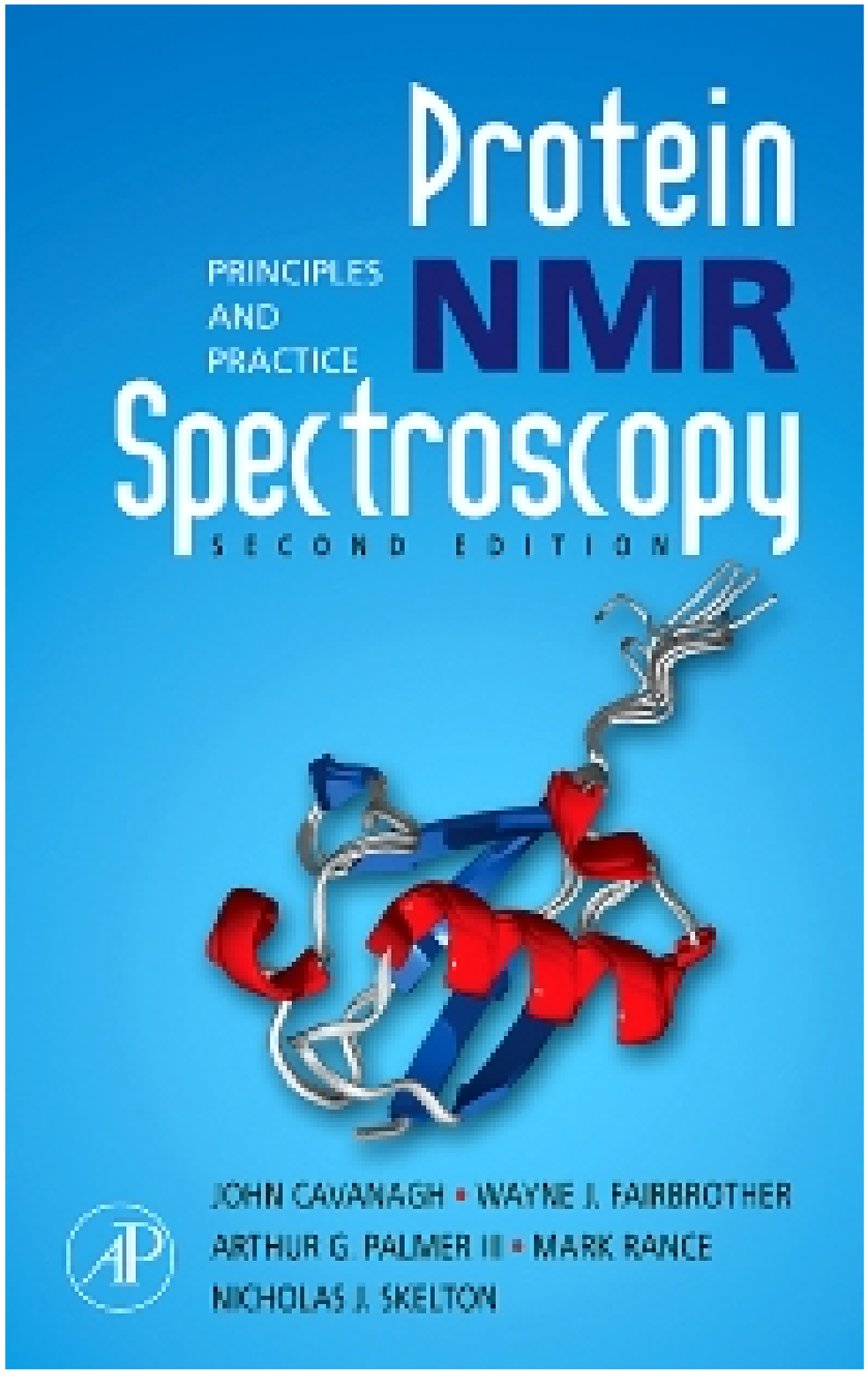
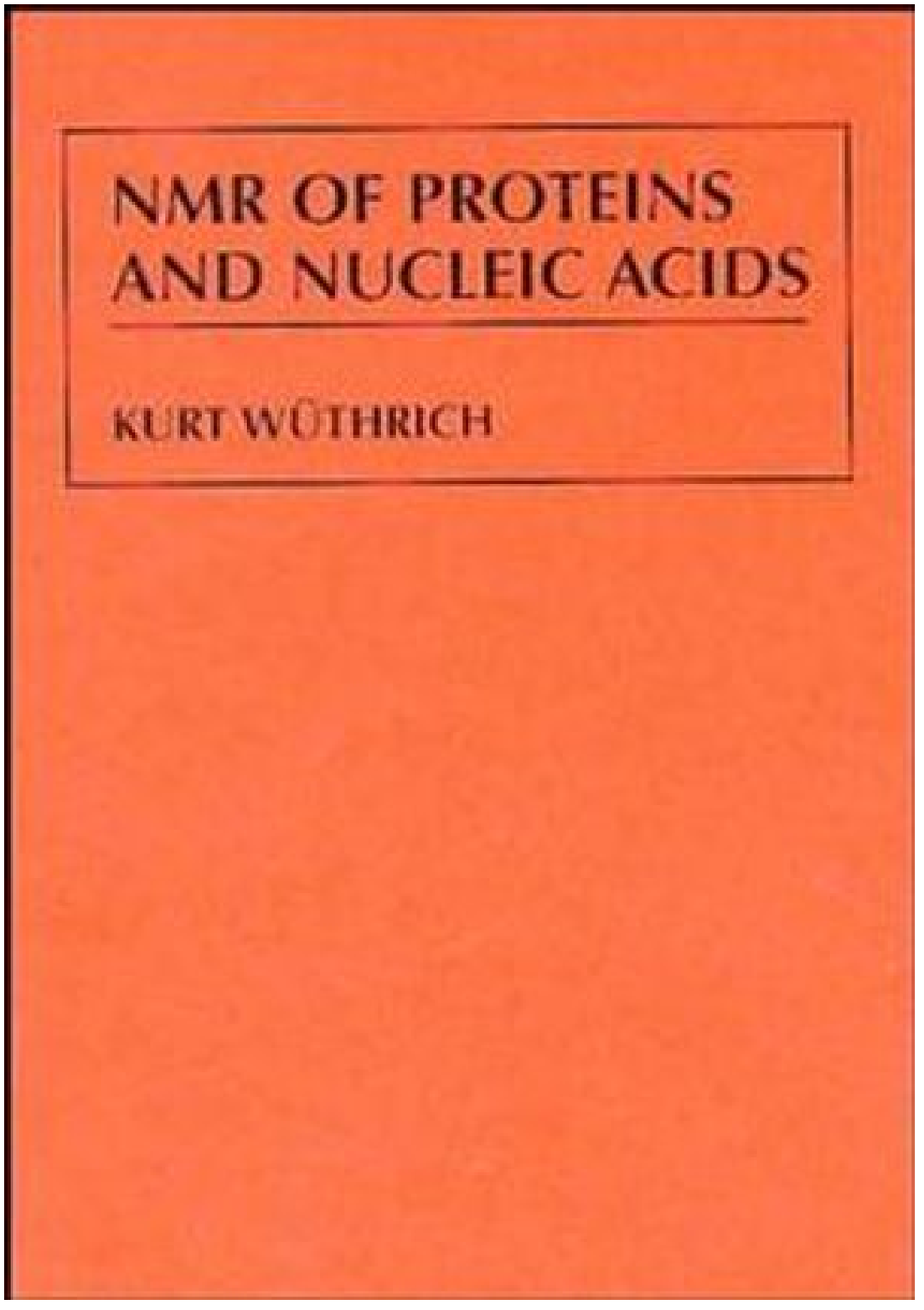
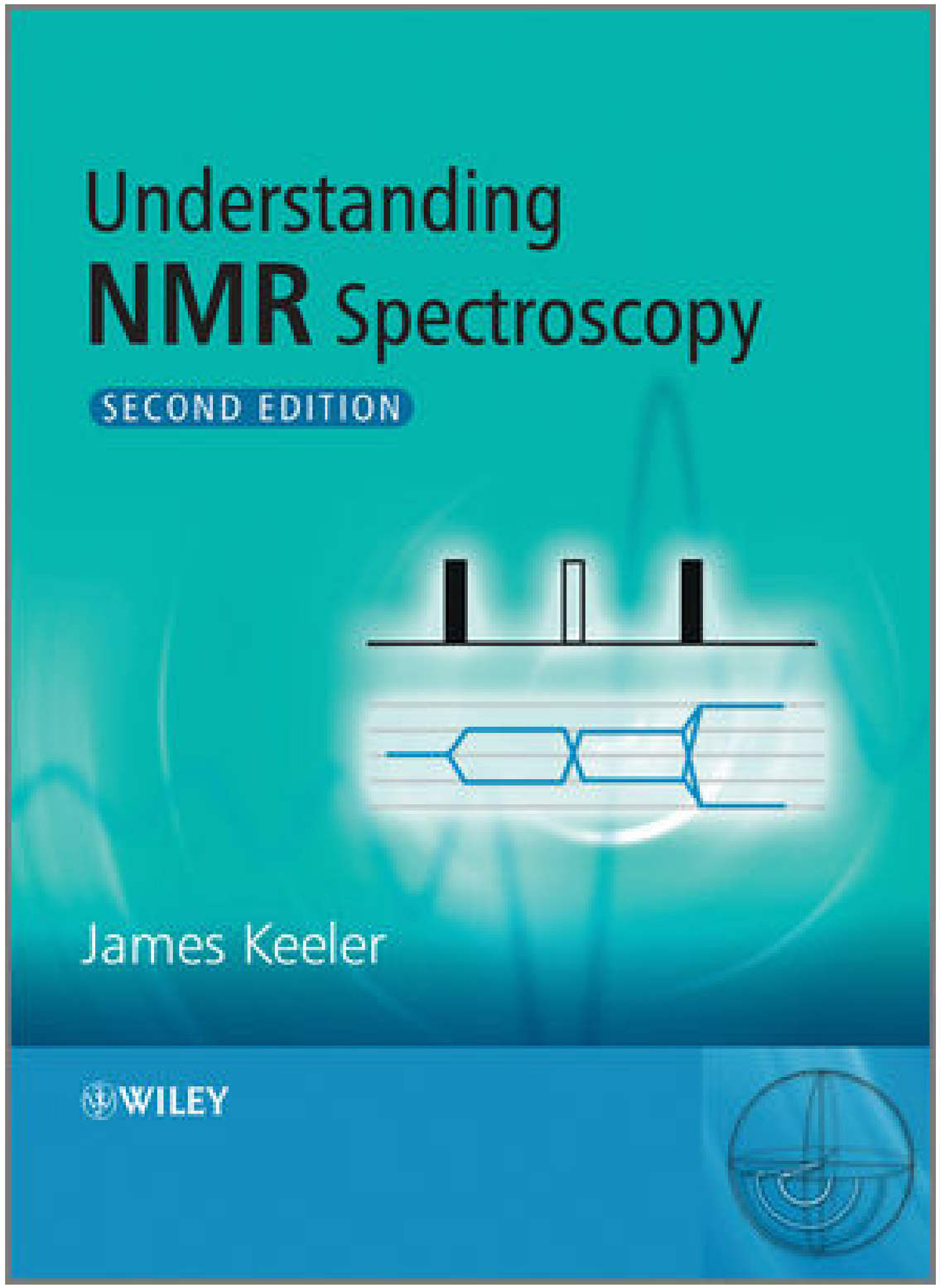
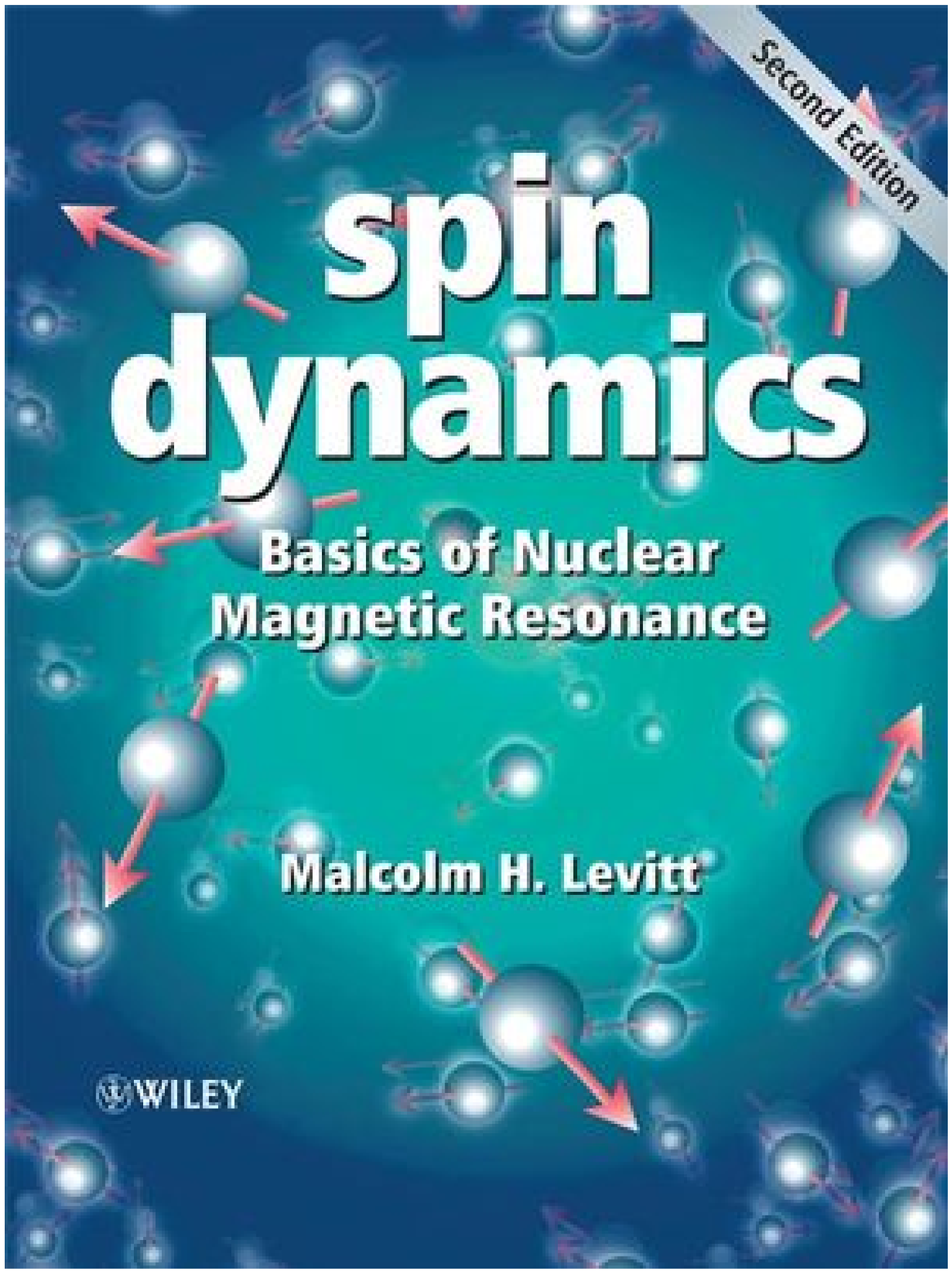
LECTURE 1a


Protein
NMR
Spectroscopy
PRINCIPLES
AND
PRACTICE
SECOND EDITION
JOHN CAVANAGH • WAYNE J. FAIRBROTHER
ARTHUR G. PALMER III • MARK RANCE
NICHOLAS J. SKELTON

