Configuration Model

Session: Contrast Educational

ISMRM 2018. Program #5663

Extended Phase Graphs (EPG)

- **Extended phase graphs (EPG)** are an indispensable tool to understand and simulate the generation of echoes in multi-pulse sequences.
- Idea: **Gradients** cause specific **non-local dephasing patterns** in **periodic** sequences.
- The magnetization is expressed in terms of **EPG states**, which are associated with these patterns and **populated** in the course of time.
- An excellent review has been given by Weigel in: JMRI (2014) 41:266-295

Common EPG Limitations

- Technically, EPG states are usually not defined **microscopically**, but in terms of somewhat fuzzy **voxel-scale** Fourier integrals.
- In consequence, the requirements on **crusher** gradients, to suppress unwanted echoes in the reconstructed voxel, are difficult to understand.
- Considering dephasing due to gradients alone, also impedes the proper inclusion of **susceptibility** effects.
- The scope is limited to **periodic** sequences.

Alternative: Configuration Model (CM)

- In the following, we show that these limitations can be overcome in the **configuration model (CM)**, which differs from EPG in a few technical aspects:
  - We define **configurations**, the analogue of EPG states, purely **microscopically** and solve the **Bloch(-Torrey) equations** for them.
  - The transition to the **voxel-scale** is **postponed**, until actually needed.
  - We discuss a **multidimensional** variant, valid for **non-periodic** sequences or sequence blocks.

Configuration Model Toolkit (CoMoTk)

- Before we proceed with the CM model, it should be mentioned that a free CM implementation is available:
  - Simulation of arbitrary sequences and sequence blocks, whether idealized or as actually played out on a scanner
  - Platform: Matlab (**R2016b** or newer)
  - Download at: **https://github.com/cganter/CoMoTk**
  - Includes full documentation and theoretical background

Microscopic Scale

Model specification

- Spin ensemble
  - **static** (except for **diffusion**)
  - **non-interacting**
  - **pure** (1-peak model)
- Sequence = alternating train of **arbitrary**
  - **instantaneous** RF pulses
  - **time intervals**

Microscopic Scale

Spin ensemble

- Intra-voxel position $\boldsymbol{x}$
- Proton density $\boldsymbol{m}_{eq}(\boldsymbol{x})$
- Relaxation times $T_1(\boldsymbol{x})$, $T_2(\boldsymbol{x})$
- Off-resonance frequency $\omega(\boldsymbol{x})$
- Diffusion tensor $\boldsymbol{D}(\boldsymbol{x})$
- Notation: In the following, we drop the implicit dependence on the position $\boldsymbol{x}$, if not explicitly relevant.

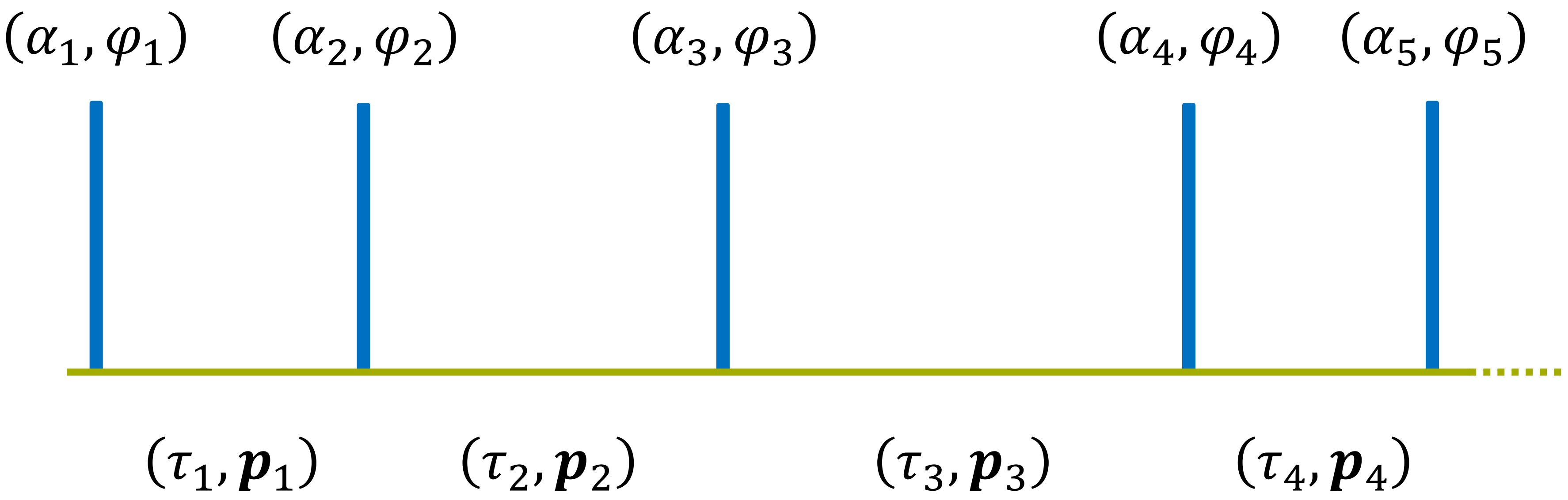
Microscopic Scale

RF pulses and time intervals

- RF pulse ($\nu = 1, 2, \ldots$)
  - Flip angle α_ν
  - Phase φ_ν
- Time interval ($\nu = 1, 2, \ldots$)
  - Duration τ_ν
  - Gradient moment $\boldsymbol{p}_\nu(t) := \gamma \int_0^t d\tau\, \boldsymbol{G}_\nu(\tau)$
  - Gradient moment over whole interval $\boldsymbol{p}_\nu := \boldsymbol{p}_\nu(\tau_\nu)$

Microscopic Scale

Pictorial view of non-periodic sequence



Microscopic Scale

Equality of time intervals

- Over the whole time interval τ_ν, the phase, accumulated by **static** spins, does not depend on the precise gradient form $\boldsymbol{p}_\nu(t)$, but only on the total gradient moment $\boldsymbol{p}_\nu$.
- Two intervals $(\tau_a, \boldsymbol{p}_a)$ and $(\tau_b, \boldsymbol{p}_b)$ shall therefore be considered as **equal**, if, and only if, $\tau_a = \tau_b$ **and** $\boldsymbol{p}_a = \boldsymbol{p}_b$.
- The number of **different** intervals, d, is called the **dimension** of the configuration model.

