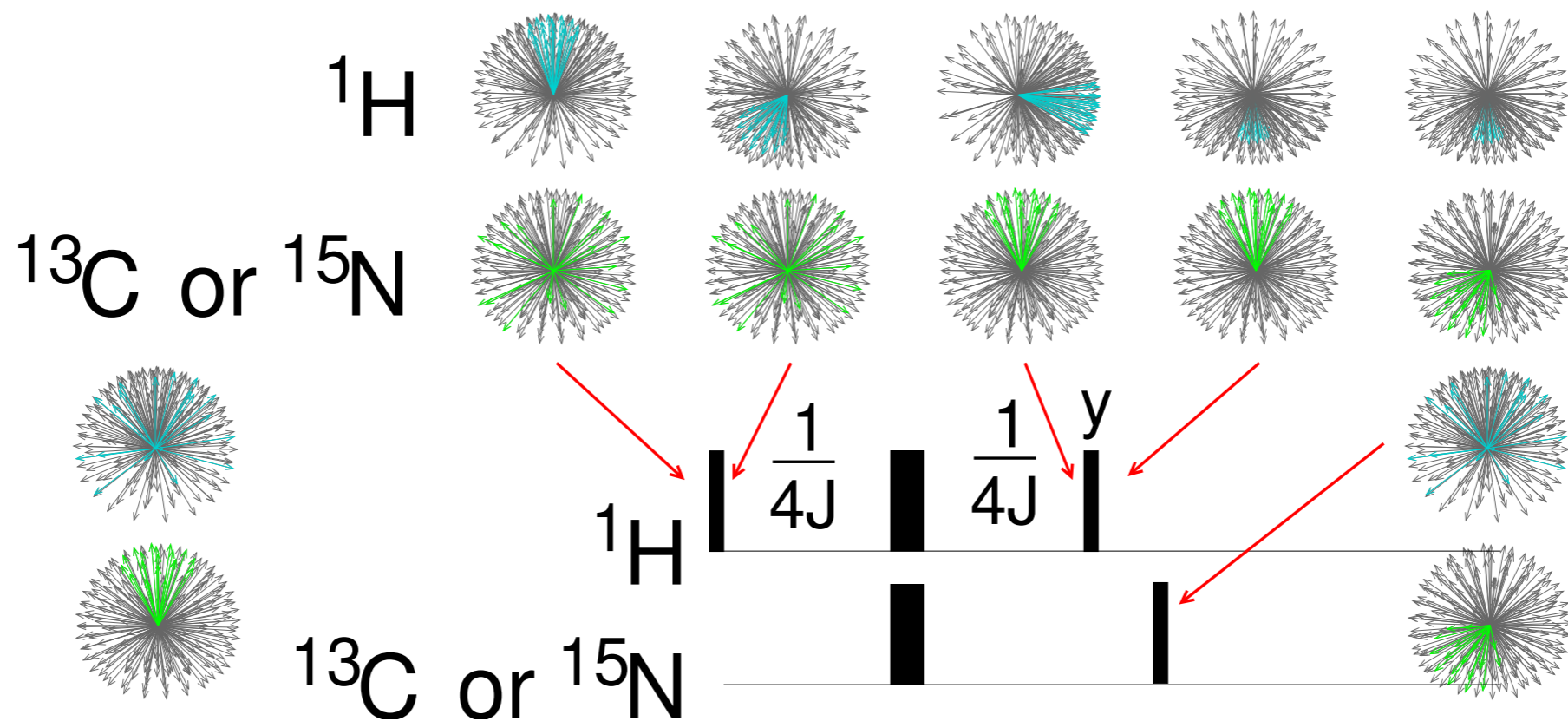
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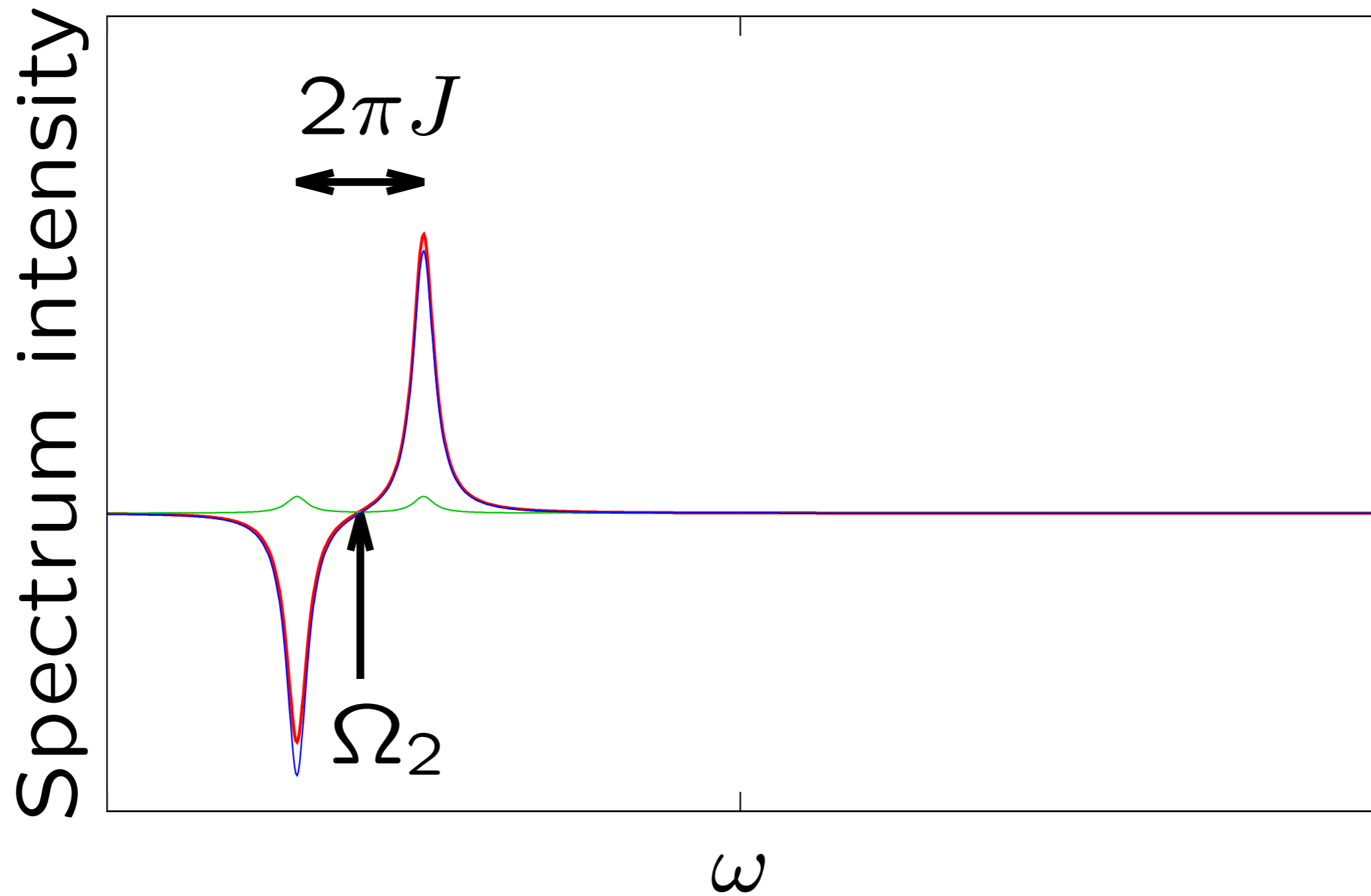
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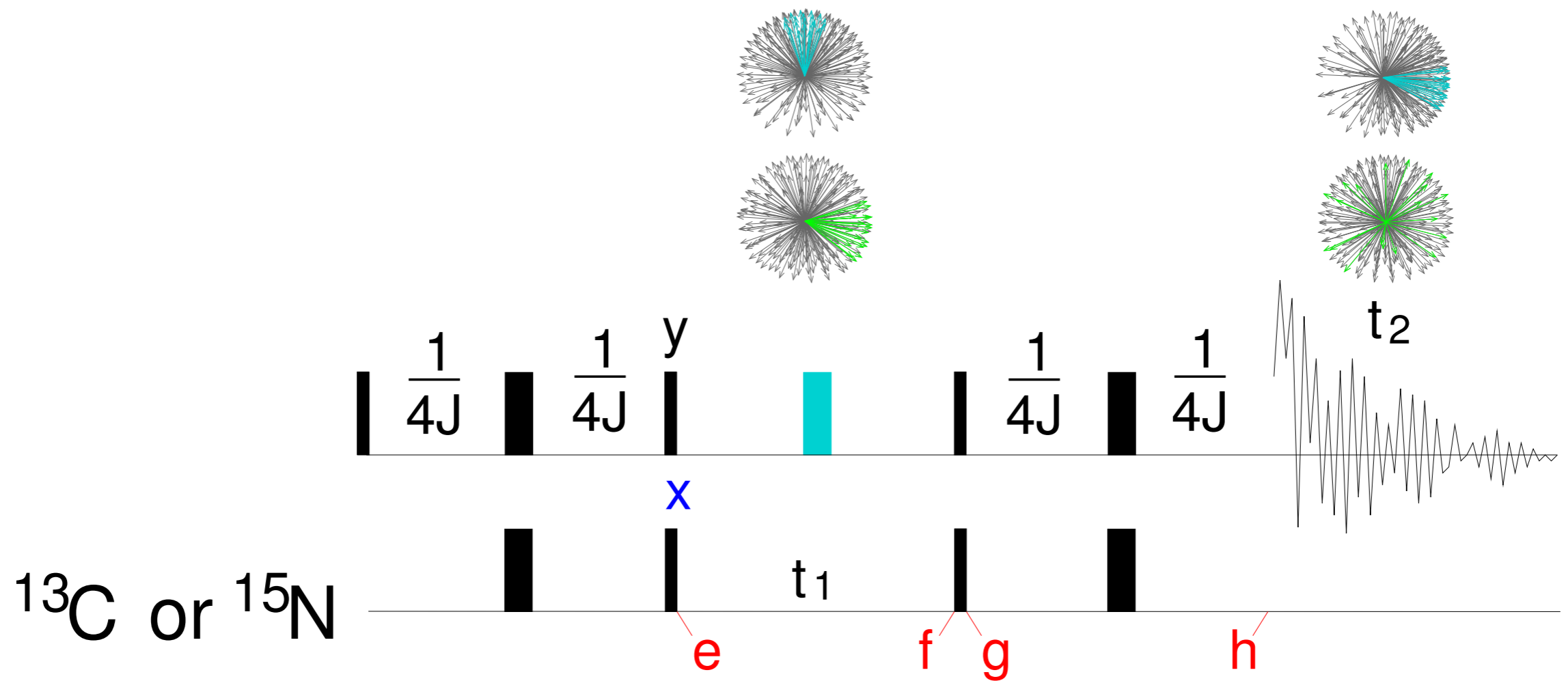
INEPT vs. direct excitation