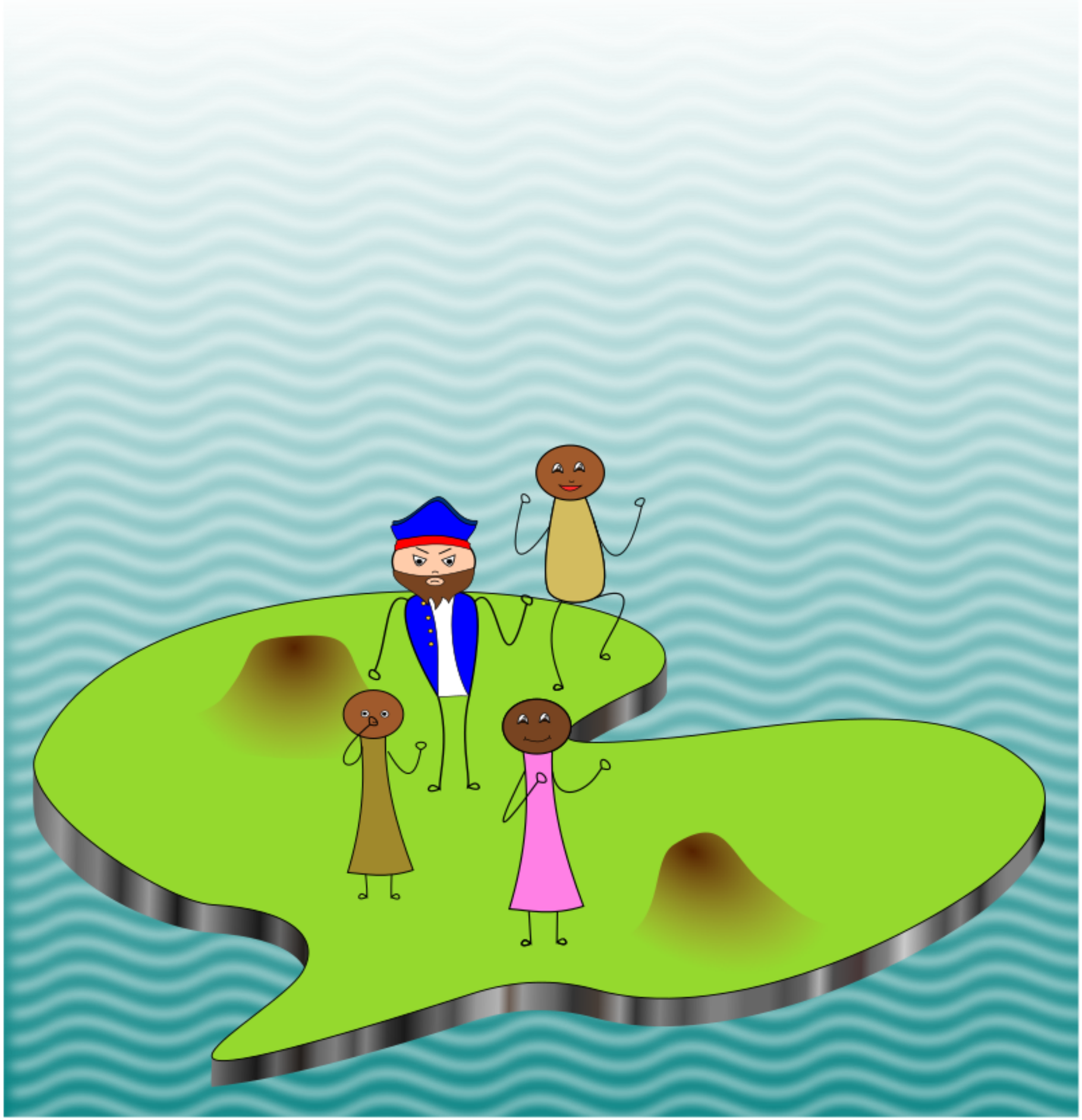

NMR OF PROTEINS
AND NUCLEIC ACIDS
KURT WÜTHRICH

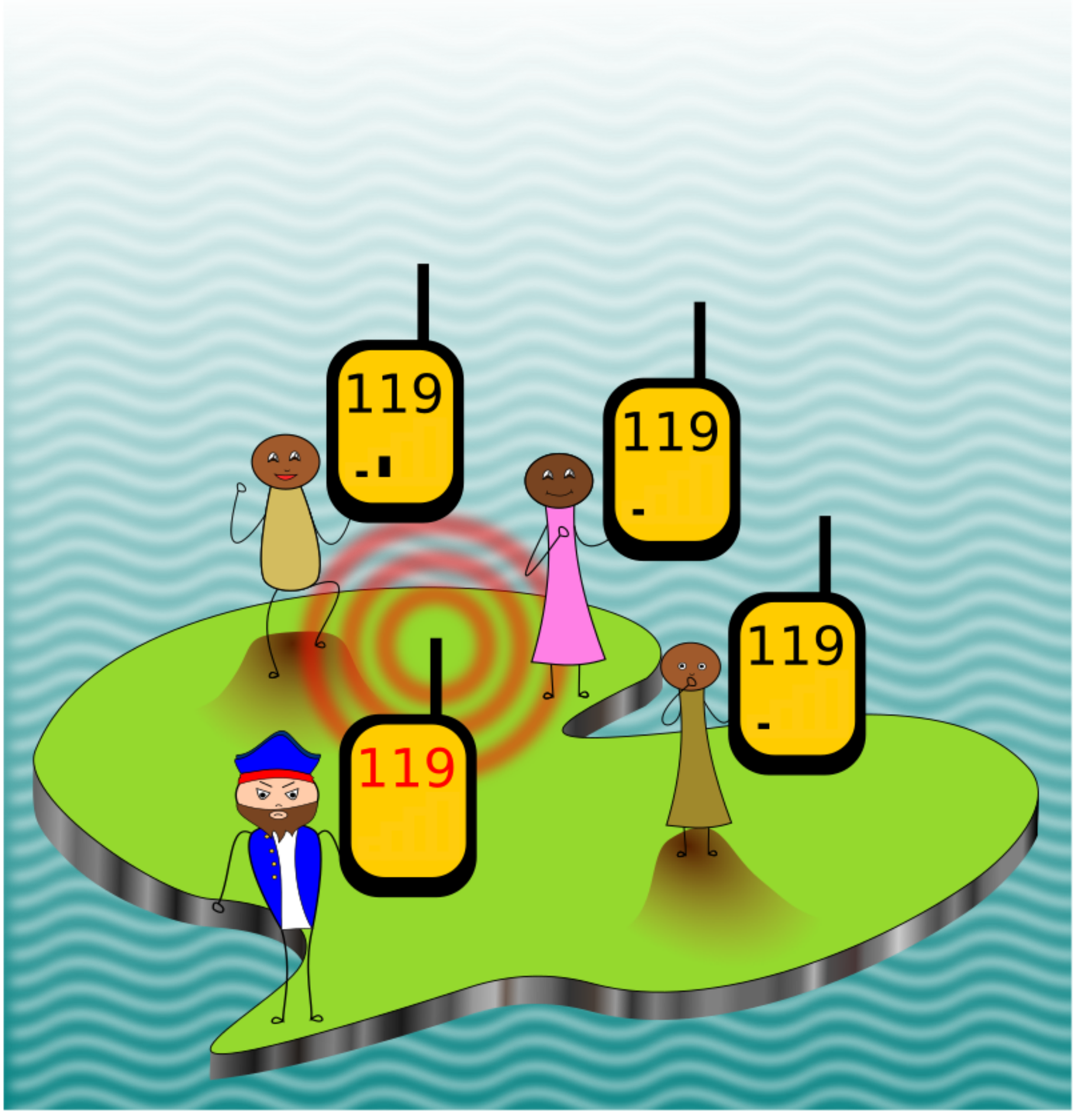

Understanding
NMR Spectroscopy
SECOND EDITION
James Keeler
WILEY


Second Edition
spin dynamics
Basics of Nuclear Magnetic Resonance
Malcolm H. Levitt
WILEY

- *Is my protein folded?*
- *3D structure determination*
- *Specific structural details*
- *Intermolecular interactions*
- *Molecular motions* (hydrodynamics, internal)
- *Kinetics and thermodynamics*
- *In vivo measurements*
- *Spatial resolution*

- *Solubility*
- *Stability*
- *Stable isotope labeling*
- *Scaling up production*
- *Size*
- *Separation from impurities*
- *Salt content*