Microscopic Scale

Equality of time intervals

- We assign a **unique** identifier $\mu = 1, \dots, d$ to all **different** intervals, based on some **mapping**

$$\mu \;:\; \mathbb{N} \longrightarrow \{1, \dots, d\} \;:\; \nu \longmapsto \mu(\nu)$$

- The **phase** ϑ_μ, accumulated in time interval $\mu \equiv \mu(\nu)$ due to the **combined** effect of **off-resonance** and **gradients**, is then given by

$$\vartheta_\mu = \omega\tau_\mu - \boldsymbol{p}_\mu \boldsymbol{x}$$

Microscopic Scale

Configuration model

- **Immediately after** any RF pulse or time interval, the local magnetization density vector $\boldsymbol{m}_\nu(\boldsymbol{x})$ can be written in the form

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

- The d elements of the vector $\boldsymbol{\vartheta}$ are just the accumulated phases ϑ_μ.
- $\boldsymbol{m}_\nu^{(\boldsymbol{n})}$ and $\boldsymbol{n}$ are called **configuration vector** and **configuration order**, respectively.

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

Configuration model

- Uniquely associated with any configuration order $\boldsymbol{n}$ is a time scale $\tau_{\boldsymbol{n}}$

  and a gradient moment $\boldsymbol{p}_{\boldsymbol{n}}$

$$\tau_{\boldsymbol{n}} \coloneqq \sum_{\mu=1}^{d} n_\mu \tau_\mu \qquad\qquad \boldsymbol{p}_{\boldsymbol{n}} \coloneqq \sum_{\mu=1}^{d} n_\mu \boldsymbol{p}_\mu$$

- With these definitions, the configuration model can also be written

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

Spin dynamics

- The ν^{th} RF pulse or time interval modifies the magnetization density

$$\boldsymbol{m}_{\nu,+} = \boldsymbol{B}_\nu\, \boldsymbol{m}_{\nu,-} + \boldsymbol{b}_\nu$$

- After inserting the configuration model for $\boldsymbol{m}_{\nu,\pm}$, we equate equal powers $e^{i\boldsymbol{n}\boldsymbol{\vartheta}}$ and the resulting recursion relations for $\boldsymbol{m}_{\nu,\pm}^{(\boldsymbol{n})}$ must be of the general form

$$\boldsymbol{m}_{\nu,+}^{(\boldsymbol{n})} = \sum_{\boldsymbol{q}\in\mathbb{Z}^d} \boldsymbol{B}_\nu^{(\boldsymbol{n},\boldsymbol{q})} \boldsymbol{m}_{\nu,-}^{(\boldsymbol{n}+\boldsymbol{q})} + \delta_{\boldsymbol{n}\boldsymbol{0}} \cdot \boldsymbol{b}_\nu$$

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n} \in \mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}} \, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

RF pulse

- An instantaneous RF pulse is described by a simple rotation

$$\boldsymbol{m}_{\nu,+} = \boldsymbol{R}(\alpha_\nu, \varphi_\nu) \, \boldsymbol{m}_{\nu,-}$$

- Since the phase factors $e^{i\boldsymbol{n}\boldsymbol{\vartheta}}$ do not change, the same recursion holds for every configuration vector

$$\boldsymbol{m}_{\nu,+}^{(\boldsymbol{n})} = \boldsymbol{R}(\alpha_\nu, \varphi_\nu) \, \boldsymbol{m}_{\nu,-}^{(\boldsymbol{n})}$$

Microscopic Scale

Time interval

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

- In the ν^{th} time interval, the transverse magnetization precesses by an angle $\pm\,\vartheta_{\mu(\nu)}$. This translates to a change of the configuration order

$$e^{i\boldsymbol{n}\boldsymbol{\vartheta}} \longrightarrow e^{i\boldsymbol{n}(\boldsymbol{\vartheta}\,\pm\,\vartheta_\mu\cdot\boldsymbol{e}_\mu)} = e^{i(\boldsymbol{n}\,\pm\,\boldsymbol{e}_\mu)\boldsymbol{\vartheta}}$$

where $\boldsymbol{e}_\mu$ is just the unit vector, defined by $\left(\boldsymbol{e}_\mu\right)_\eta = \delta_{\mu\eta}$.

- We therefore get a recursion of the form

$$\boldsymbol{m}_{\nu,+}^{(\boldsymbol{n})} = \sum_{j=-1}^{1} \boldsymbol{B}_\nu^{(\boldsymbol{n},\, j\cdot\boldsymbol{e}_\mu)} \boldsymbol{m}_{\nu,-}^{(\boldsymbol{n}+j\cdot\boldsymbol{e}_\mu)} + \delta_{\boldsymbol{n}\boldsymbol{0}}\cdot\left(1 - e^{-\tau_\mu/T_1}\right)\cdot\boldsymbol{m}_{eq}$$

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n} \in \mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}} \, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

Time interval

- The matrix $\boldsymbol{B}_\nu^{(\boldsymbol{n},\, j\cdot \boldsymbol{e}_\mu)}$ exclusively consists of **damping** terms due to **relaxation** and (optionally) **diffusion**.
- All **precession** effects are encoded in the phase factors $e^{i\boldsymbol{n}\boldsymbol{\vartheta}}$ only.
- Explicit expressions for $\boldsymbol{B}_\nu^{(\boldsymbol{n},\, j\cdot \boldsymbol{e}_\mu)}$ are derived in the documentation on the CoMoTk page.