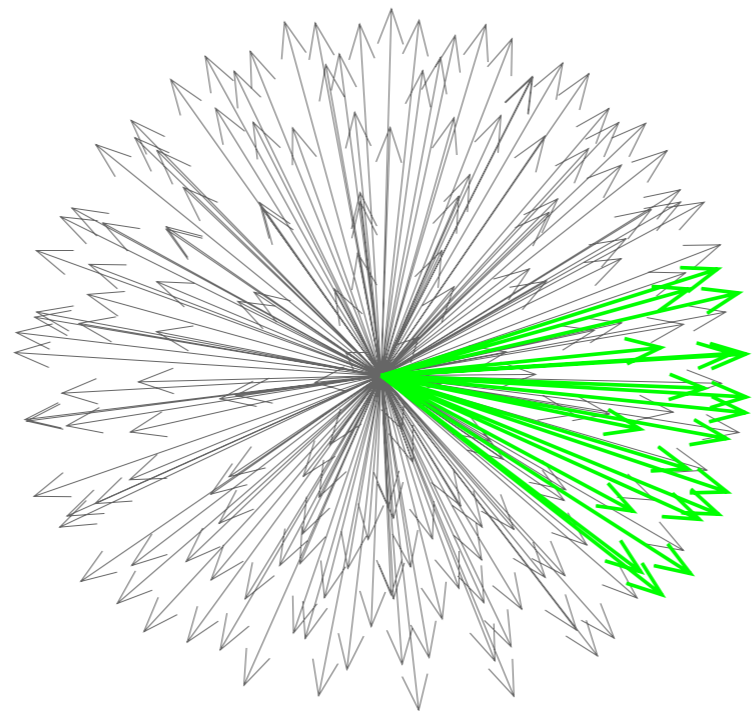
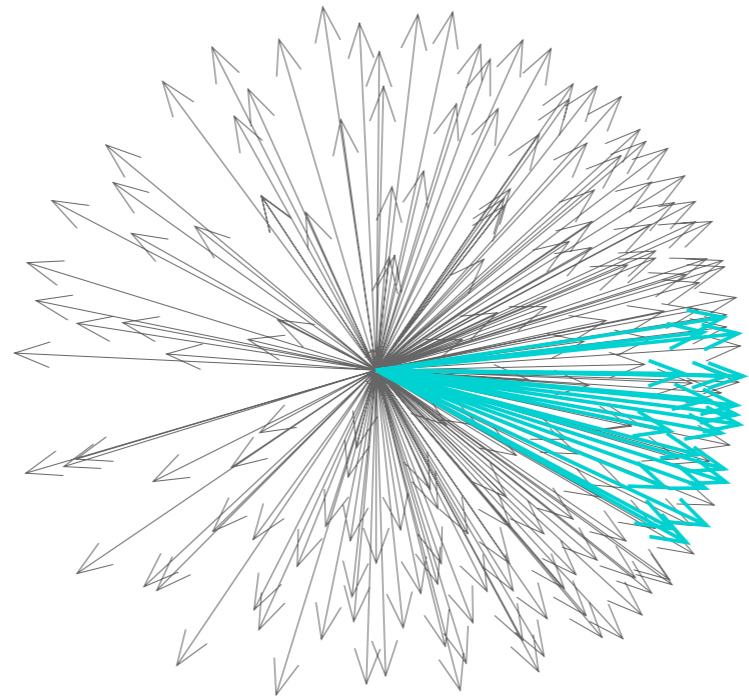
INEPT vs. direct excitation:



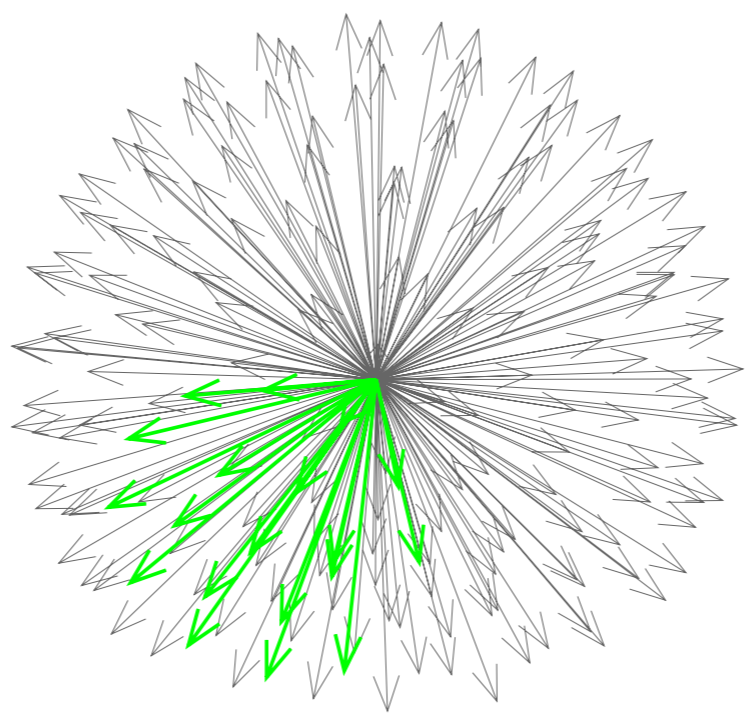
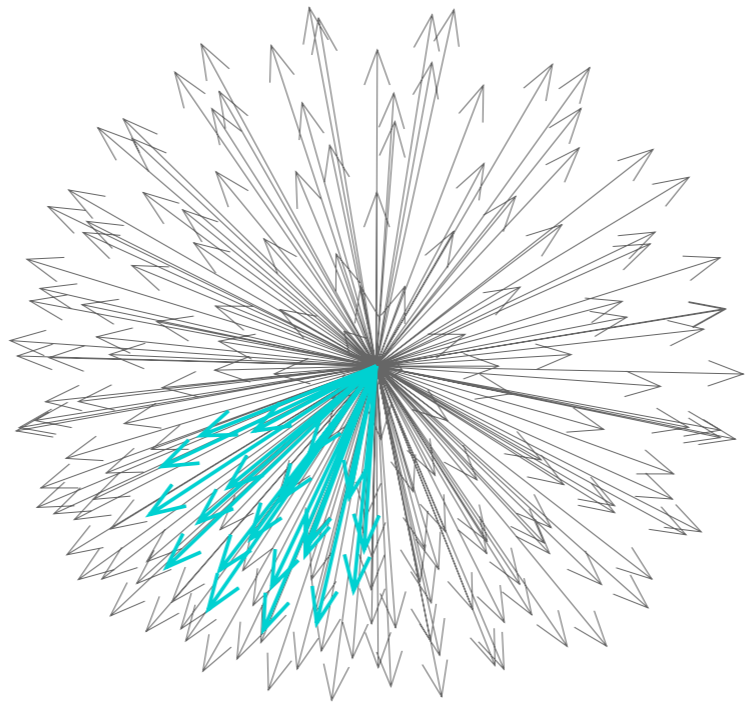
HSQC Spectroscopy



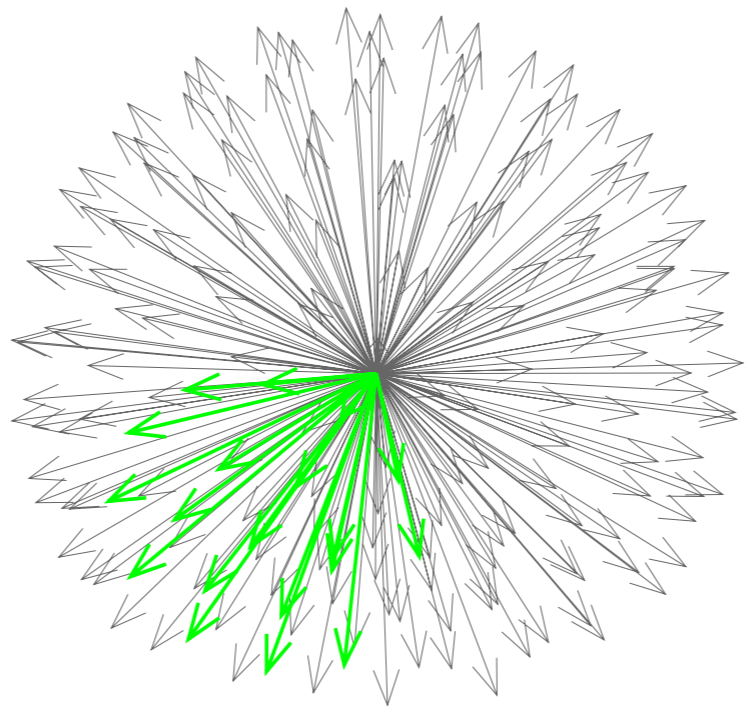
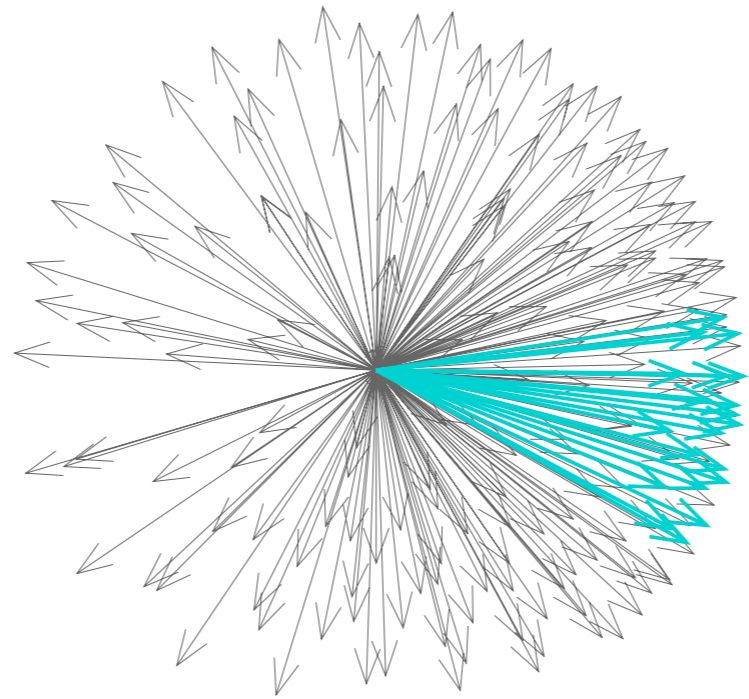
Multiple quantum coherences