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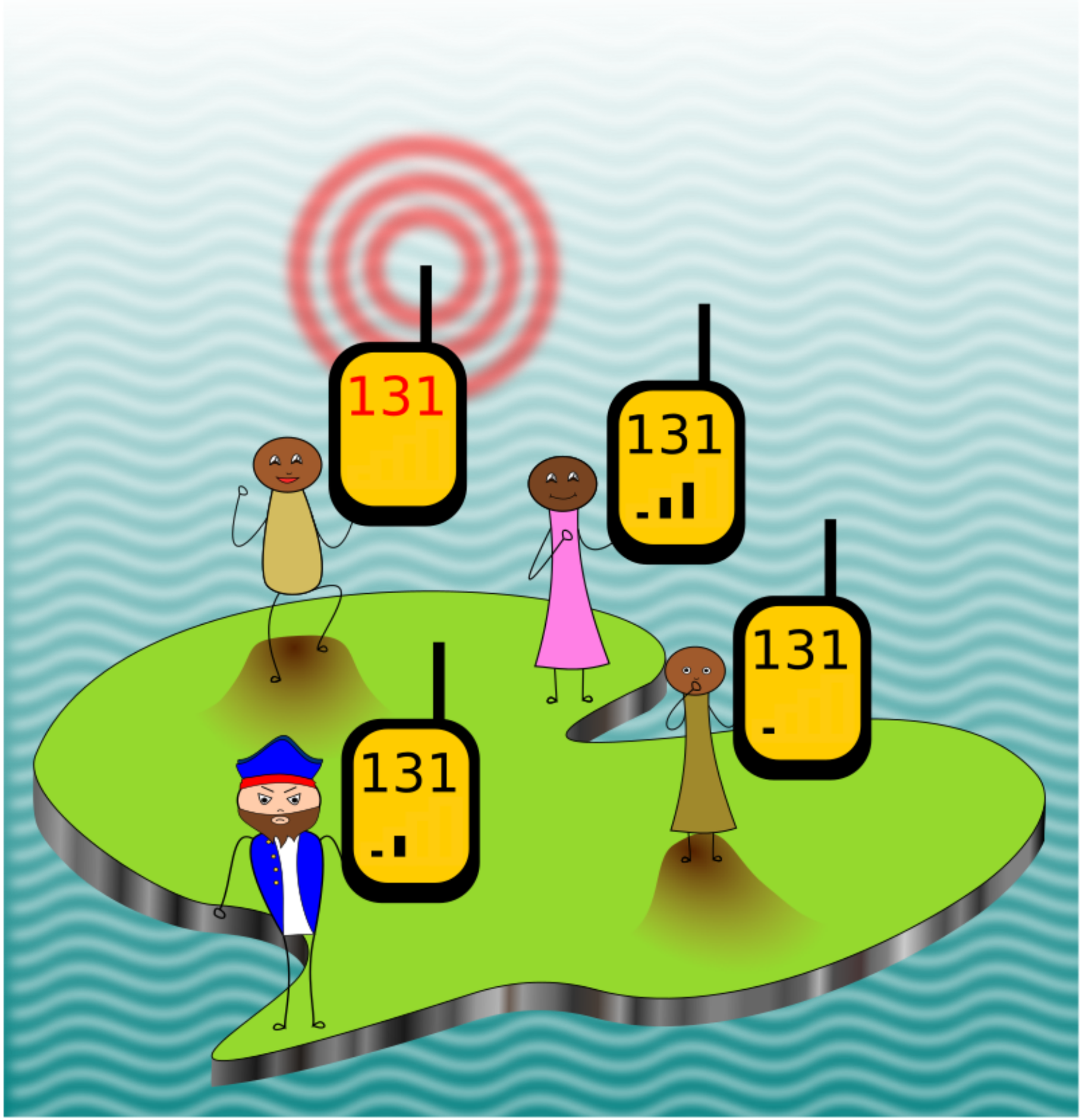
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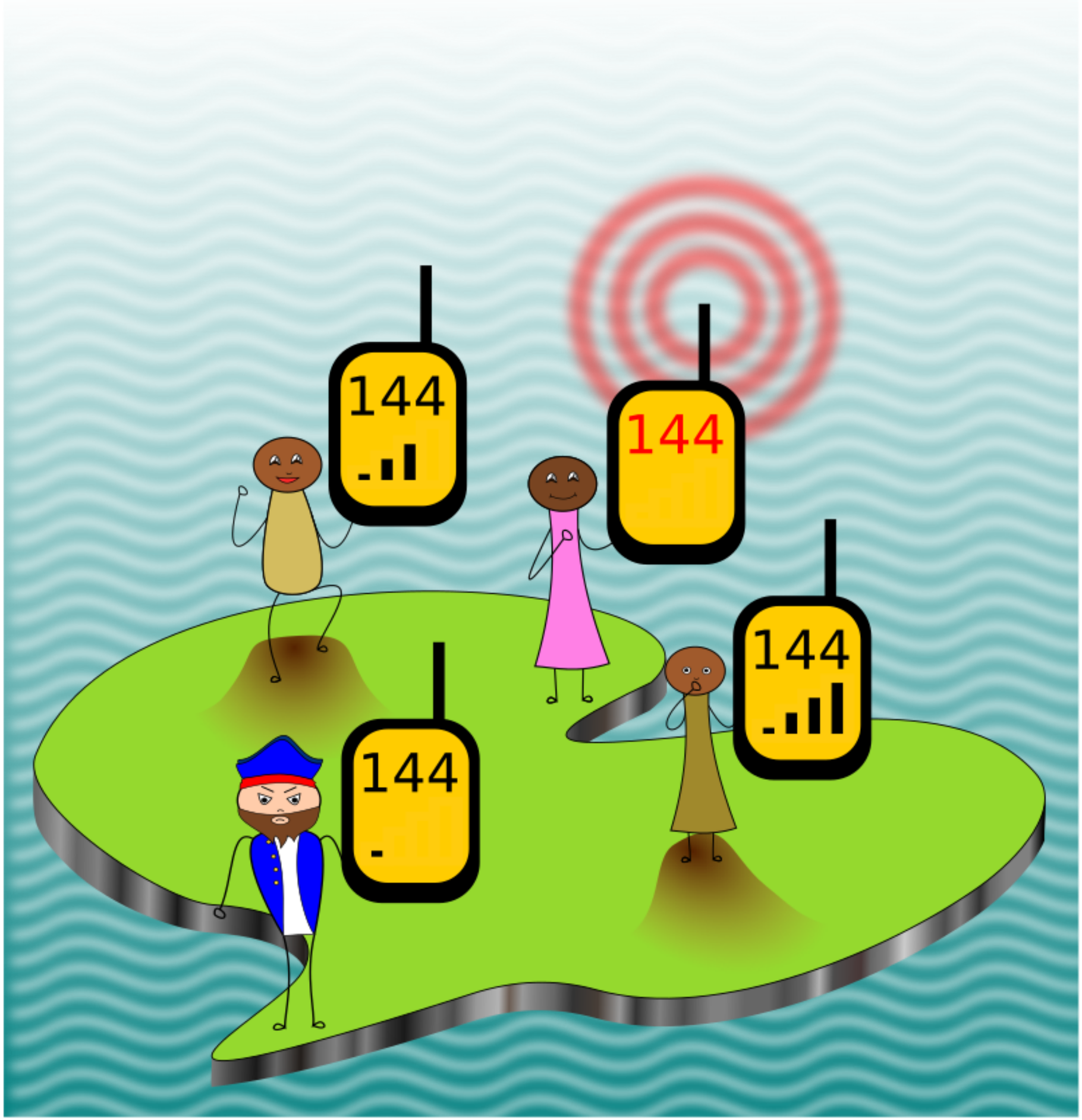
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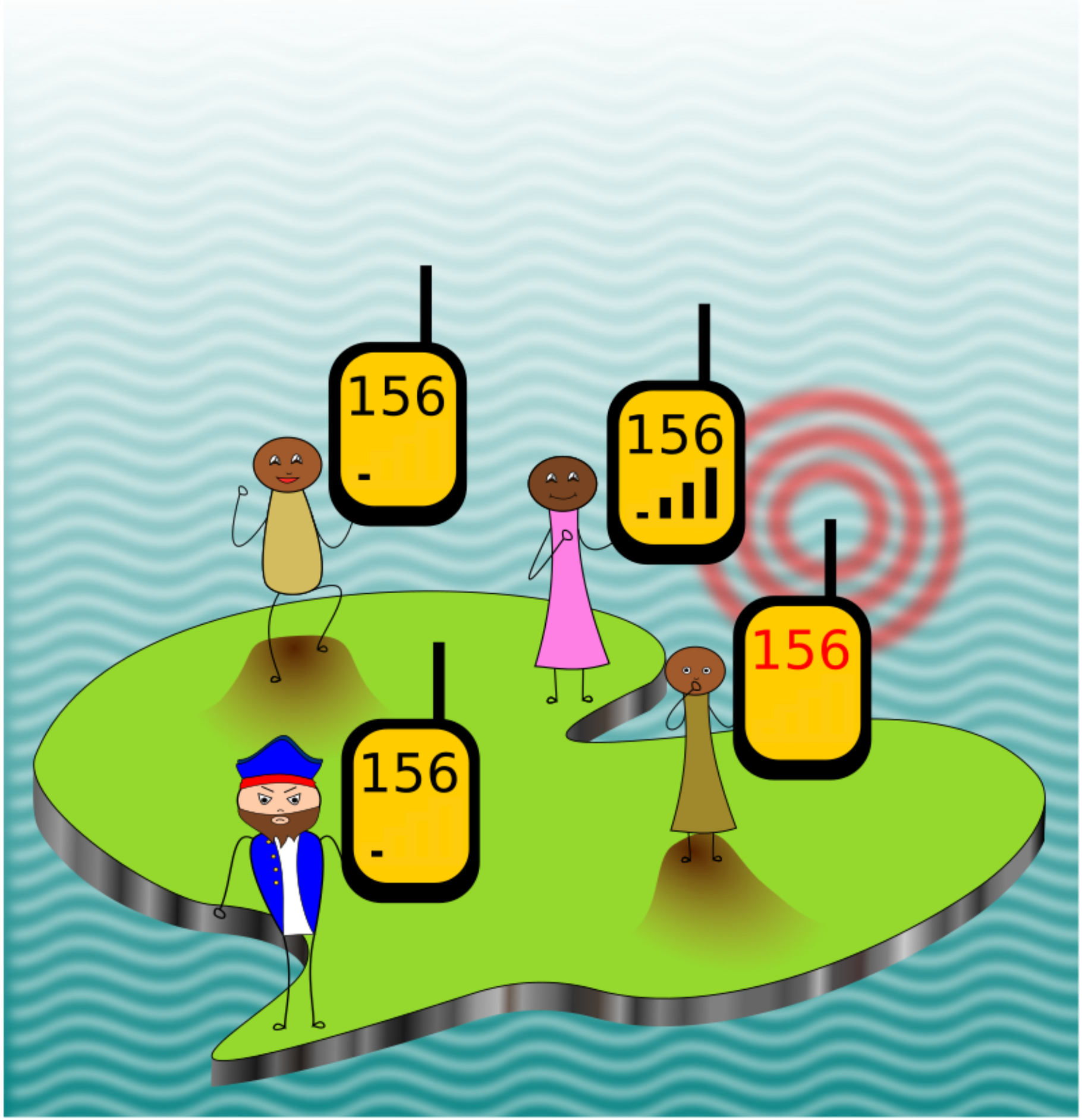
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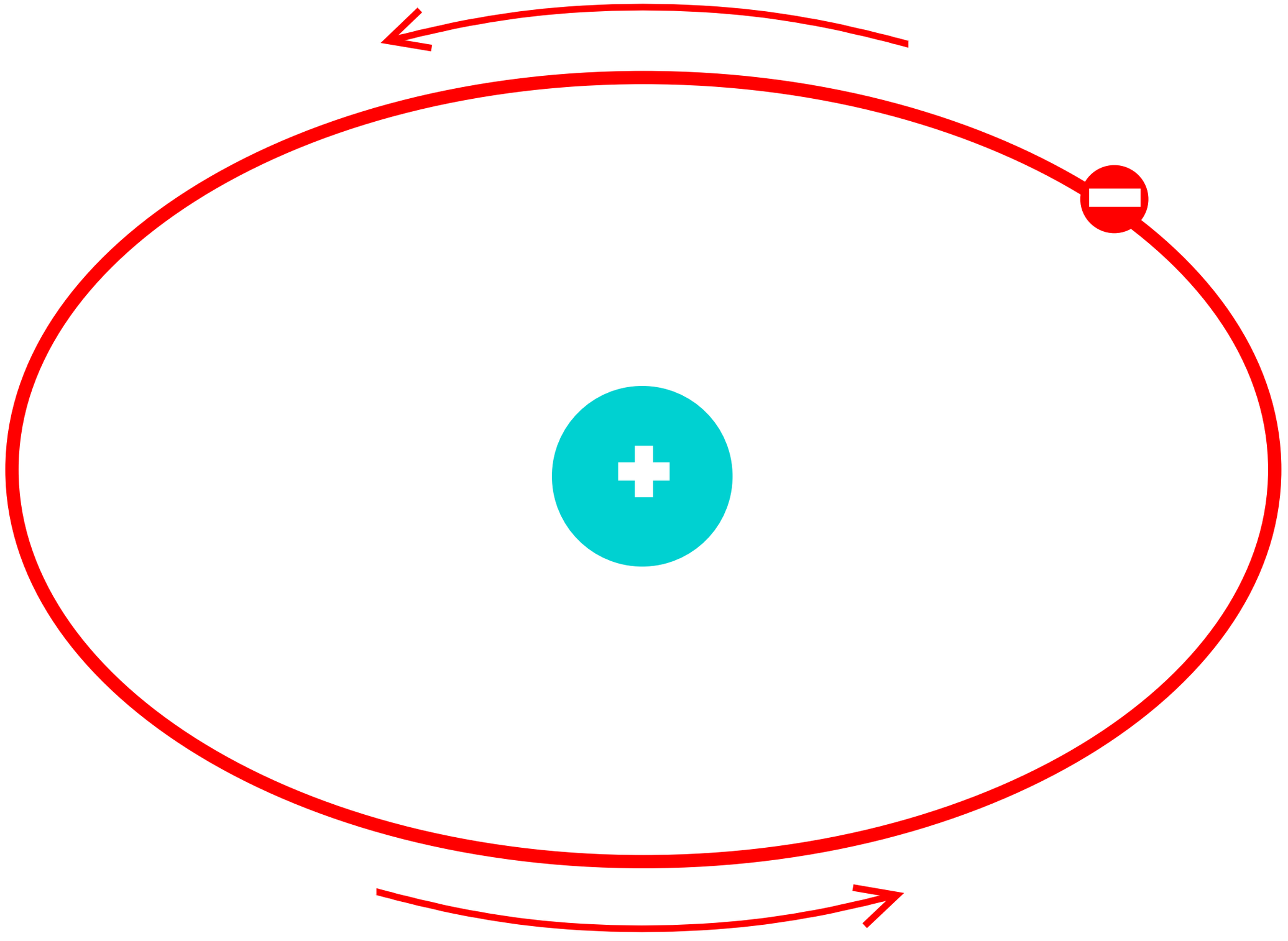
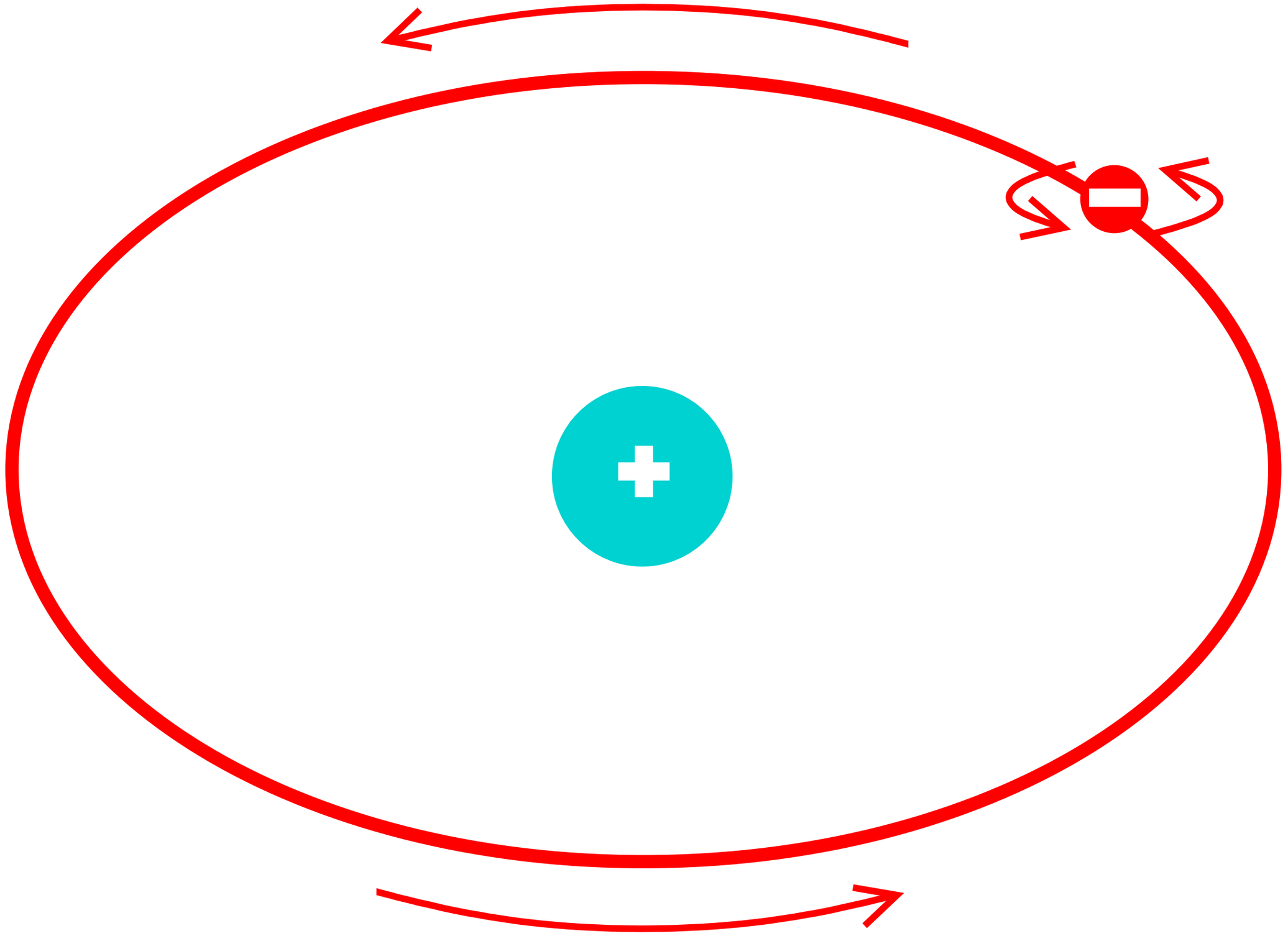
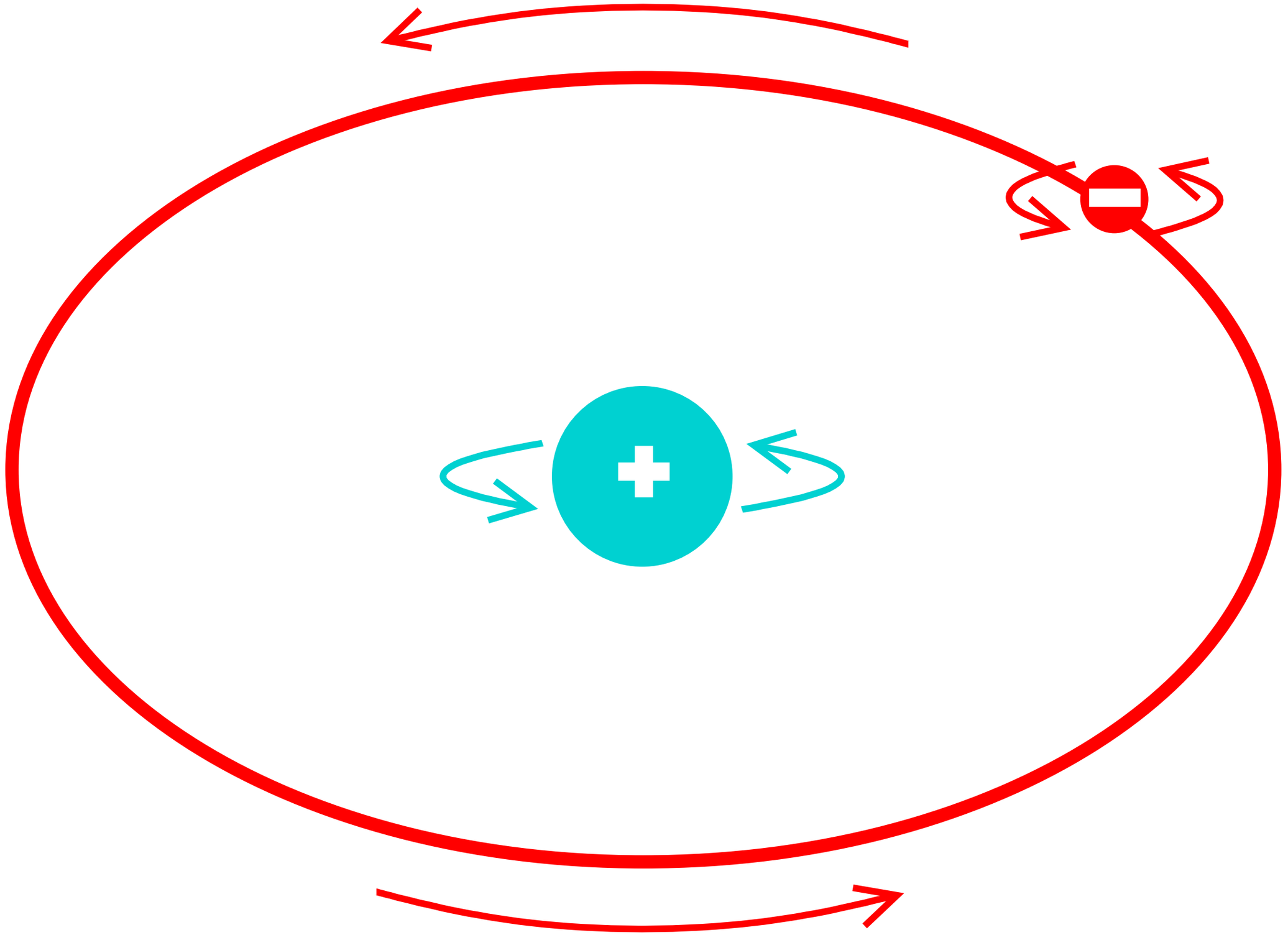
LECTURE 1b







Dirac-like nuclei:

	$\frac{10^{-9}\gamma}{\mathrm{rad\,s^{-1}T^{-1}}}$	% in Nature
e^-	-182.000	100
^{1}H	0.277	99.98
^{13}C	0.067	1.1
^{15}N	-0.027	0.4
^{19}F	0.252	100
^{31}P	0.108	100
^{129}Xe	-0.075	24.4