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

Populated configurations

- Prior to the first RF pulse, the most common initial state is just the proton density

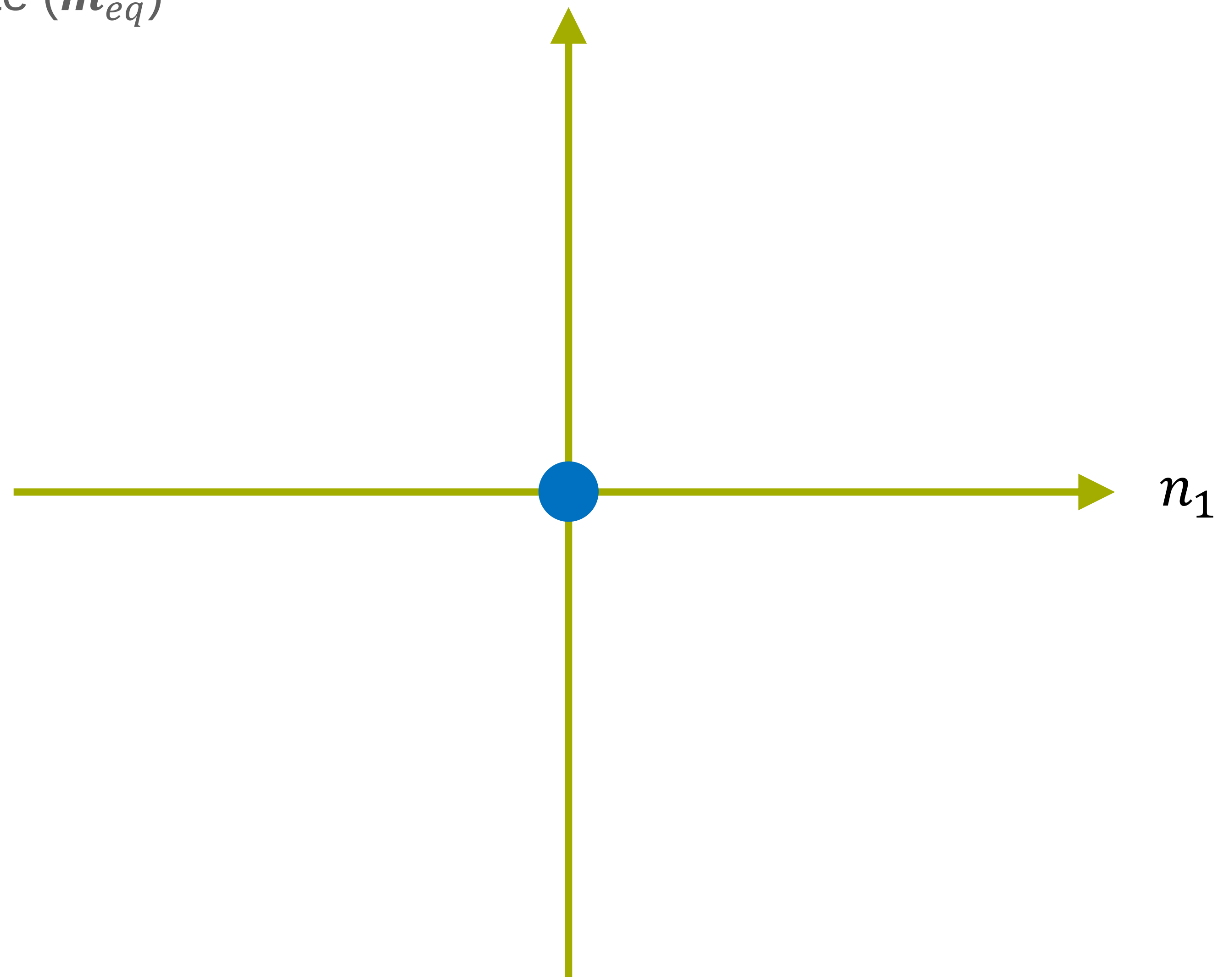
$$\boldsymbol{m}_0^{(\boldsymbol{n})} = \delta_{\boldsymbol{n}\boldsymbol{0}} \cdot \boldsymbol{m}_{eq}$$

- This means that only the configuration $\boldsymbol{n} = \boldsymbol{0}$ is **populated**.
- To get an impression, how the population evolves under subsequent RF pulses and time intervals, we now look at the case $d = 2$.

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\vartheta}\,\boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