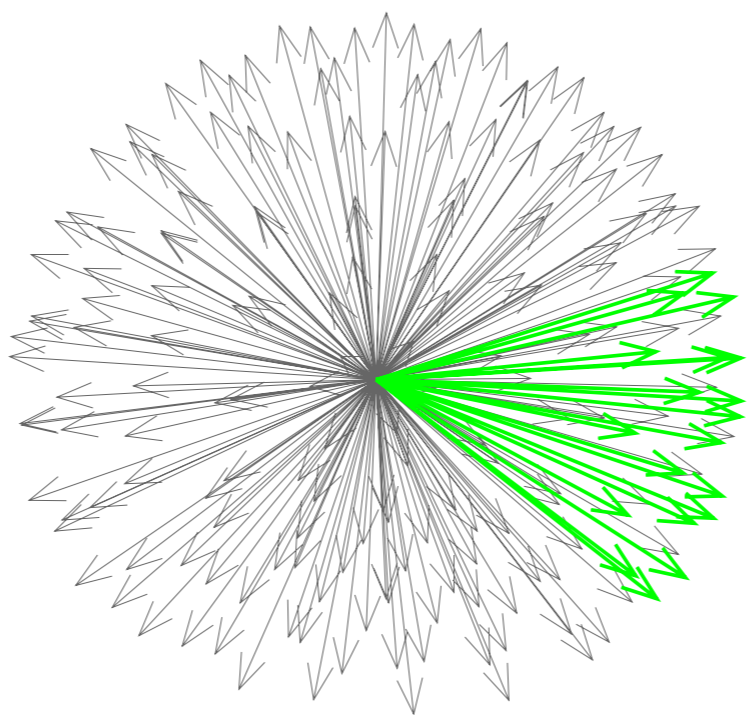
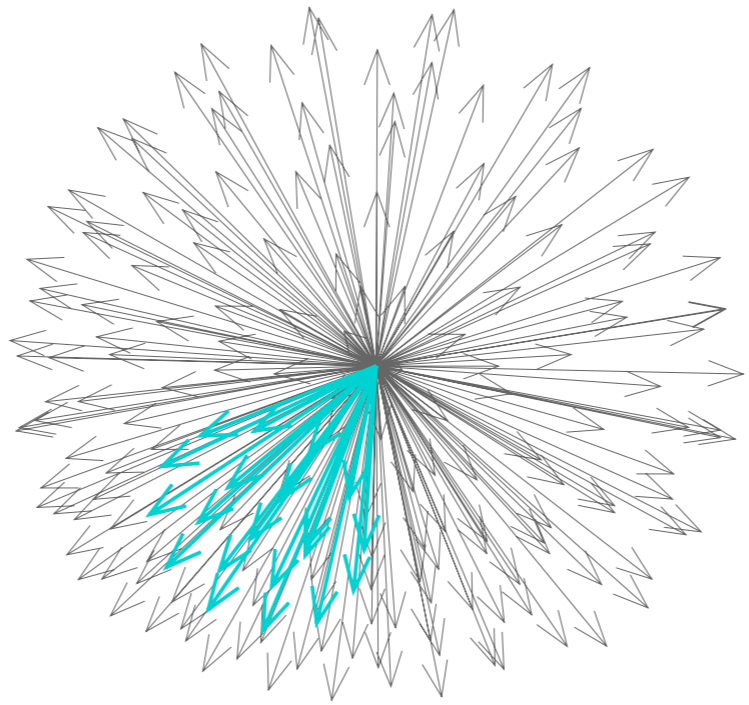
Multiple quantum coherences