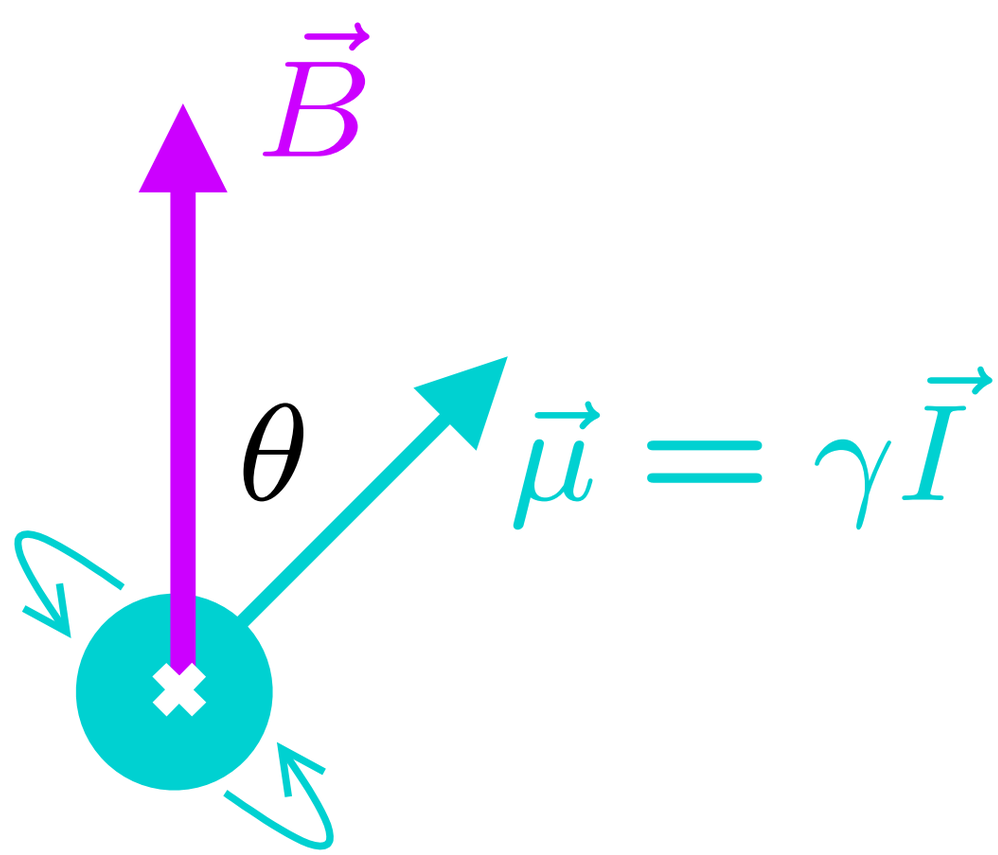
rare isotopes (require enrichment)