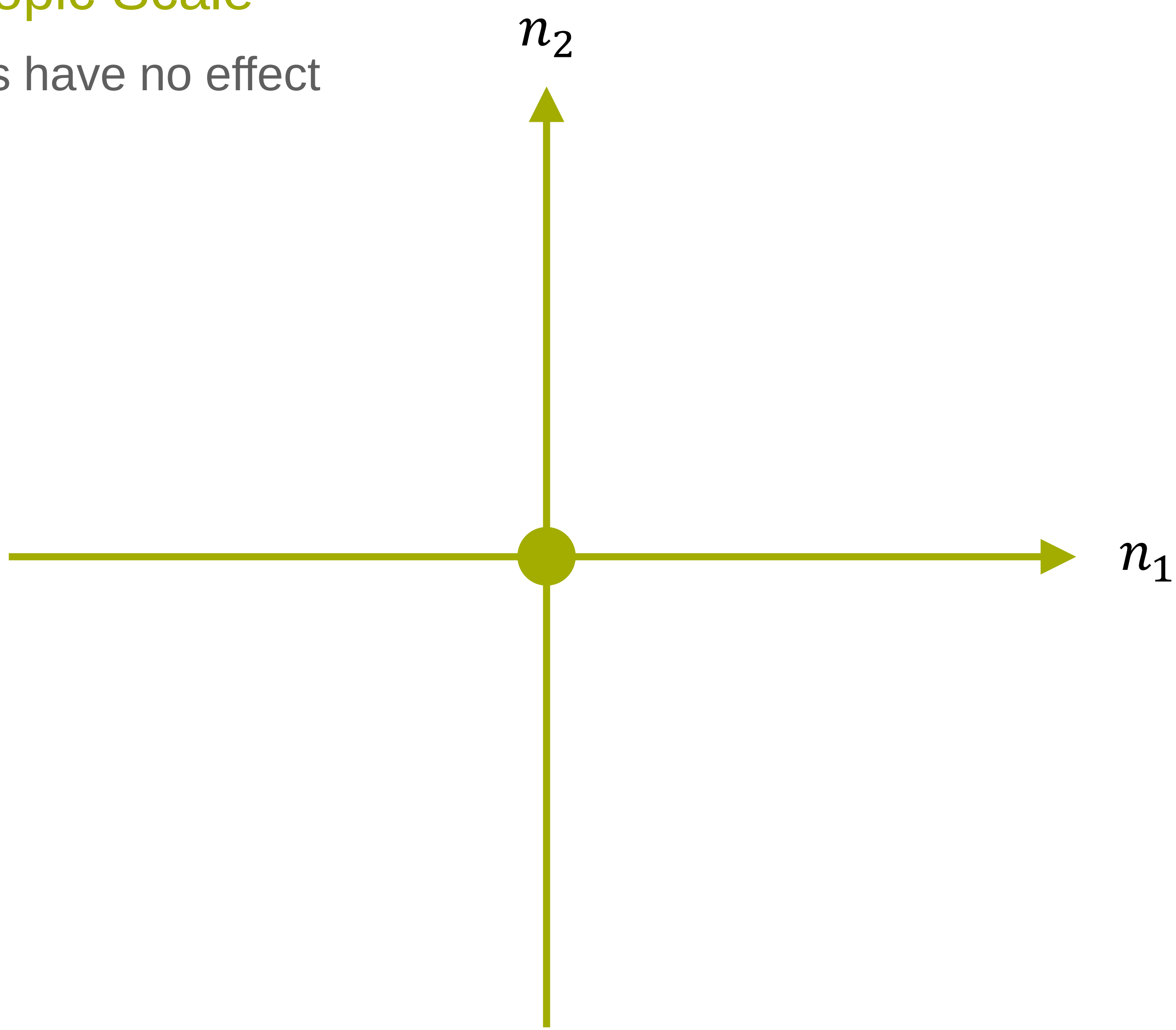
Initial state ($\boldsymbol{m}_{eq}$)



$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

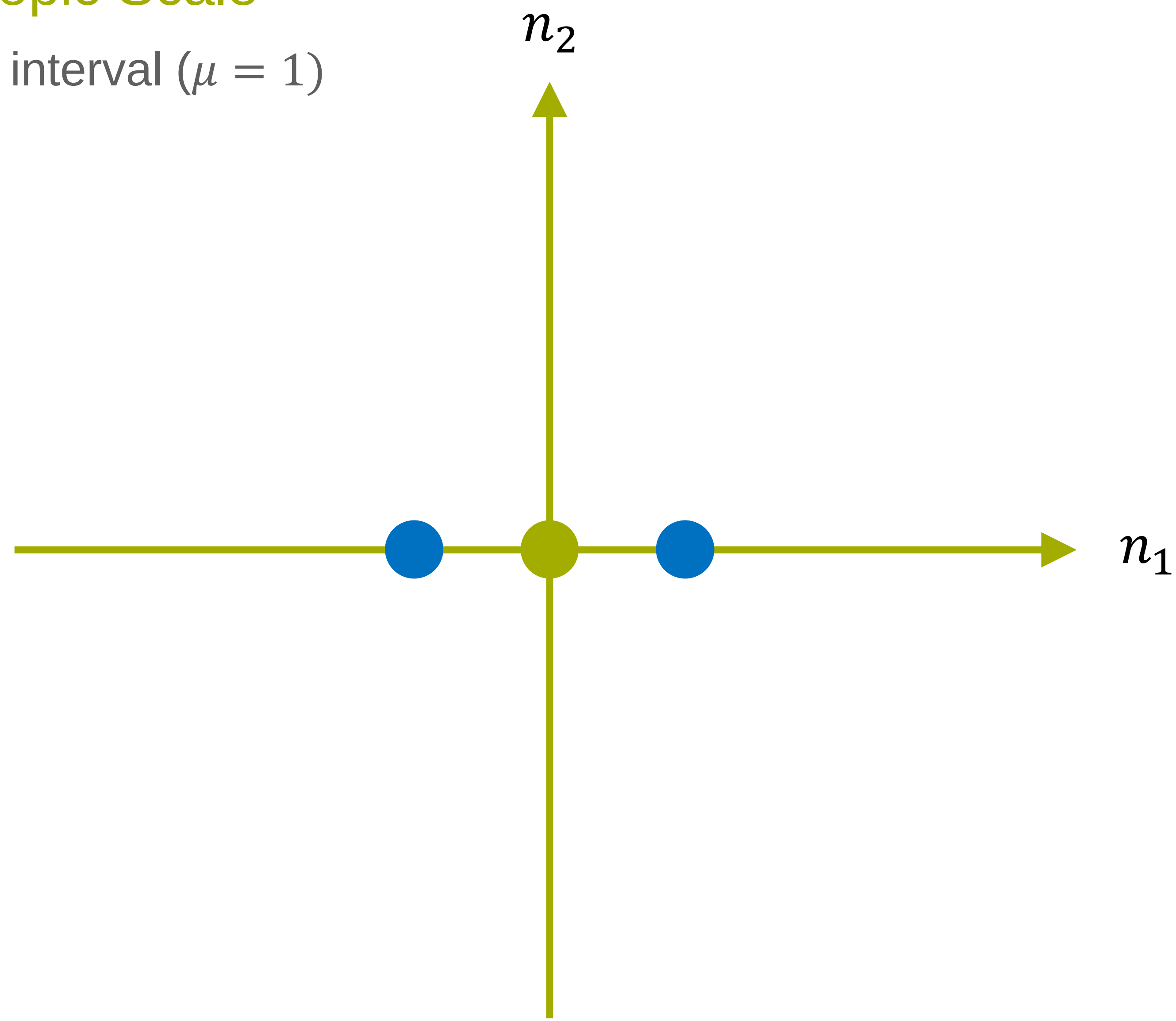
RF pulses have no effect



Microscopic Scale

First time interval ($\mu = 1$)