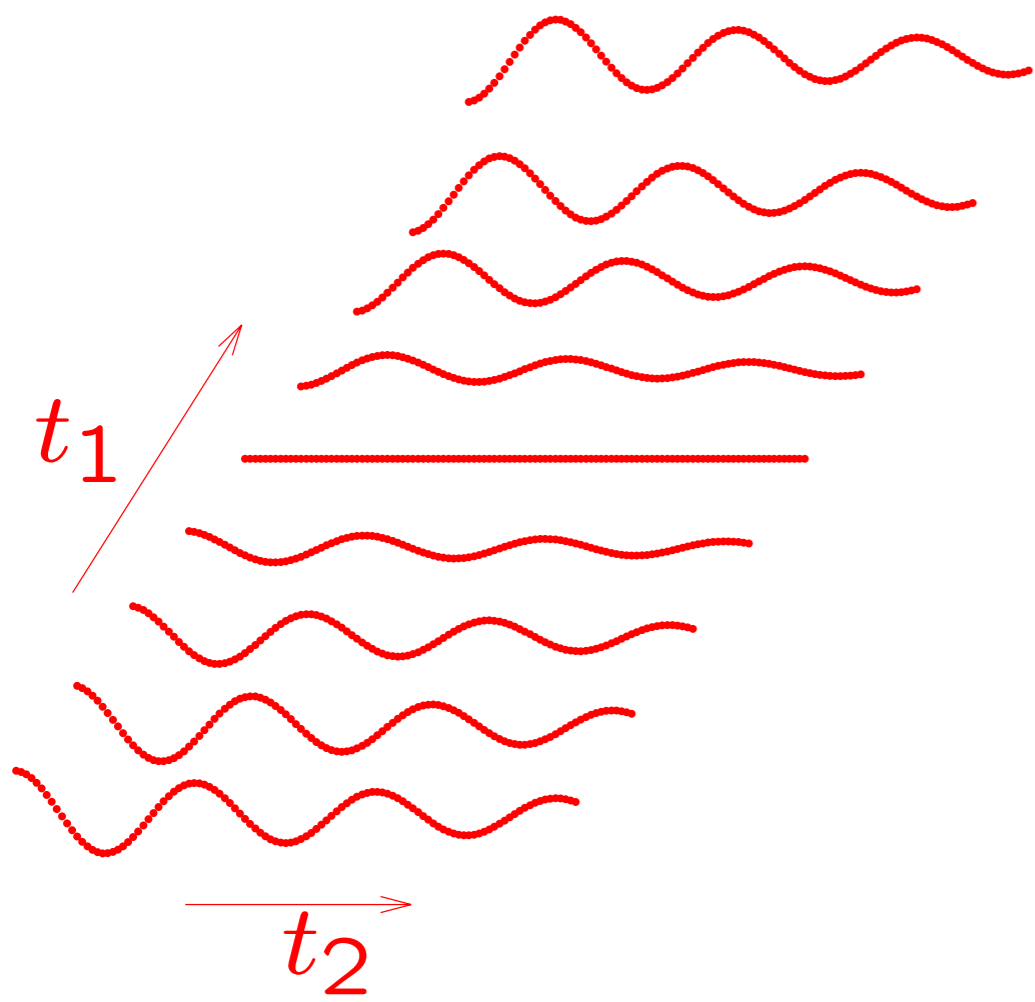


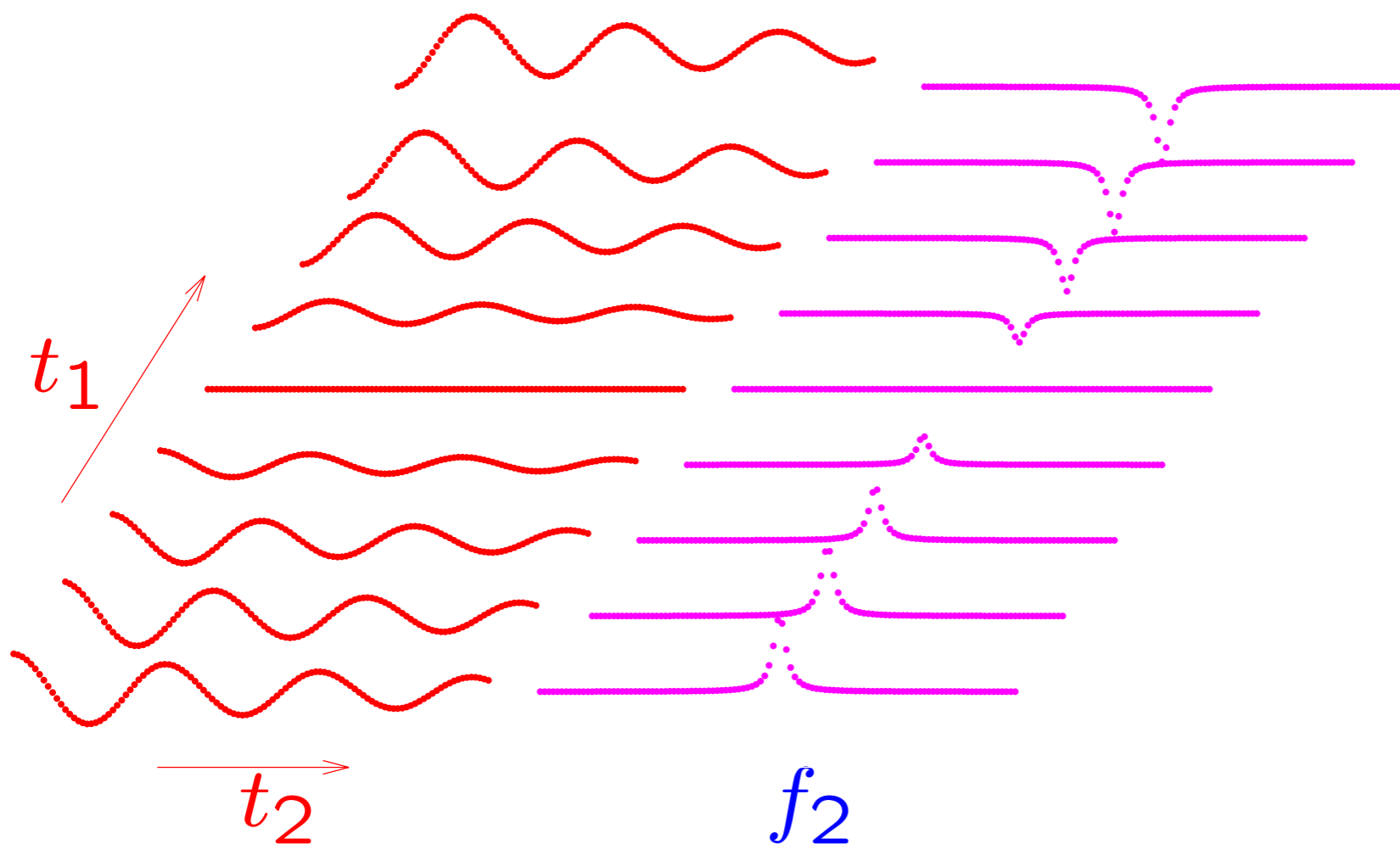
Multiple quantum coherences