Magnetic moment

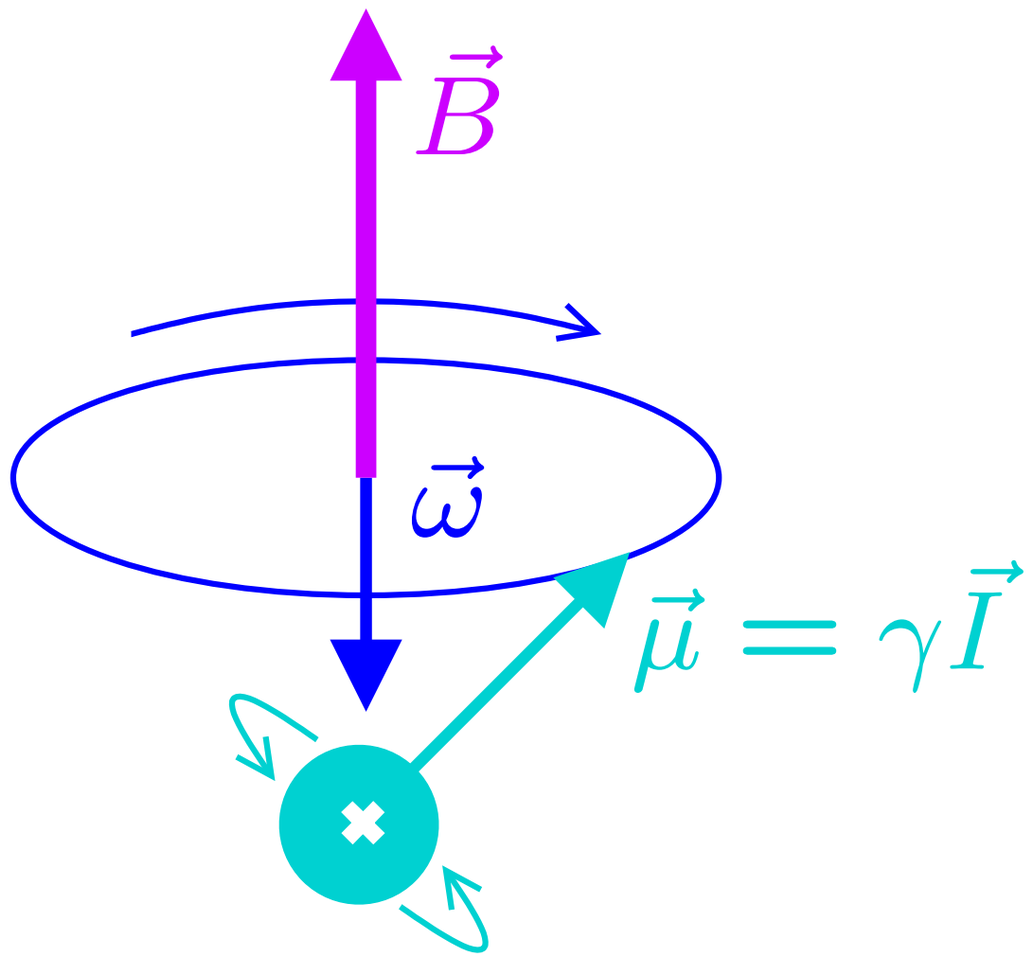
$$\vec{\mu} = -\gamma I$$

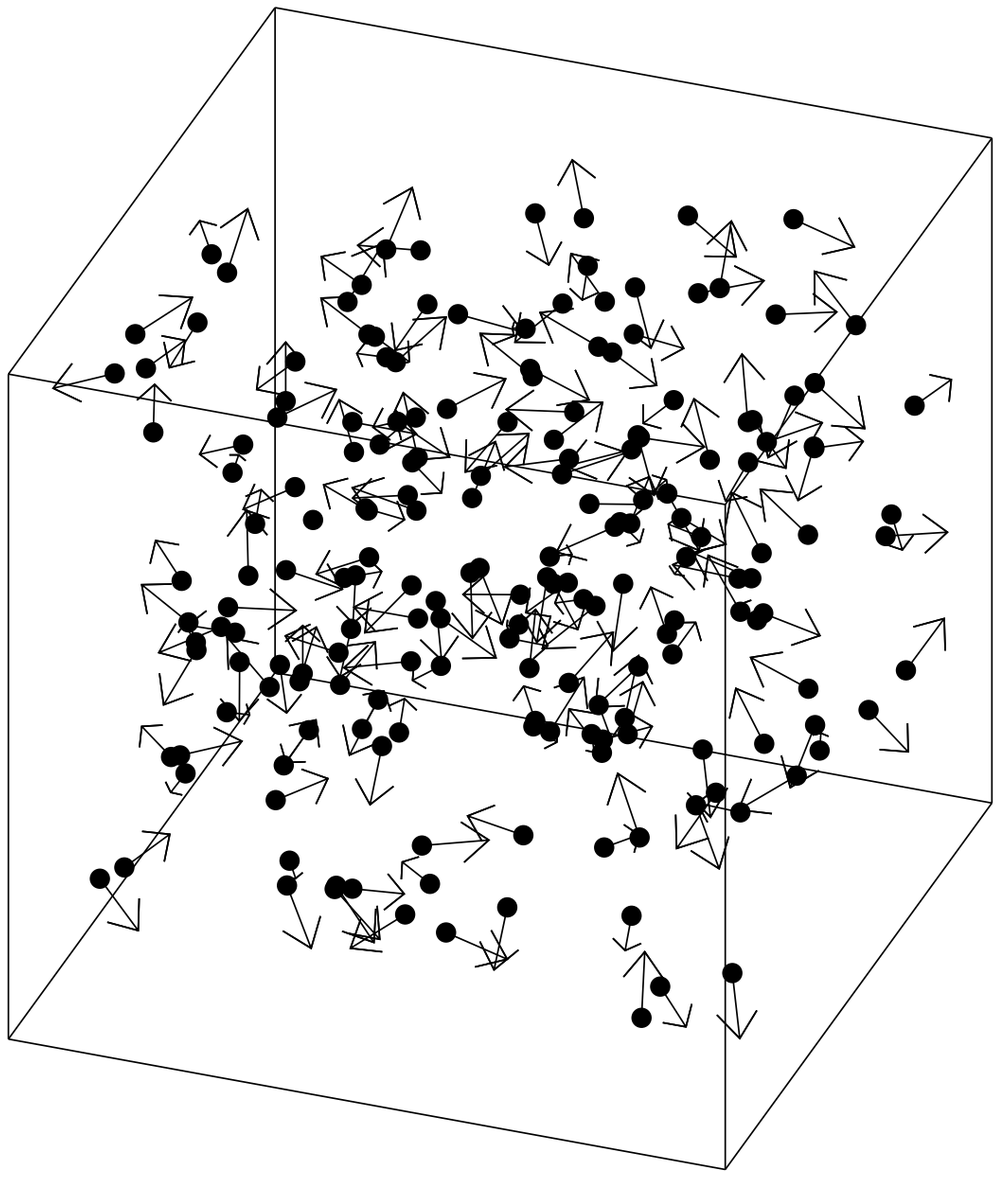
Energy

$$E = -\vec{\mu} \cdot \vec{B} = -|\mu||B| \cos\theta$$

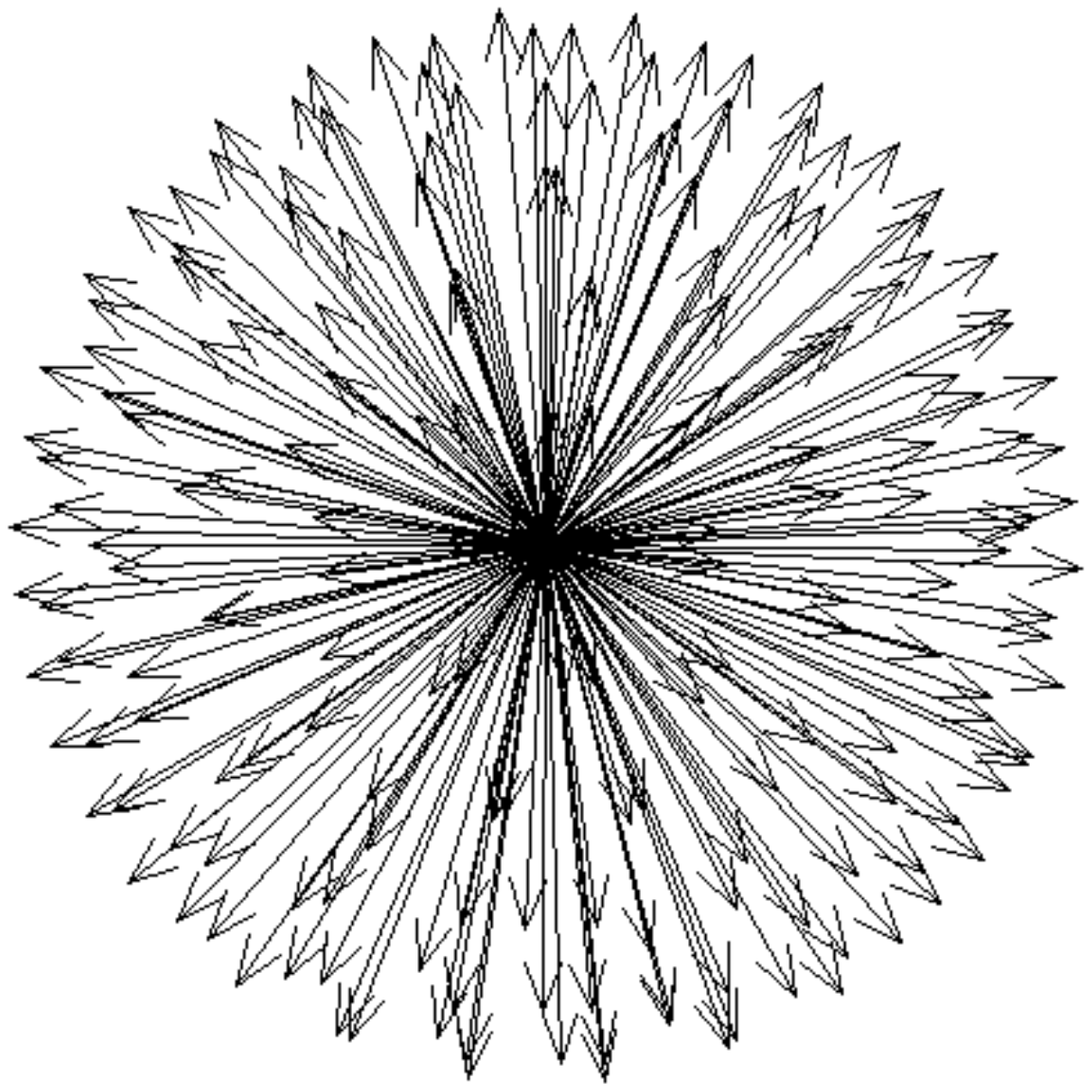


Angular precession frequency $\vec{\omega} = -\gamma \vec{B}$

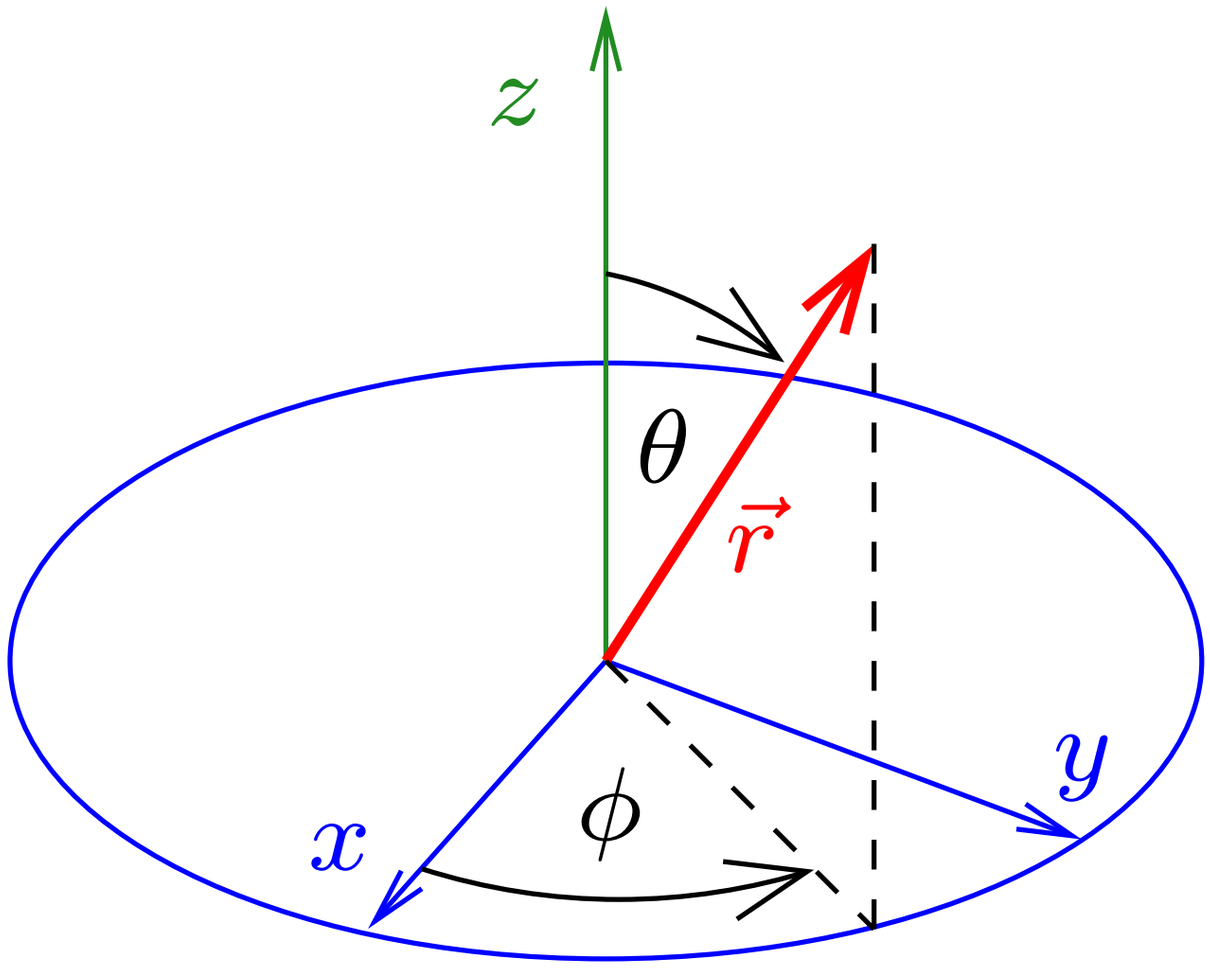


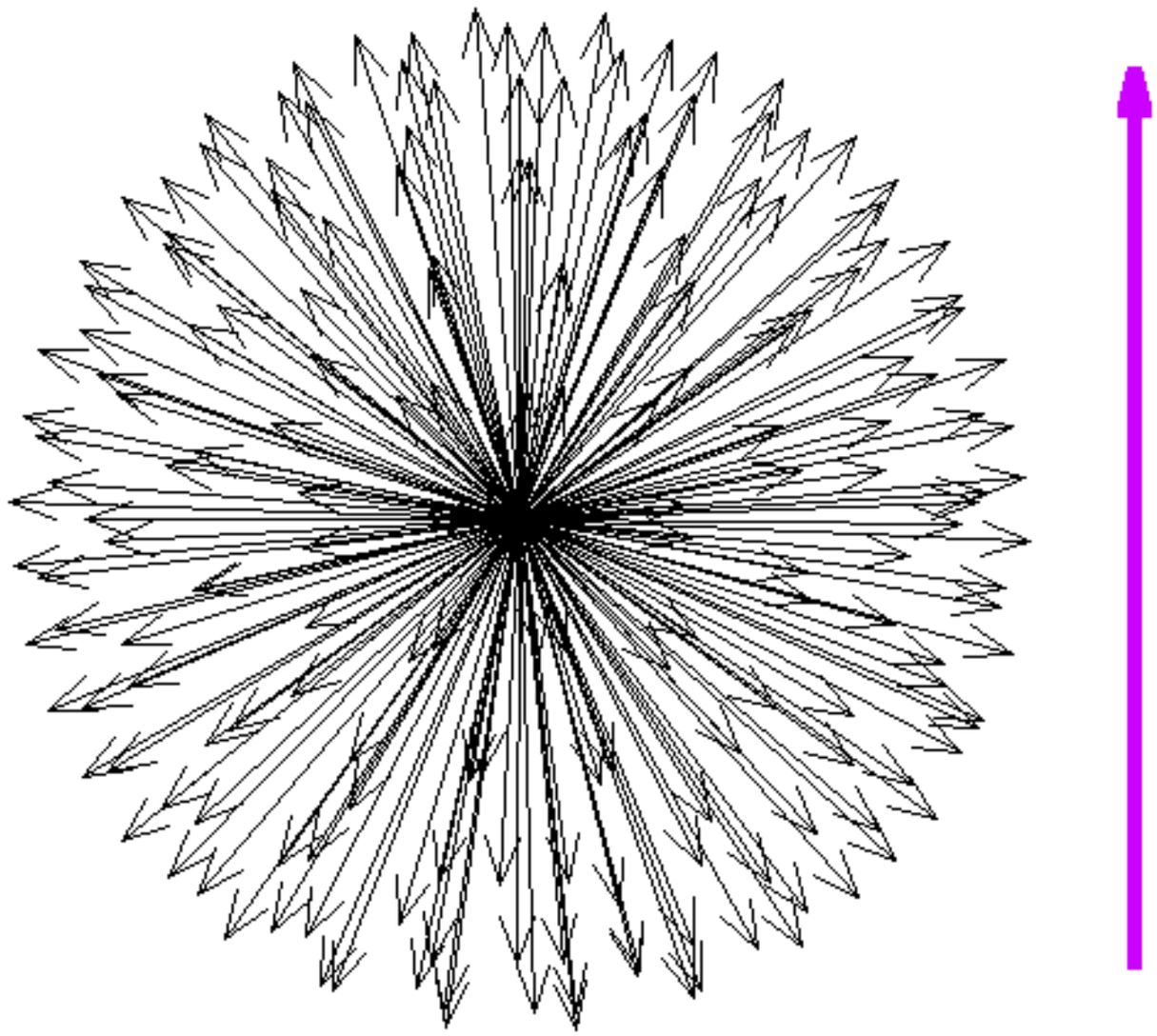


$\vec{M} = (\vec{\mu}_1 + \vec{\mu}_2 + \vec{\mu}_3 + \vec{\mu}_4 + \vec{\mu}_5 + \vec{\mu}_6 + \cdots)/V$ Magnetization