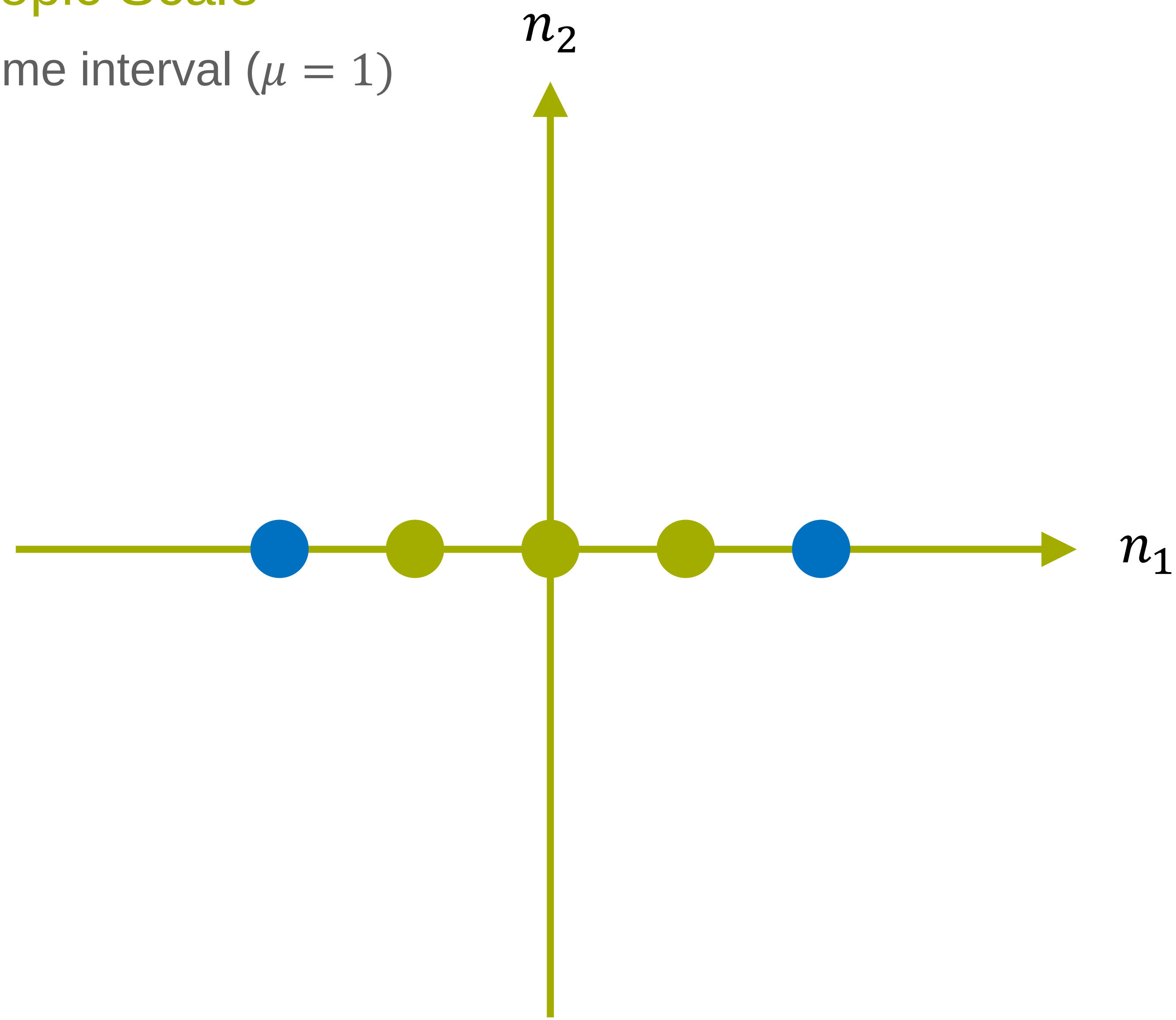
$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n} \in \mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}} \, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$



$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

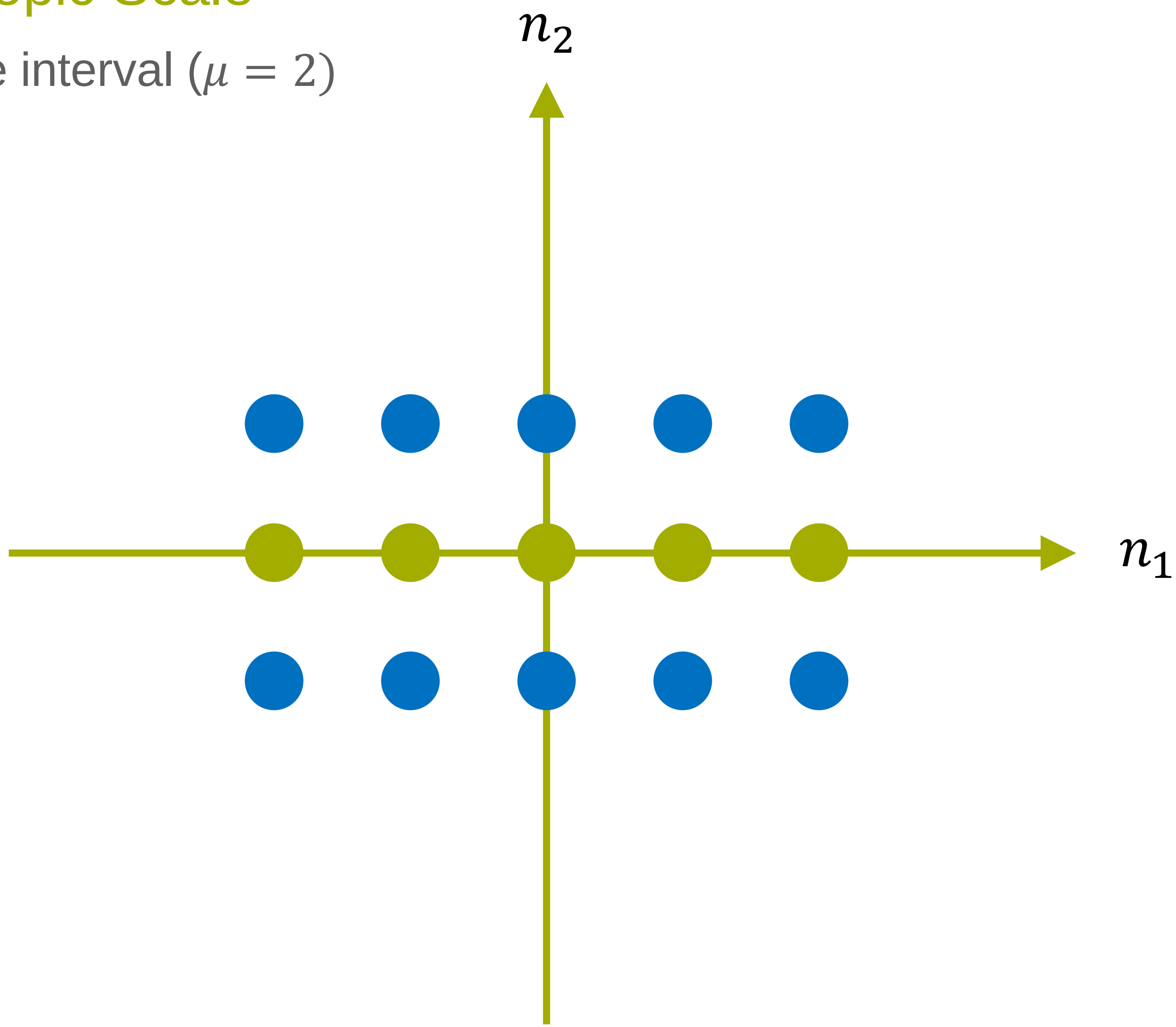
Second time interval ($\mu = 1$)