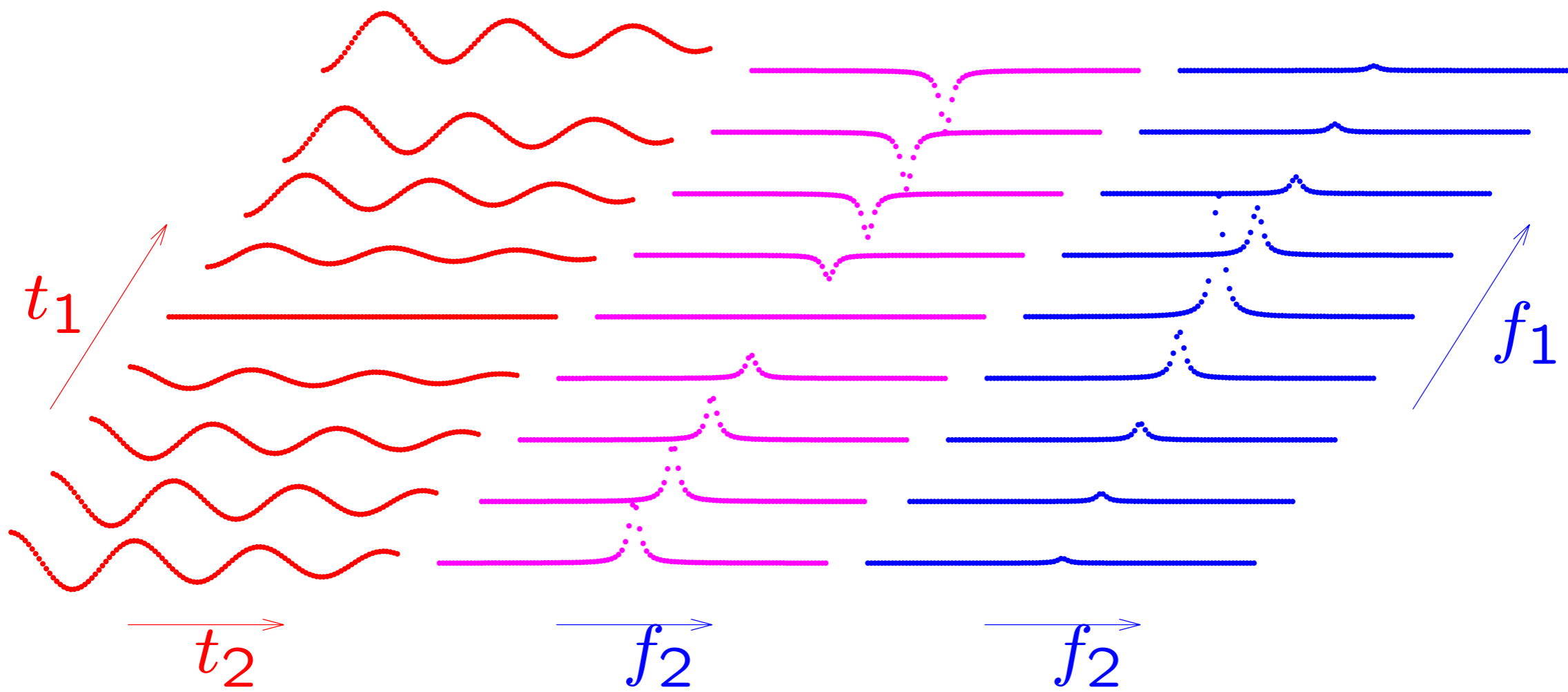


Multiple quantum coherences

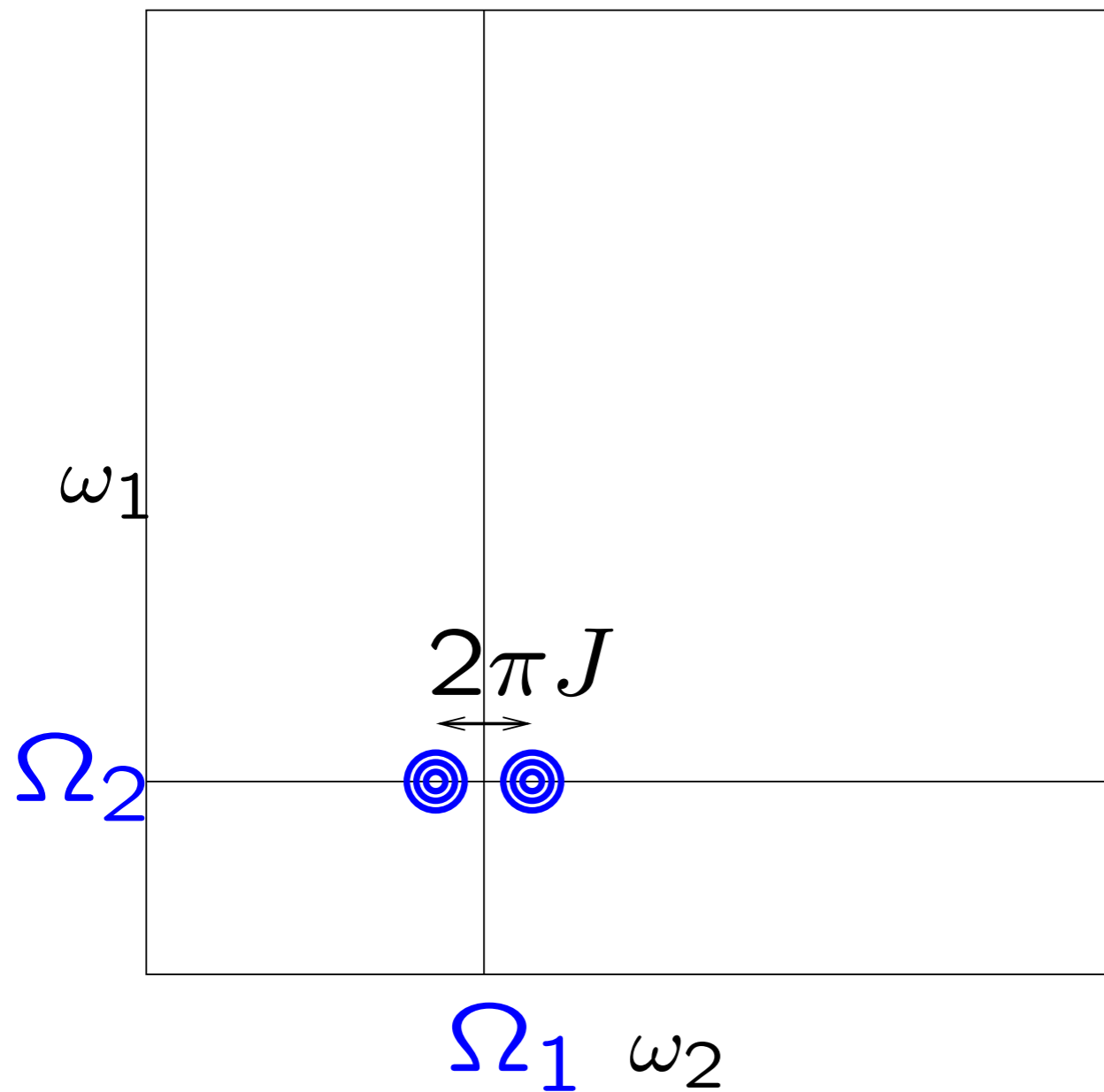




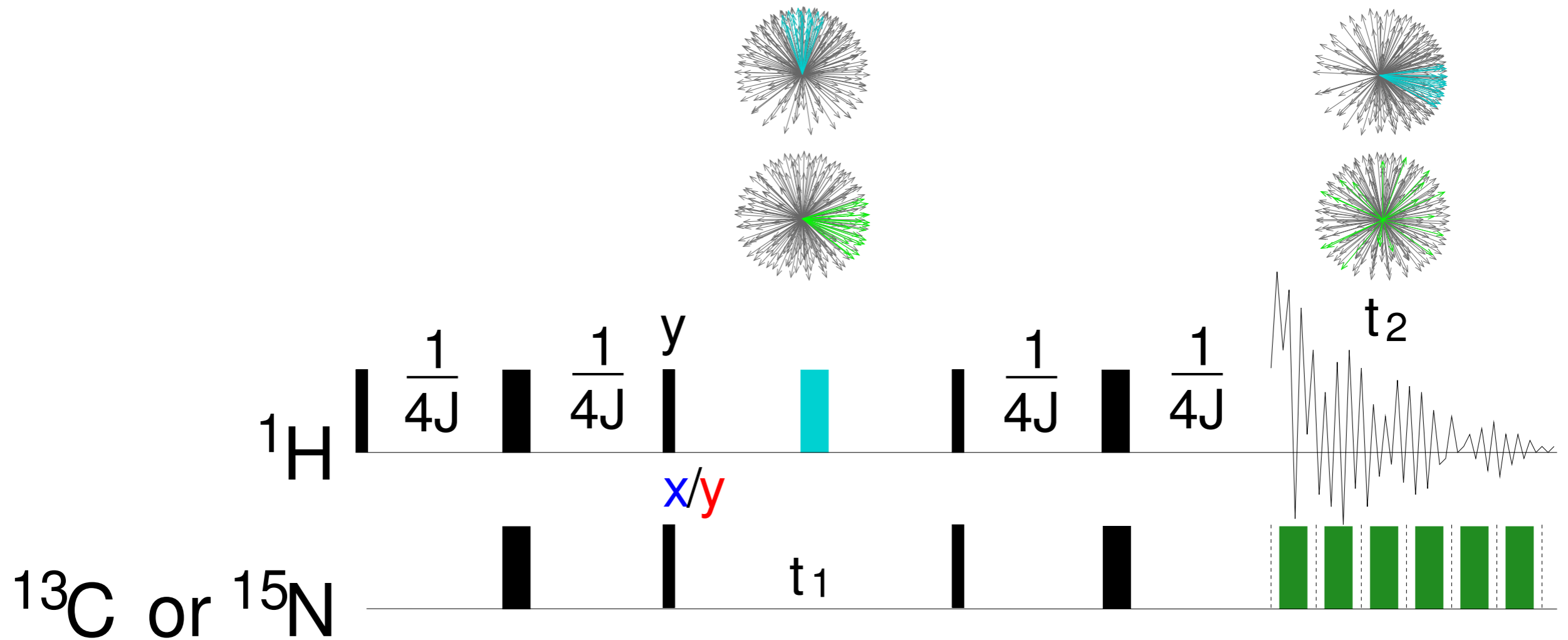