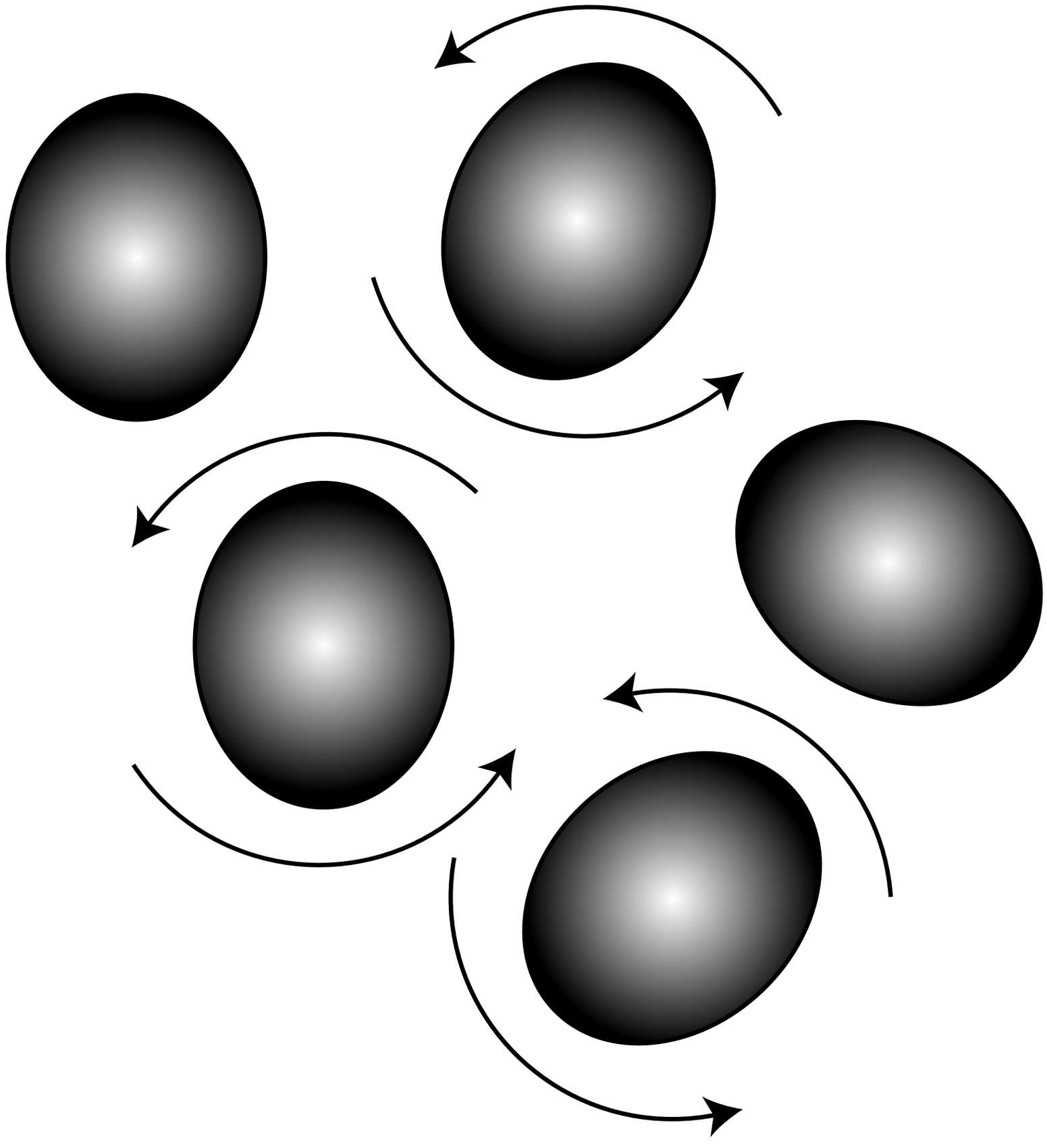


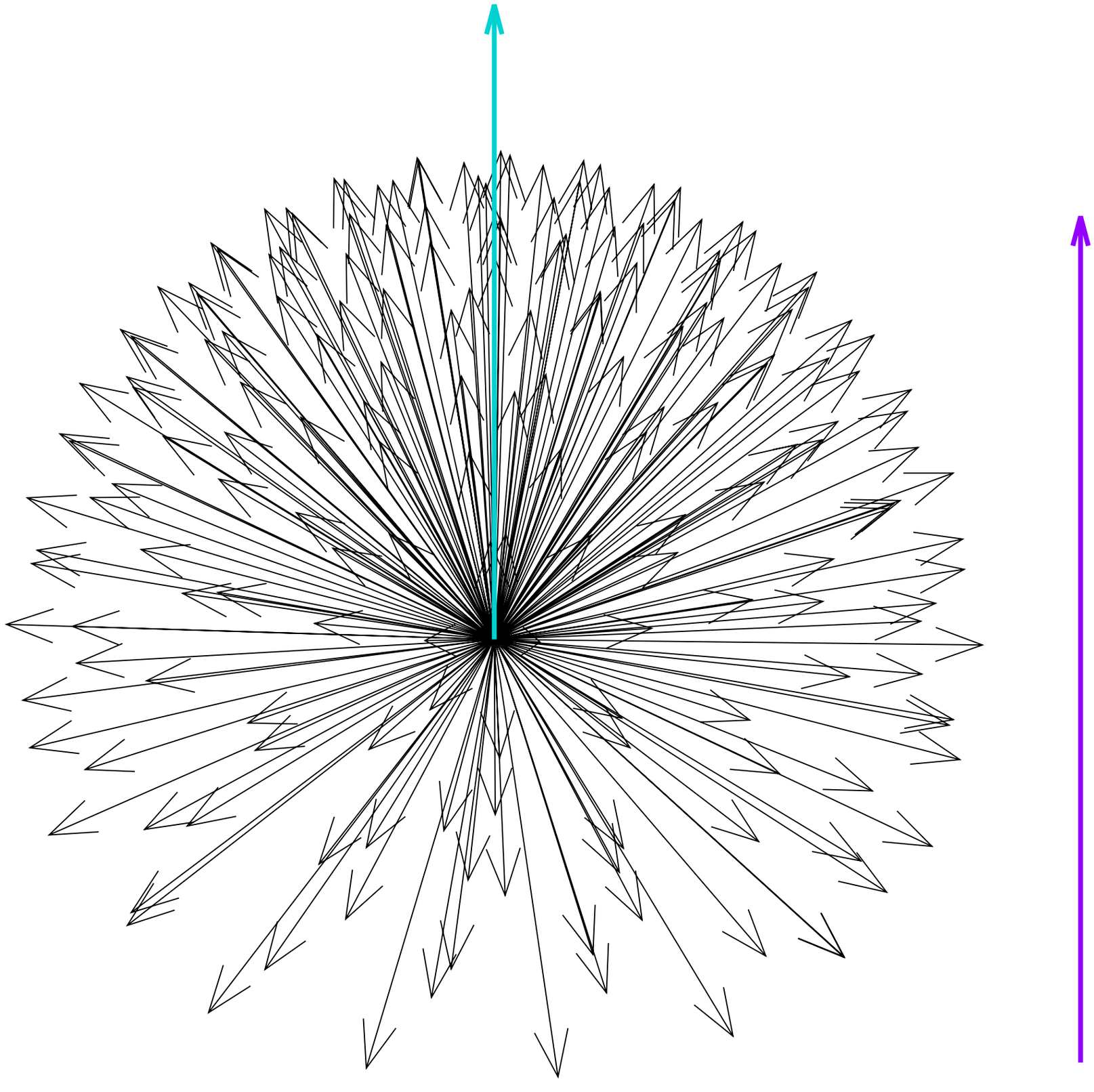
Spherical coordinates



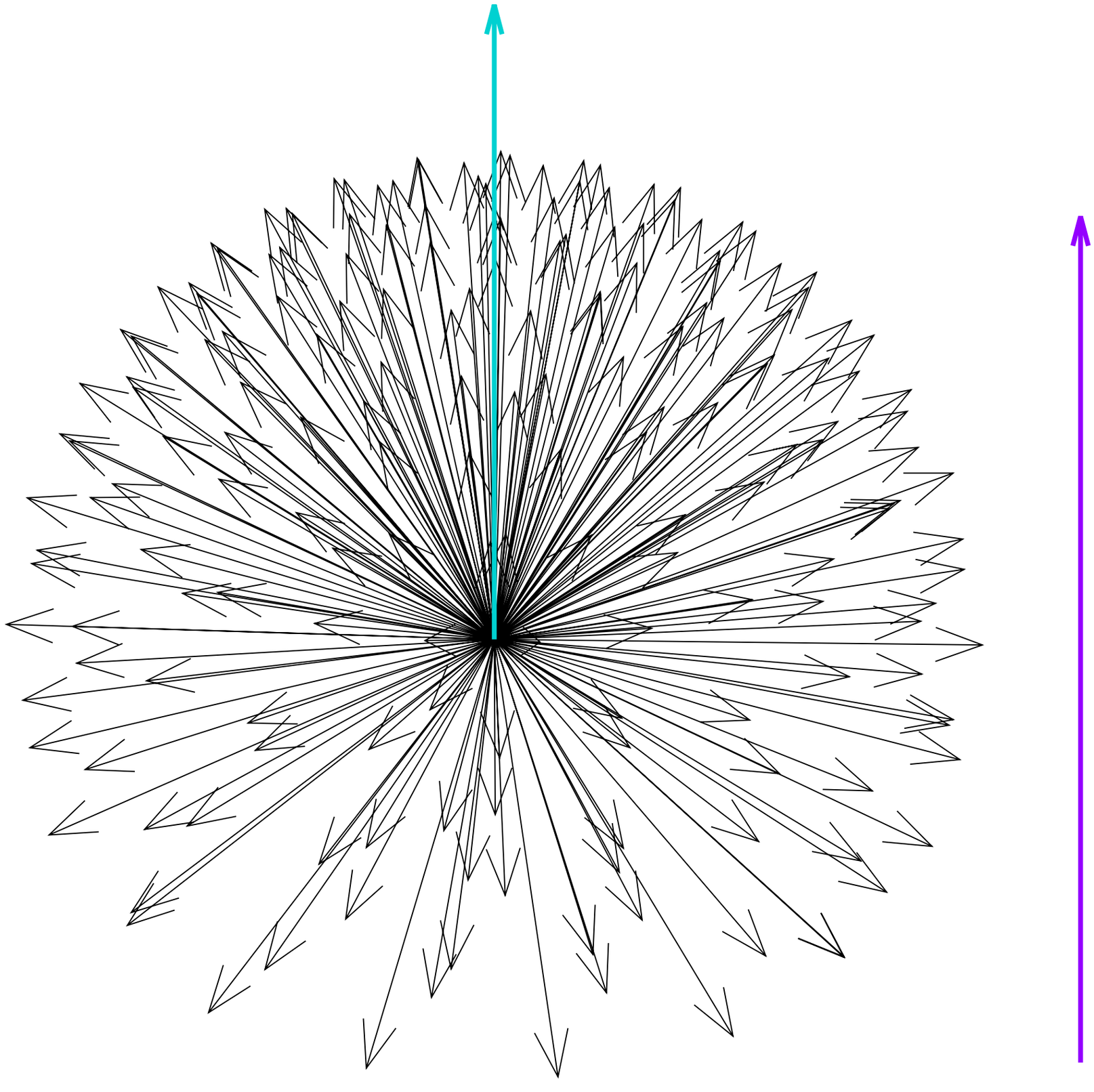


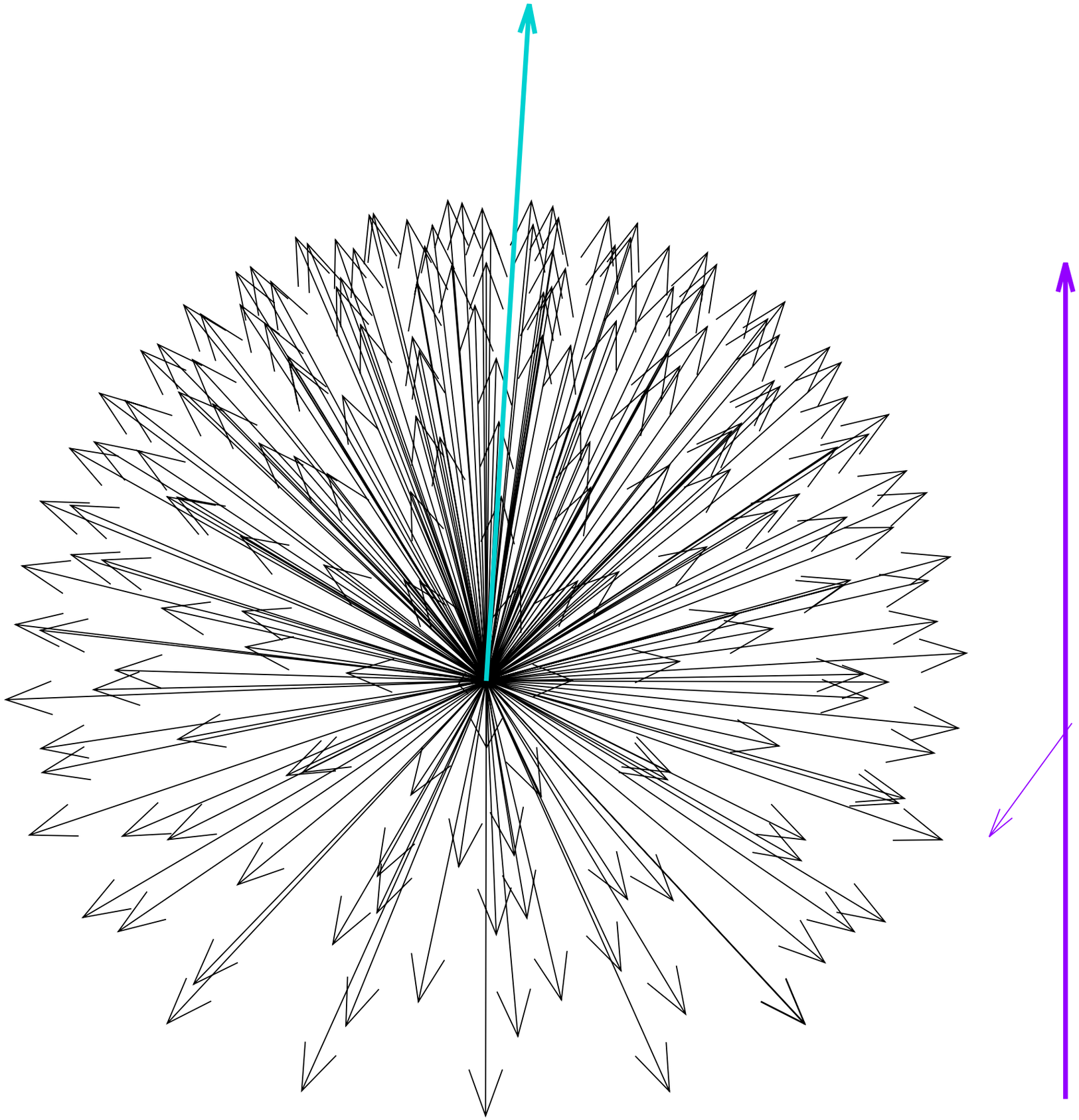
Magnetic moments in magnetic field

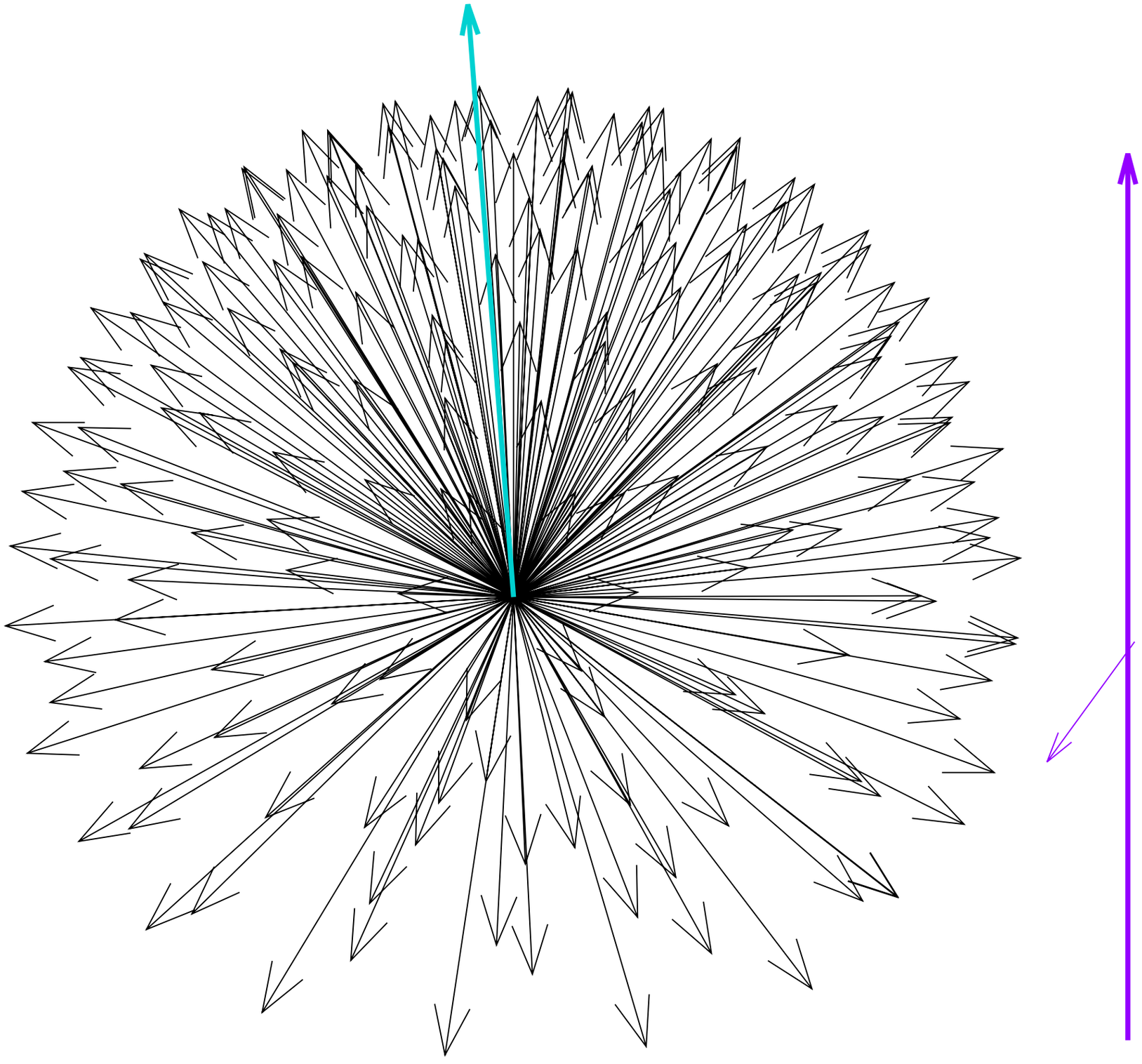