$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

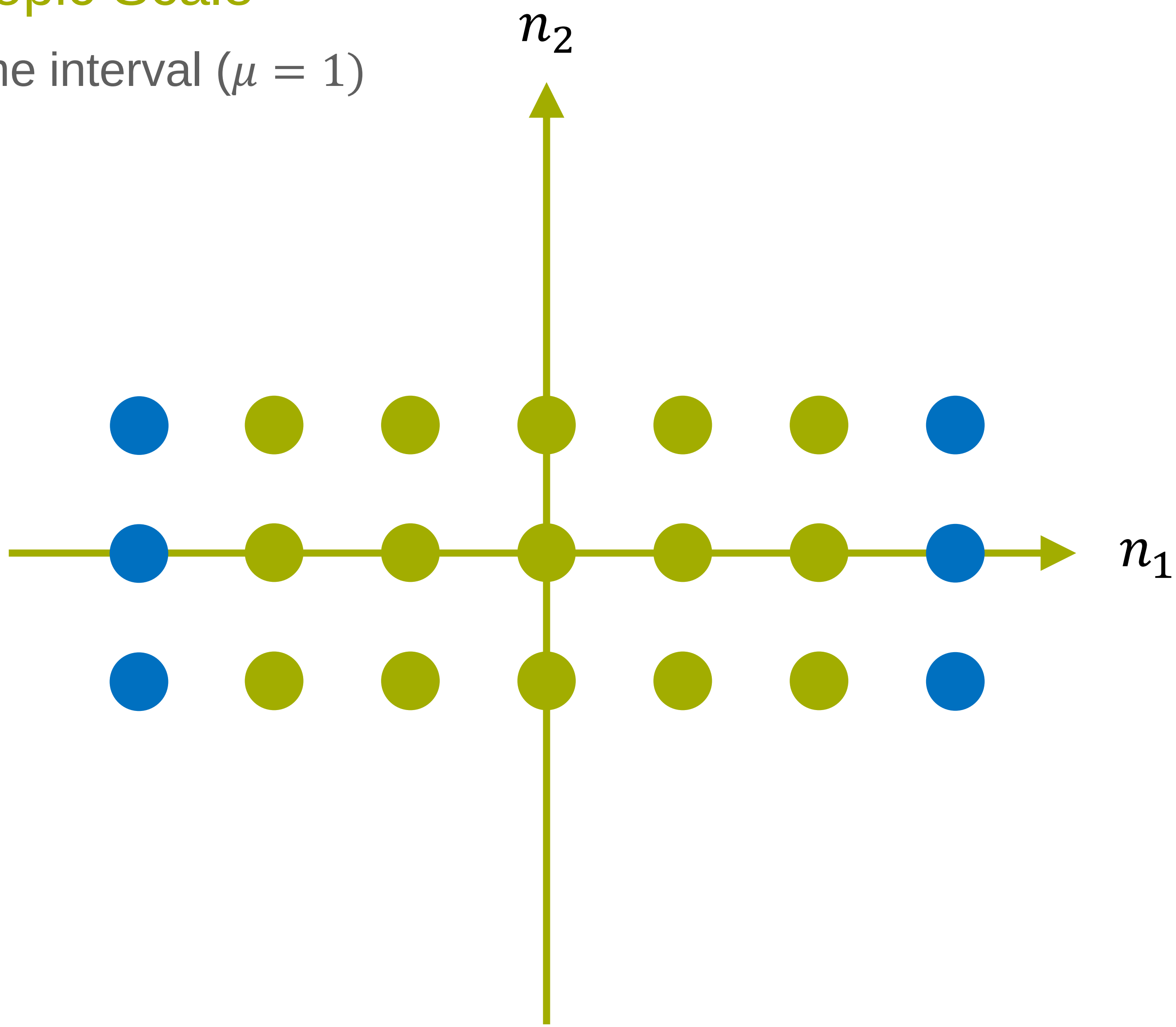
Third time interval ($\mu = 2$)