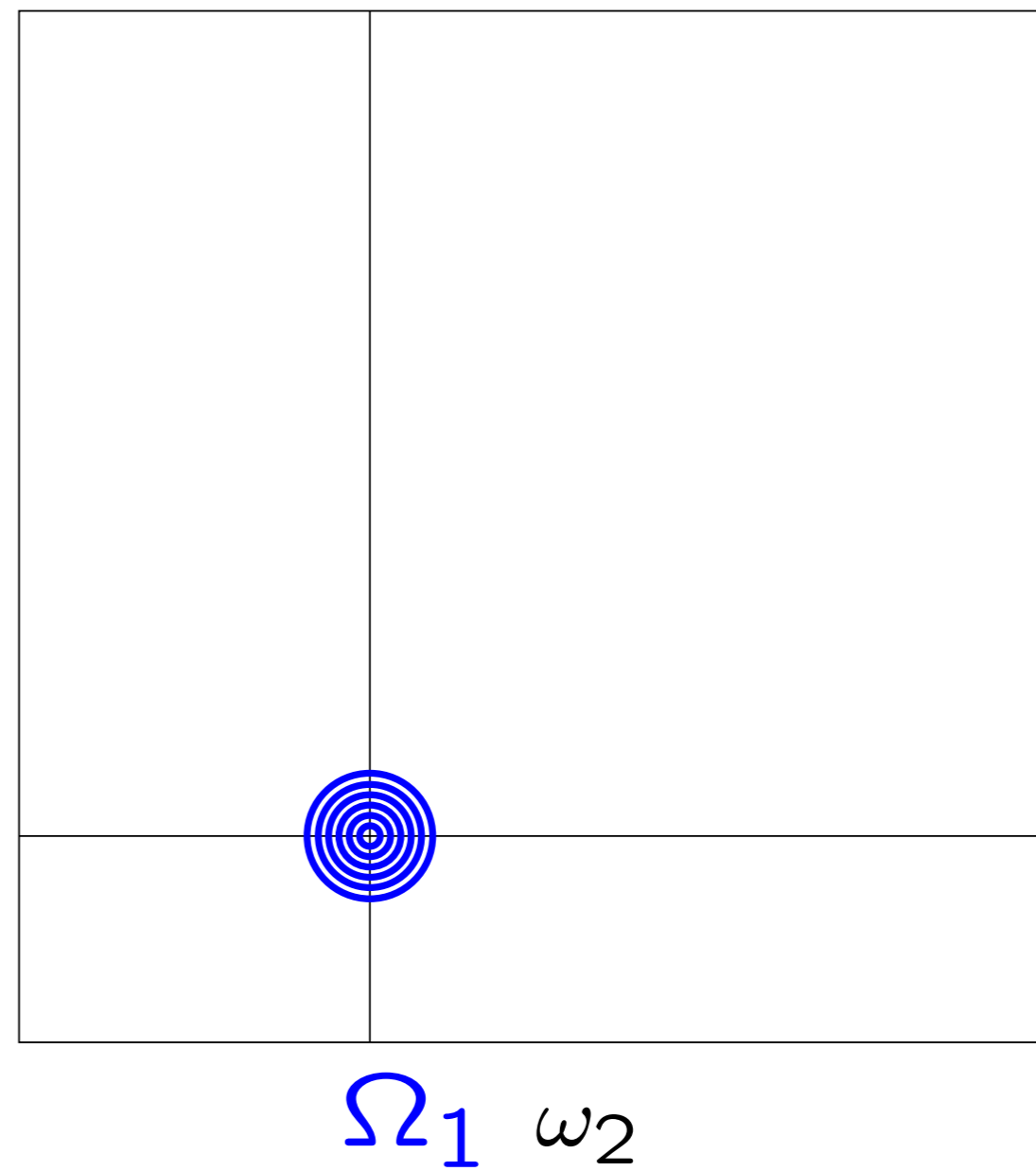
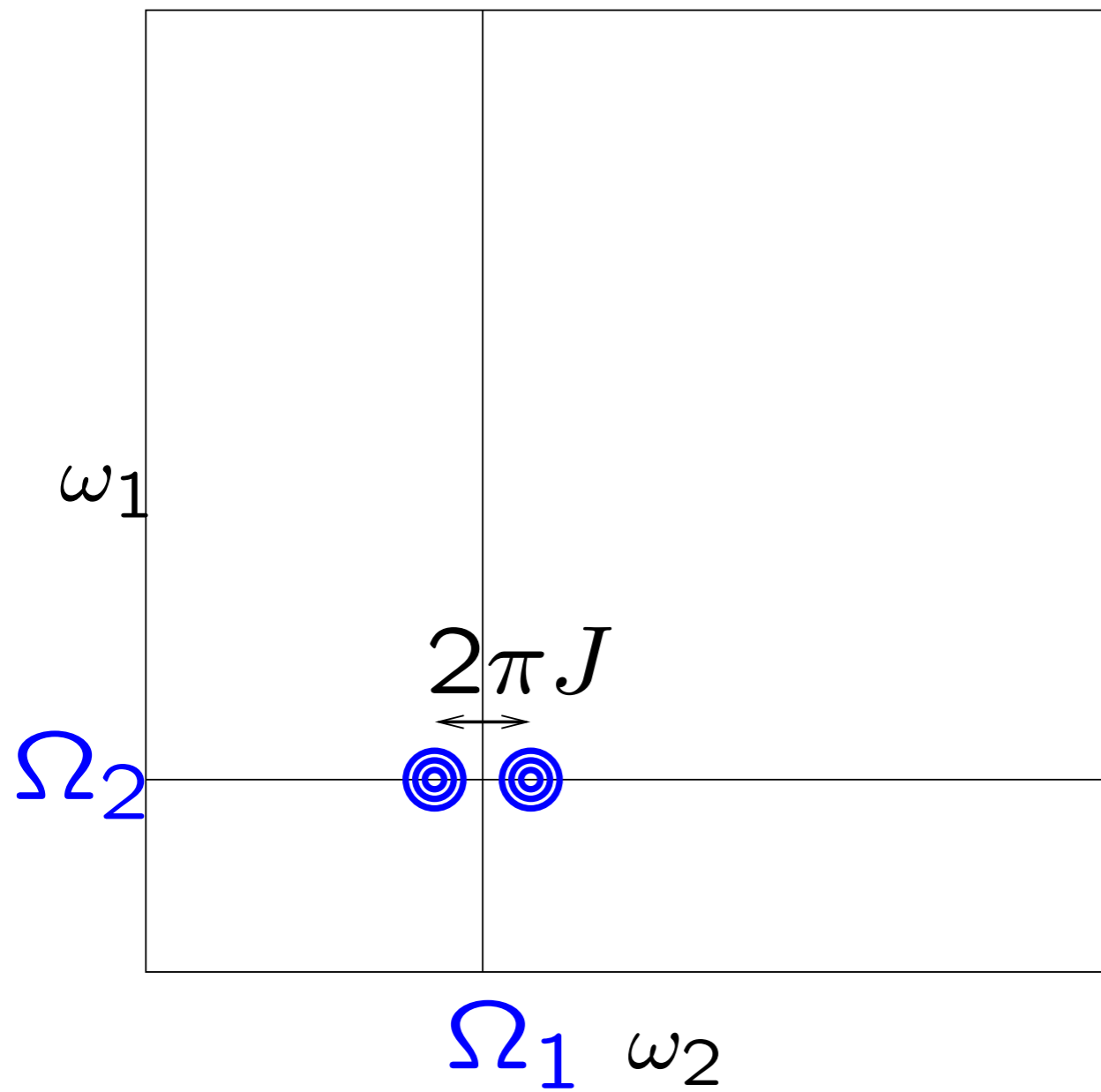
Decoupling in direct dimension