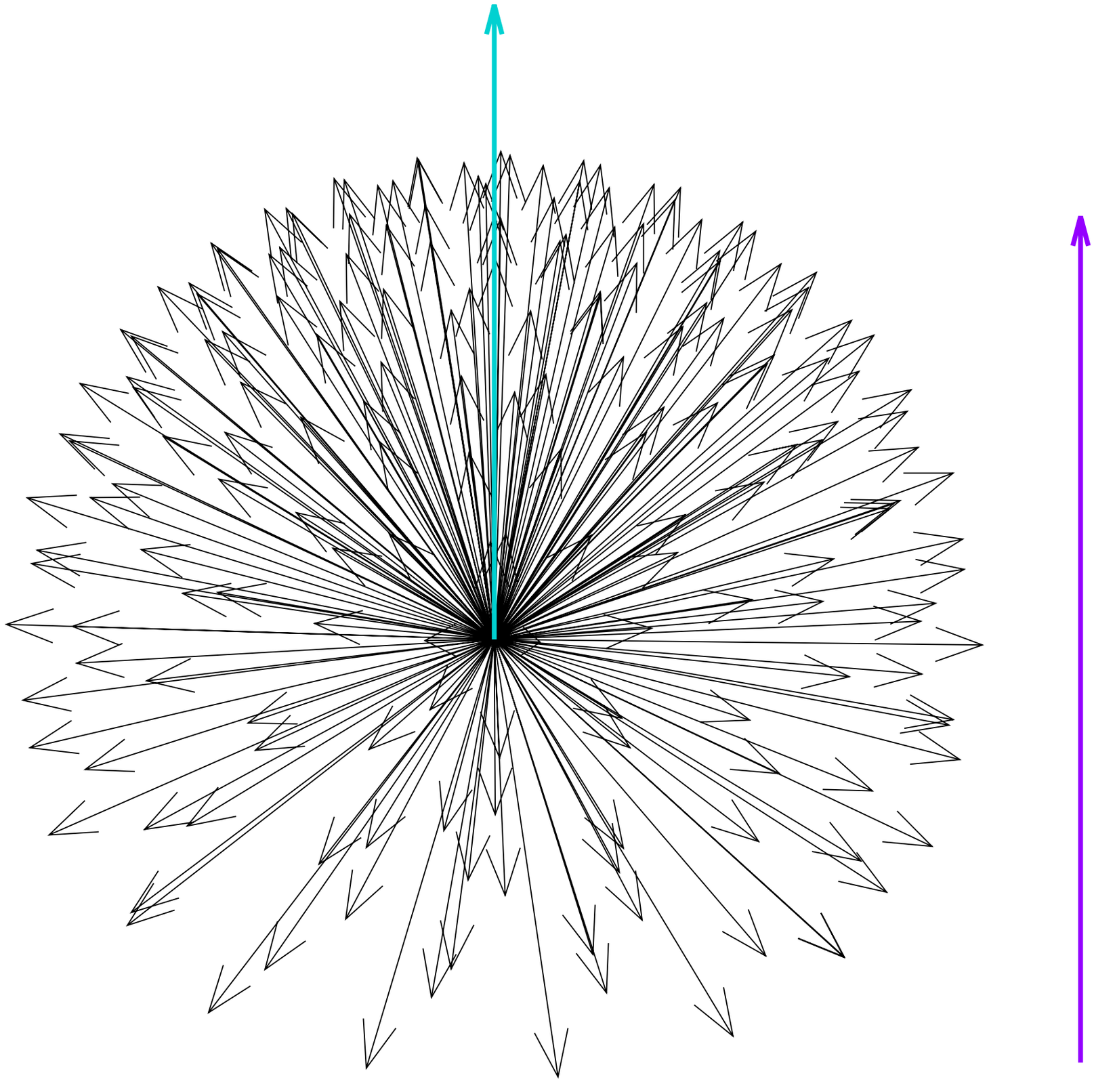


Longitudinal polarization

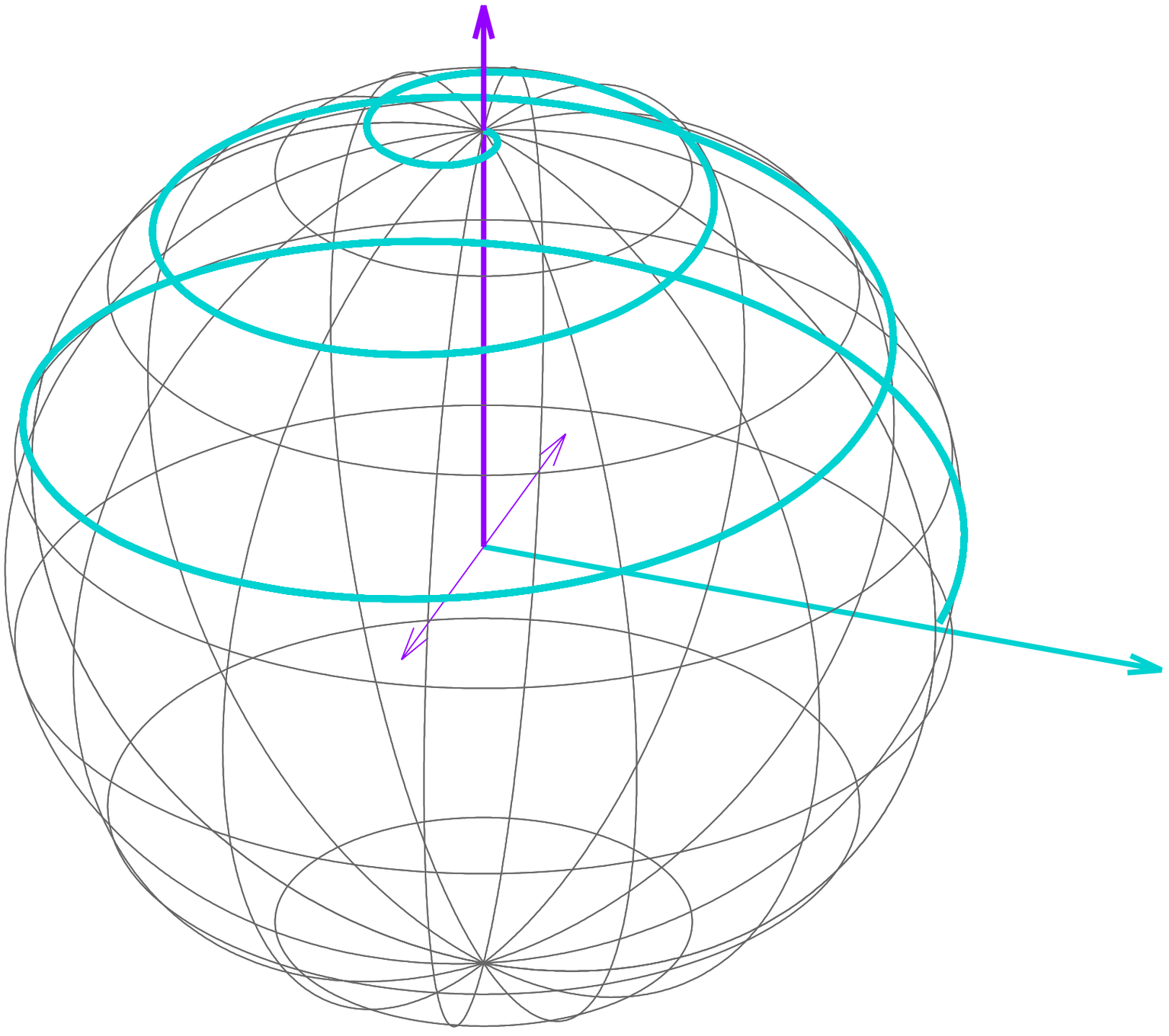


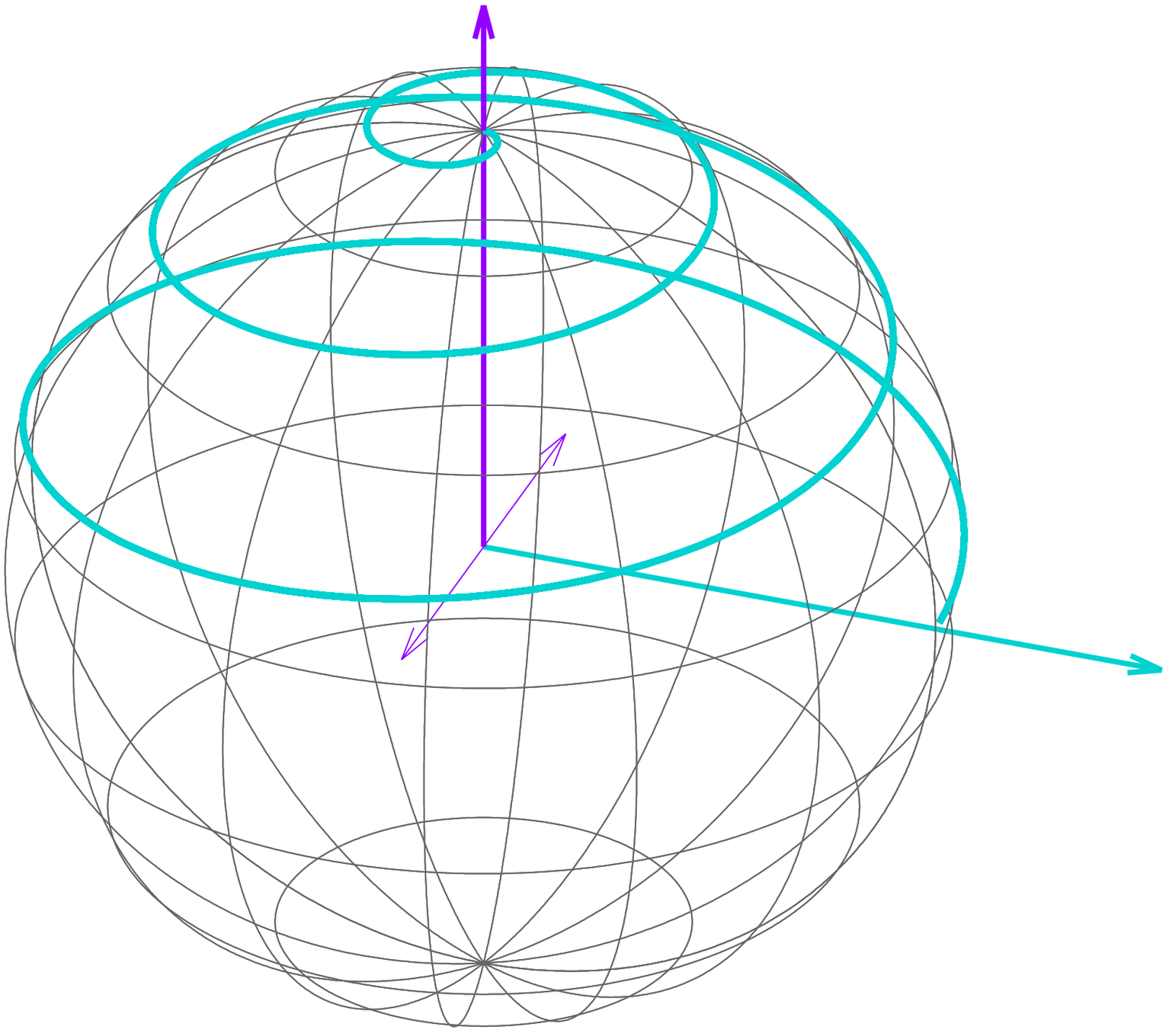


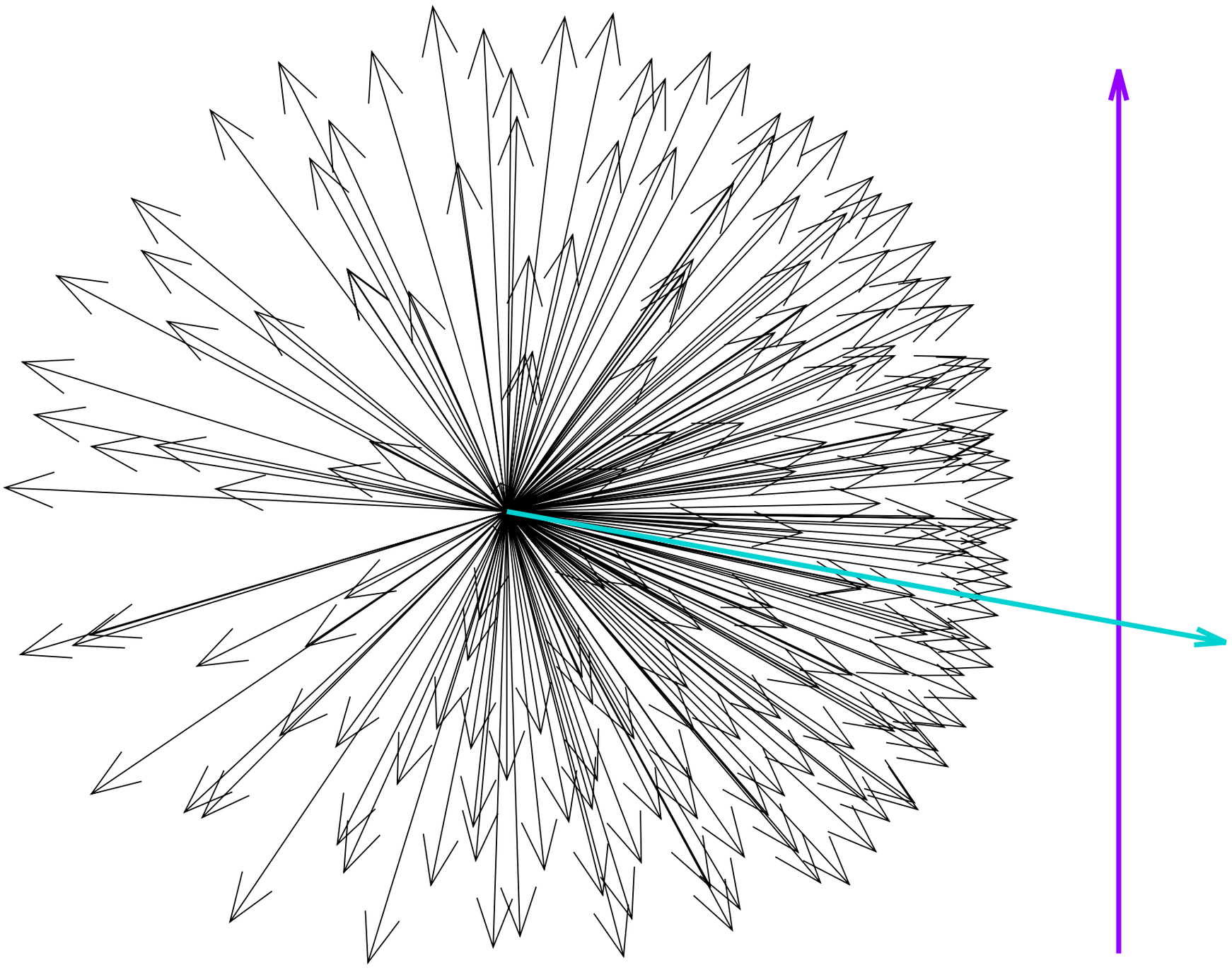




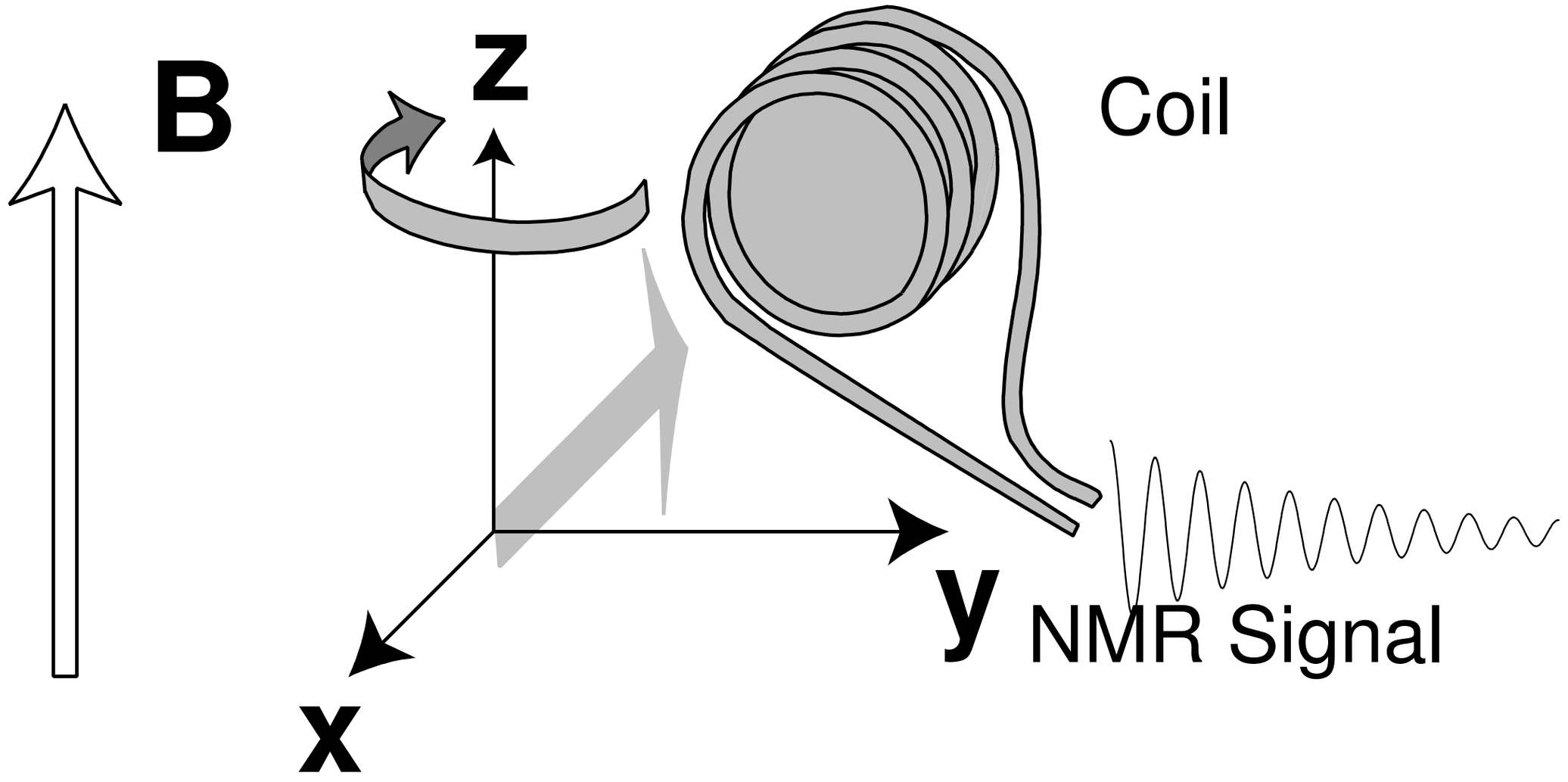
Flipping magnetization