$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

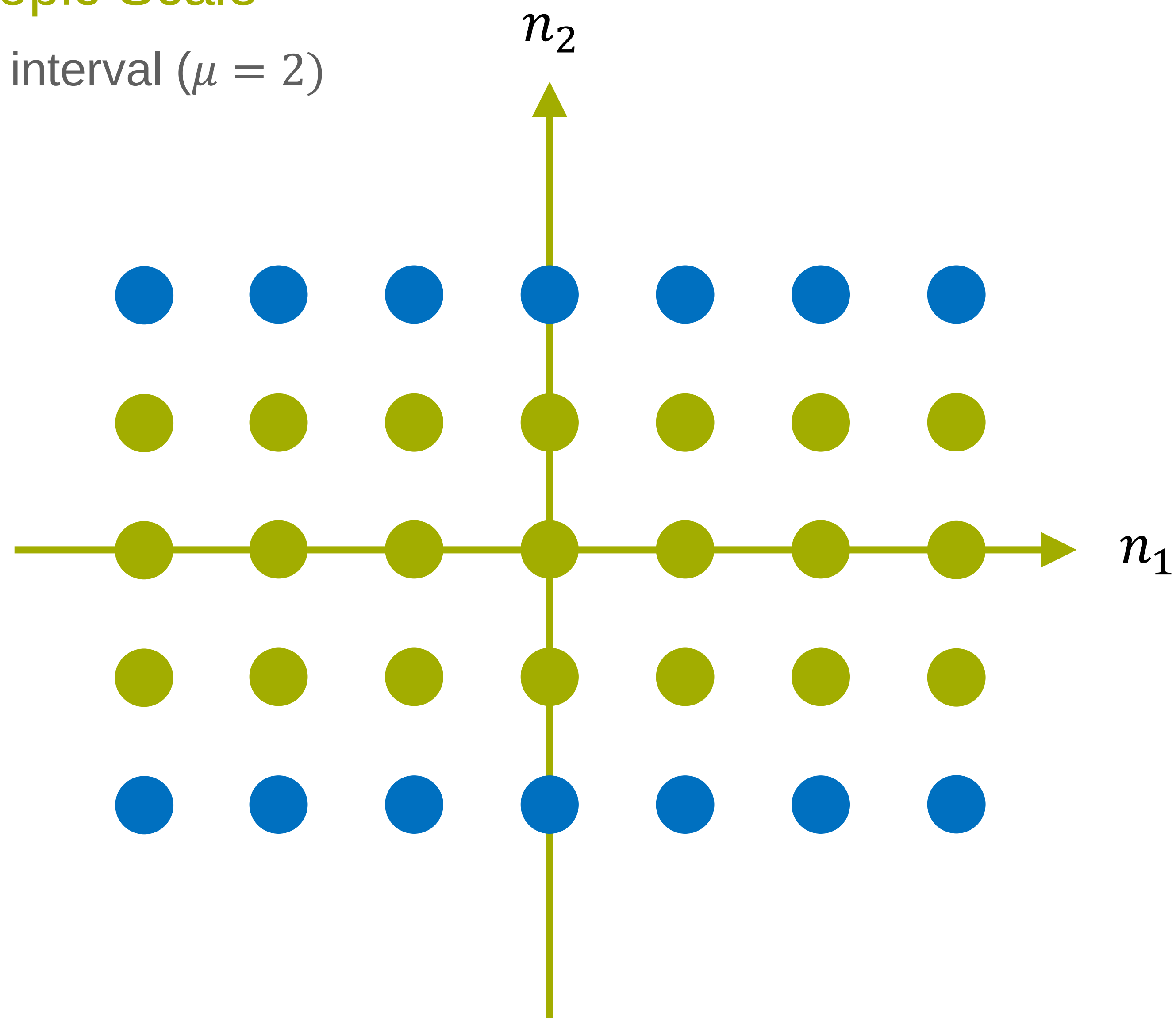
Fourth time interval ($\mu = 1$)



$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

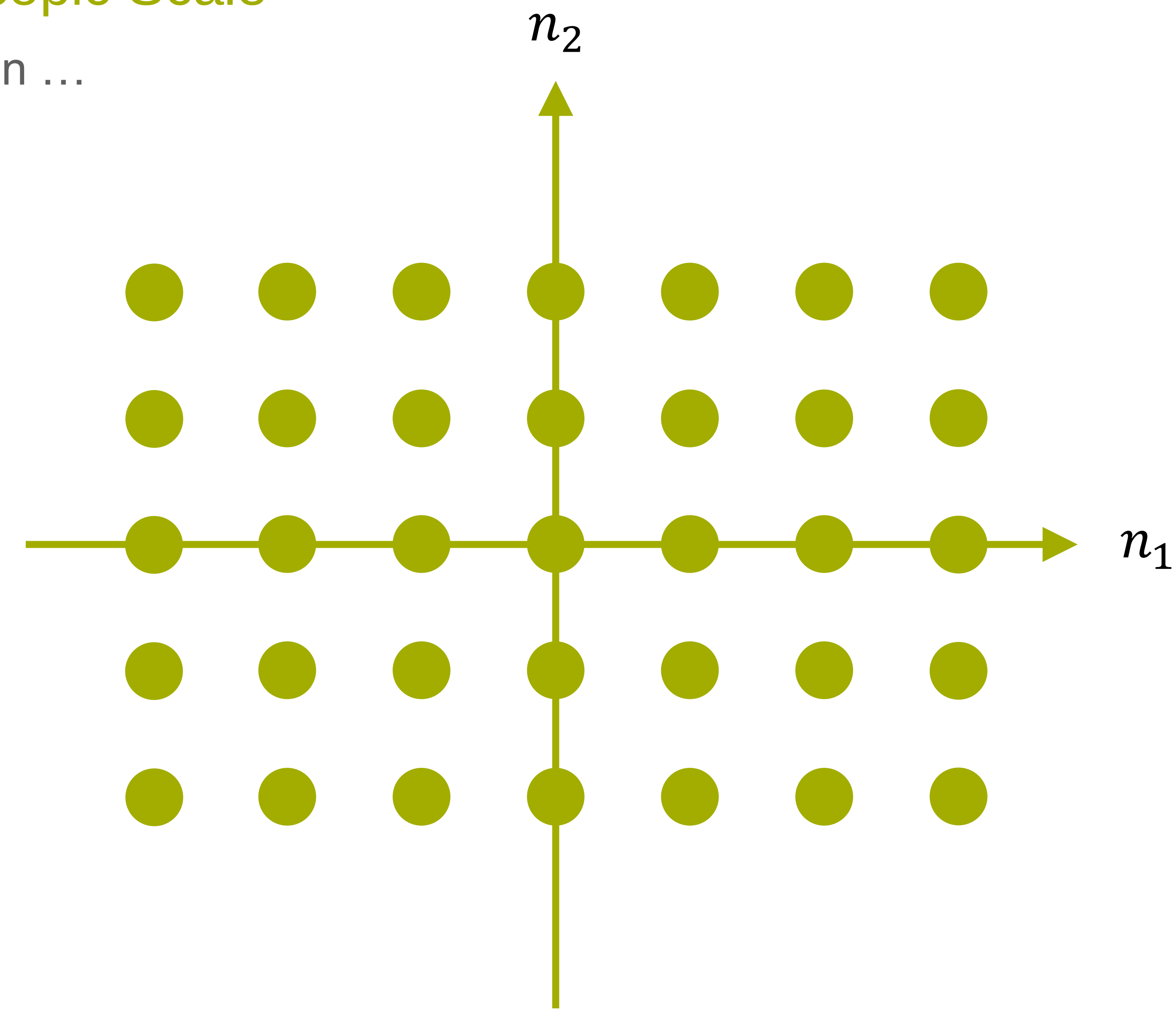
Fifth time interval ($\mu = 2$)