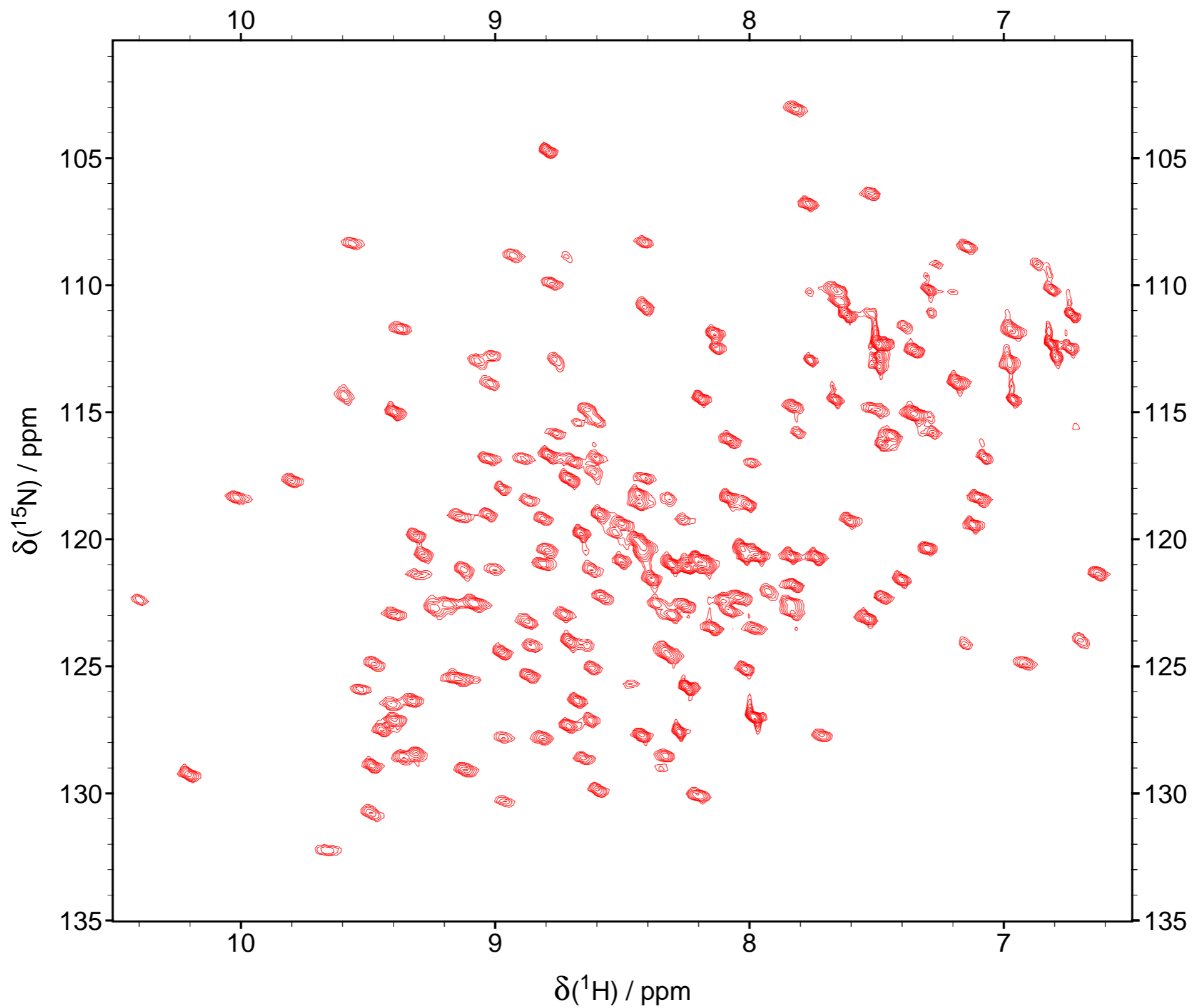
Decoupling in direct dimension



Decoupling in direct dimension



$^1\text{H}, ^{15}\text{N}$ HSQC spectrum of a 20 kDa protein



Benefits of HSQC

- *High sensitivity* for ^{13}C or ^{15}N
(higher by $(\gamma_1/\gamma_2)^{5/2}$ than by the direct detection)
- *High resolution*
Second dimension and less peaks in spectrum
(only $^{13}\text{C}/^{15}\text{N}$ -bonded protons and protonated $^{13}\text{C}/^{15}\text{N}$ visible)
- *Important structural information*
 ^1H - ^{13}C and ^1H - ^{15}N correlation
(it tells us which proton is attached to which ^{13}C or ^{15}N).