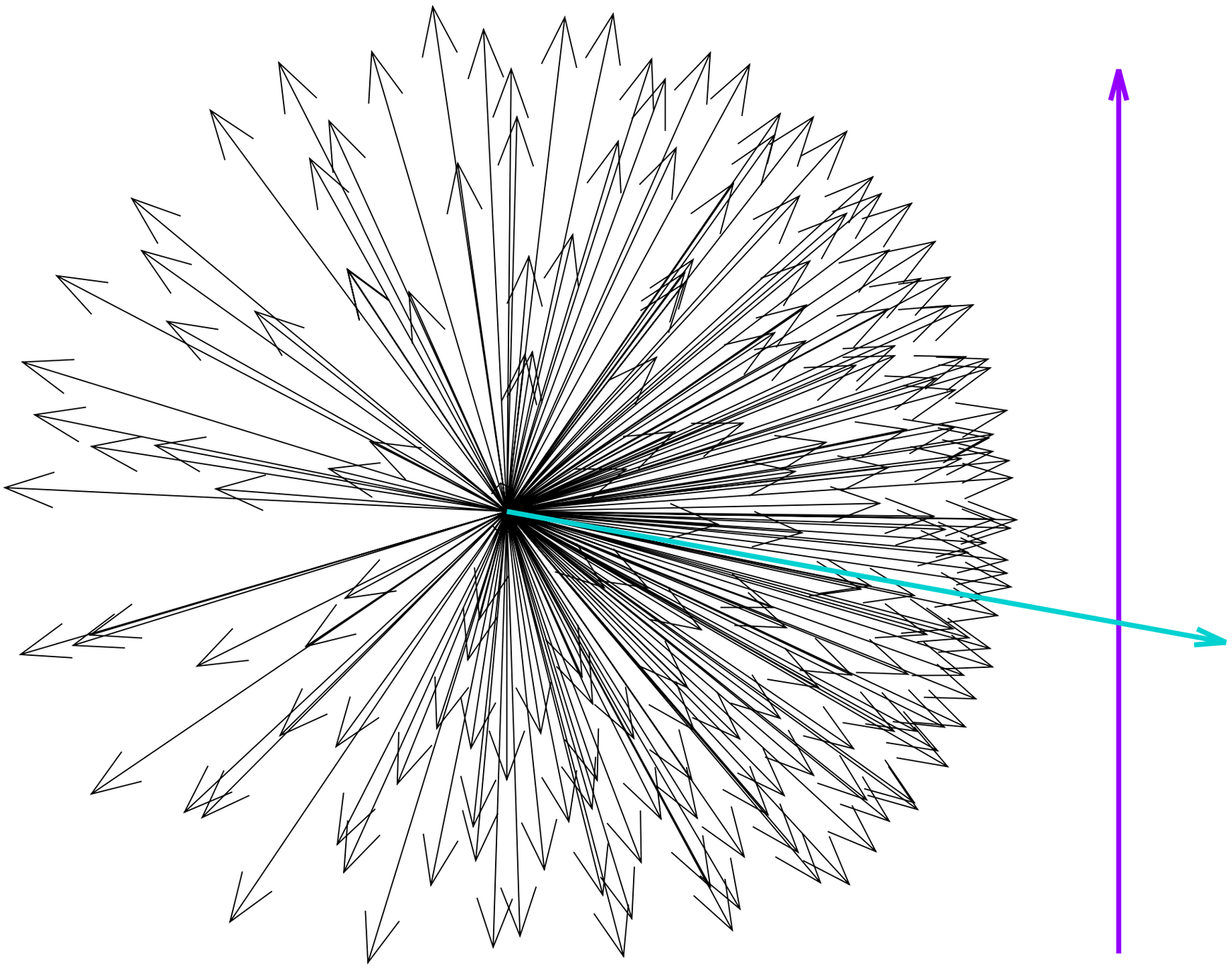


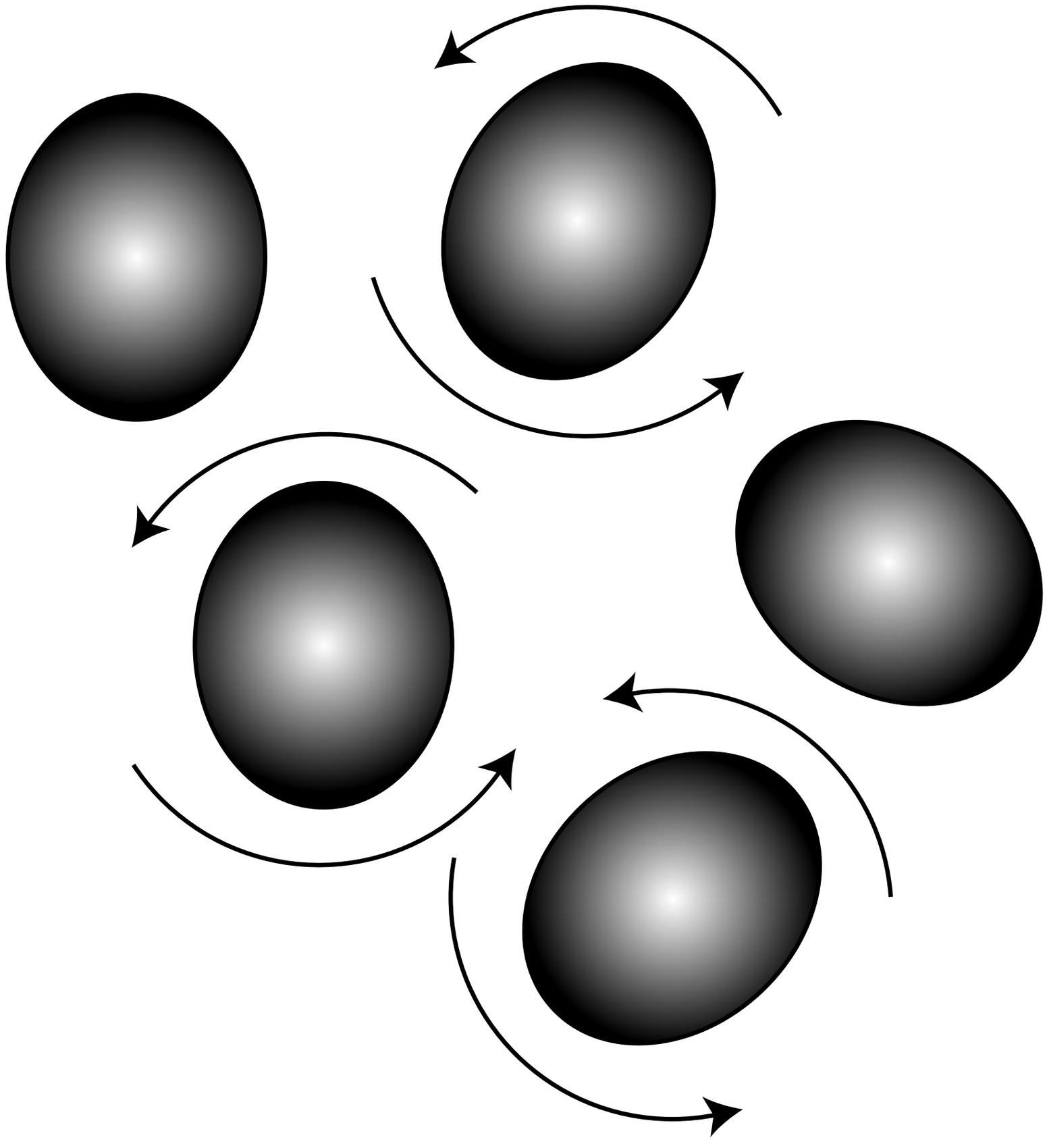


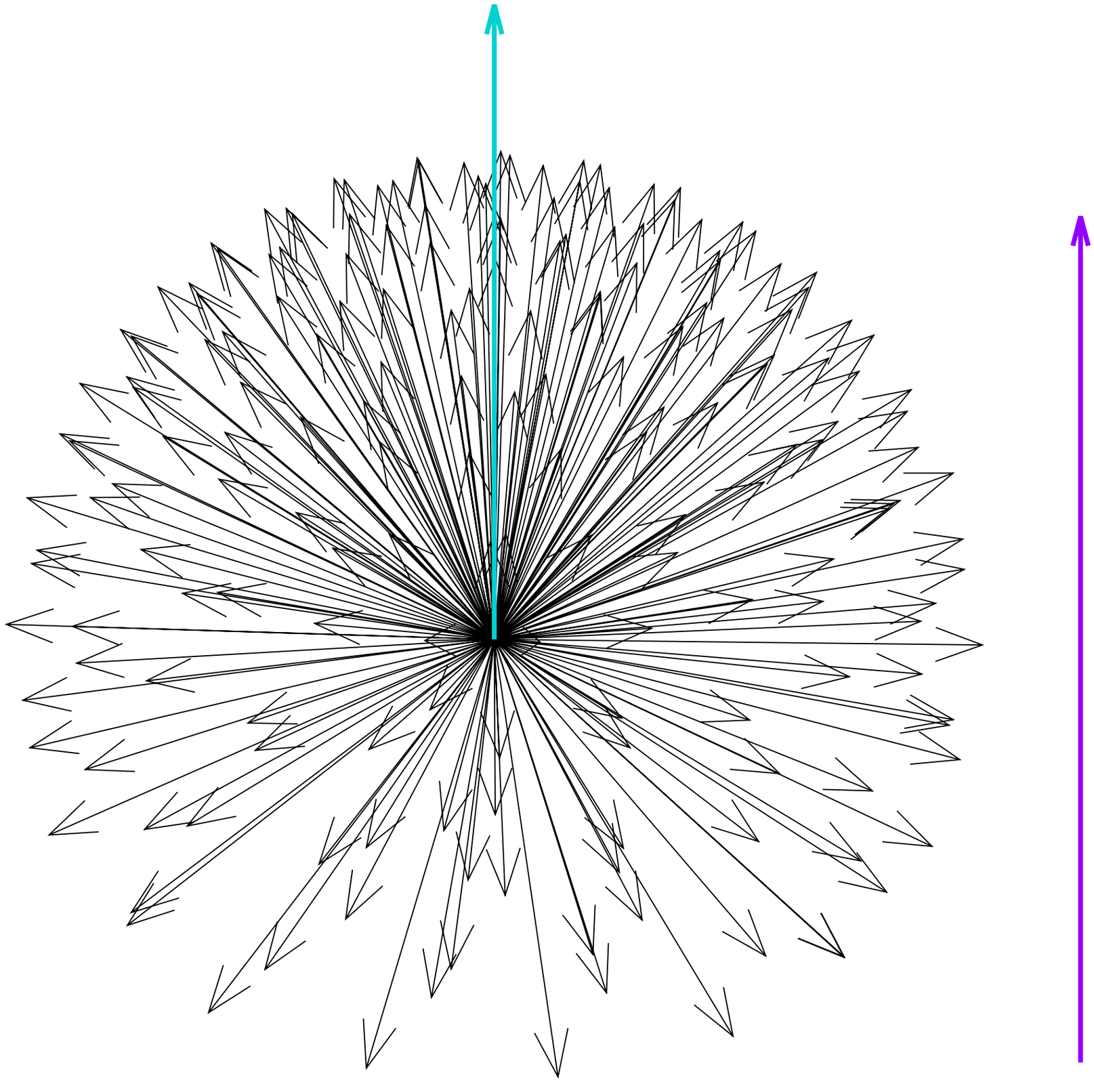


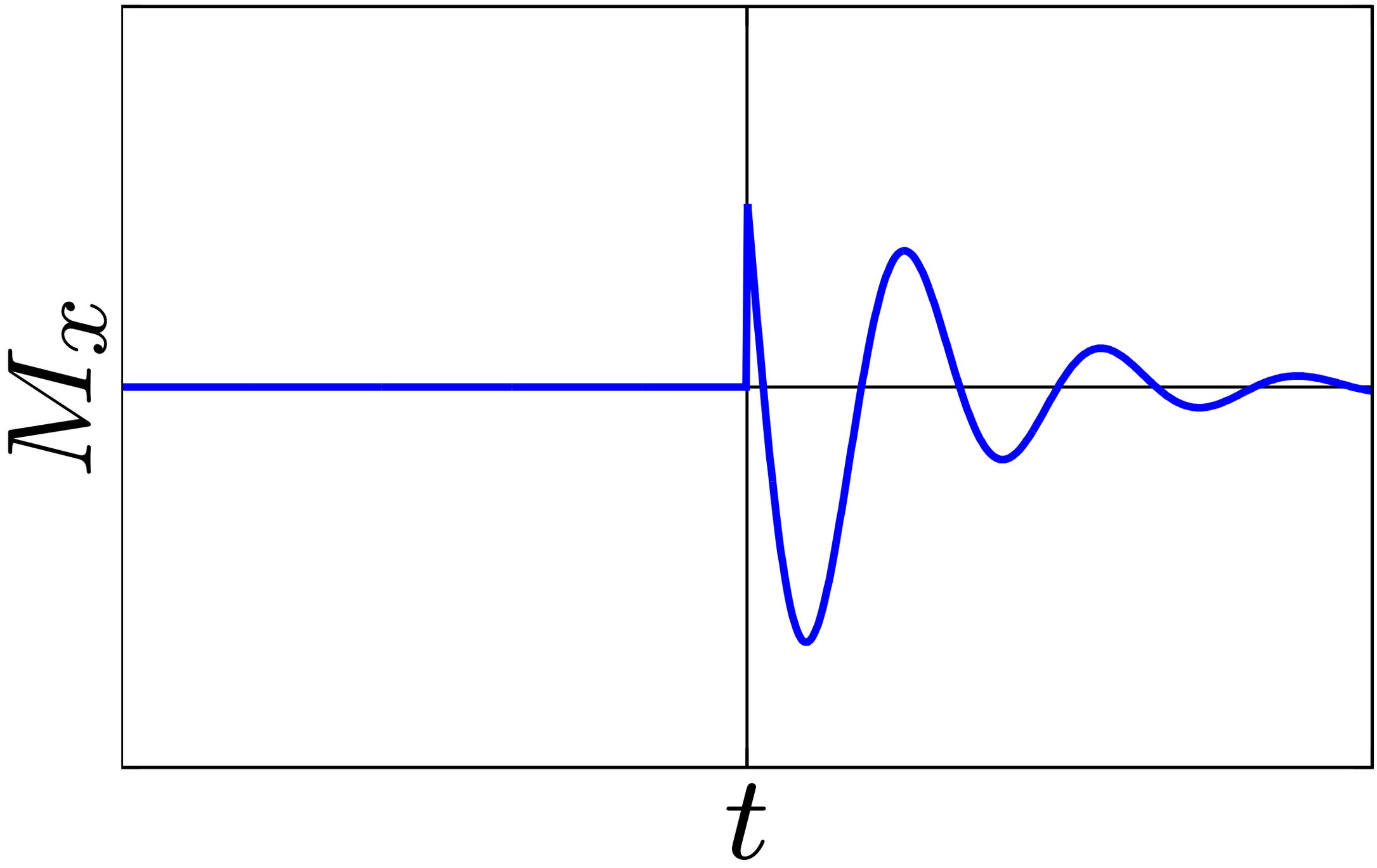
Transverse polarization

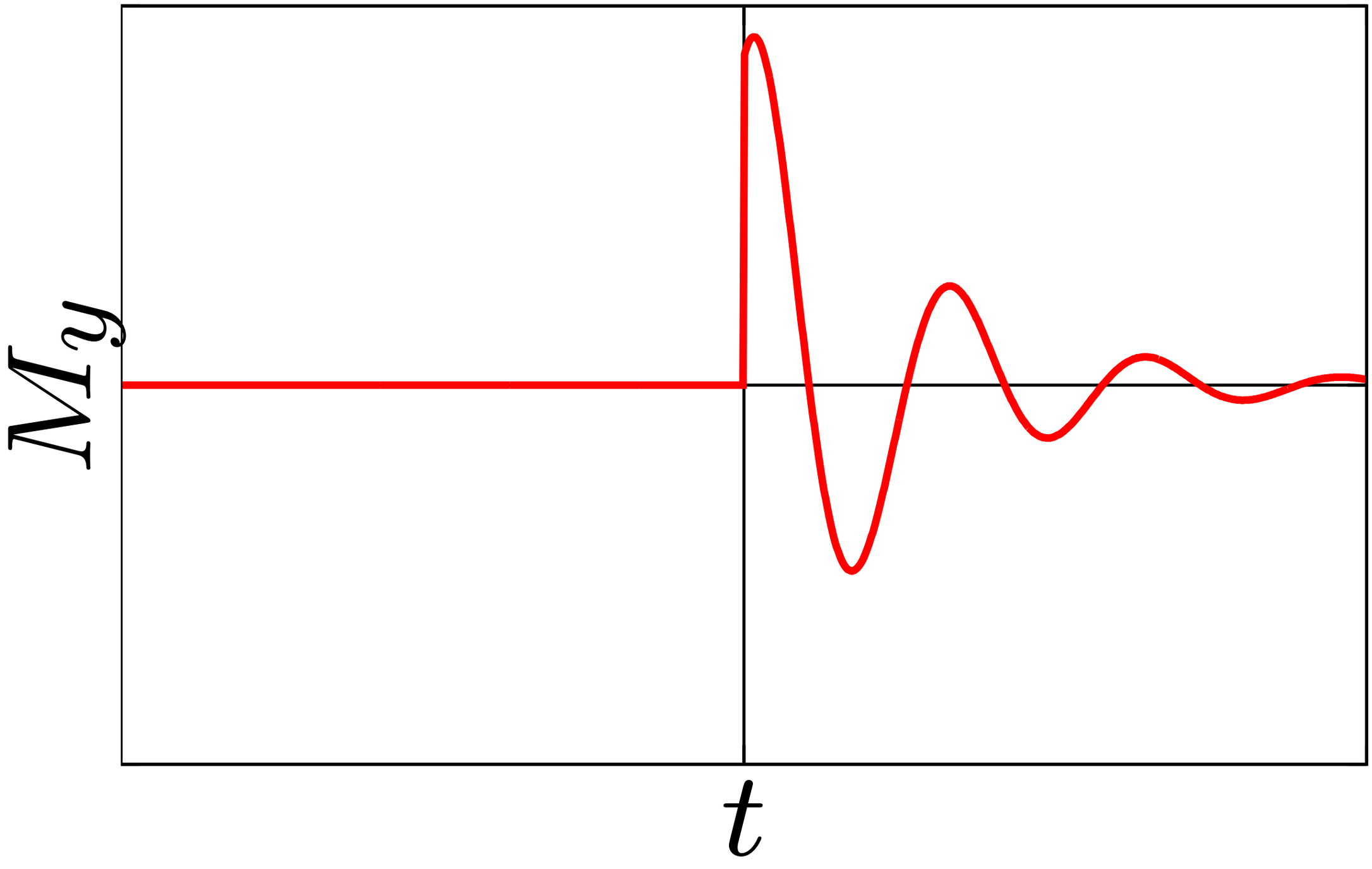

B
z
Coil
y
NMR Signal
x








M_x
t


M_y
t