$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i\boldsymbol{n}\boldsymbol{\vartheta}}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Microscopic Scale

And so on …



$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Beyond the Microscopic Scale

Use of the configuration model

- The configuration model appears to be just a cumbersome and highly redundant representation of the magnetization density $\boldsymbol{m}(\boldsymbol{x})$.
- Its true value becomes apparent only beyond the microscopic scale, specifically for the **voxel scale**, i.e. the reconstructed signal m_ρ.
- Two fundamental mechanisms for signal **localization** are available:
    - **Selective excitation**
    - **Spatial Encoding**

$$\boxed{\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}}$$

Voxel Scale

CM encodes local variations

- Both methods rely on **gradient induced modulations** of the magnetization in the vicinity of $\boldsymbol{x}$.
- If we assume the tissue to be essentially homogeneous on the voxel scale, the superposition of configurations encodes just this information via the phase factors $e^{-i\boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x}}$.
- To illustrate the concepts, we consider a 2D sequence with Cartesian sampling and slice selective excitation.

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Voxel Scale

Spatial encoding

- Due to **finite sampling**, the discrete reconstructed voxel signal m_ρ at position $\boldsymbol{x}_\rho$ results from **convolution** of the transverse magnetization density $m(\boldsymbol{x})$ with a **point spread function** $\phi(\boldsymbol{x})$

$$m_\rho \propto m * \phi(\boldsymbol{x}_\rho)$$

- which in our example is just a **scaled sinc** function

$$\phi(\boldsymbol{x}) = \prod_{j=1}^{2} \operatorname{sinc}\left(\frac{x_j}{\Delta x_j}\right)$$

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Voxel Scale

Spatial encoding

- We assumed that $\boldsymbol{x} = \sum_{j=1}^{3} x_j \cdot \boldsymbol{e}_j$ is decomposed relative to an orthonormal set of in-plane vectors $\boldsymbol{e}_{1,2}$ and the slice normal $\boldsymbol{e}_3$. Further, Δx_j denotes the **in-plane resolution**.
- With $f^{(\boldsymbol{n})} := e^{i\omega\tau_{\boldsymbol{n}}}\, m^{(\boldsymbol{n})}$, we insert the configuration model and get

$$m_\rho \propto \sum_{\boldsymbol{n}\in\mathbb{Z}^d} \int d\boldsymbol{k}\; e^{i\boldsymbol{k}\boldsymbol{x}_\rho} \hat{f}^{(\boldsymbol{n})}(\boldsymbol{k}) \cdot \prod_{j=1}^{2} u\left(\frac{\pi}{\Delta x_j} - \left|k_j + p_{\boldsymbol{n},j}\right|\right)$$

after short calculation. $u(x)$ is the unit step function.

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Voxel Scale

Spatial encoding

- If the support of $\hat{f}^{(\boldsymbol{n})}(\boldsymbol{k})$ is approximately bounded by $\pi/\Delta x_j$ in direction $\boldsymbol{e}_j$, configurations with

$$|p_{\boldsymbol{n},j}| > \frac{2\pi}{\Delta x_j}$$

  are essentially **suppressed** in m_ρ.

- The suppression of unwanted echoes via **crusher gradients** relies on this effect.

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Voxel Scale

Selective excitation

- Actual RF pulses can be approximated by a series of instantaneous small tip angle pulses, interleaved by equal intervals of (short) duration τ and (small) gradient moment $\boldsymbol{p}$ in direction of the slice normal $\boldsymbol{e}_3$.
- In view of the integral over x_3 in the convolution $m * \phi(\boldsymbol{x}_\rho)$, we conclude that only configurations with

$$p_{\boldsymbol{n},3} = 0$$

correspond to the selected slice and contribute to m_ρ.

Voxel Scale

Selective excitation + spatial encoding

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

- The obtained results for selective excitation and spatial encoding show that the question, which configurations $m^{(\boldsymbol{n})}$ enter the reconstructed voxel signal m_ρ, is fully determined by the vector $\boldsymbol{p}_{\boldsymbol{n}}$.

$$\boldsymbol{m}_\nu = \sum_{\boldsymbol{n} \in \mathbb{Z}^d} e^{i(\omega \tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}} \boldsymbol{x})} \boldsymbol{m}_\nu^{(\boldsymbol{n})}$$

Voxel Scale

Susceptibility effects

- Let $\omega_s(\boldsymbol{x})$ be the part of $\omega(\boldsymbol{x})$, which relates to static susceptibility variations.
- Inside the convolution $m * \phi(\boldsymbol{x}_\rho)$, let us further assume that ω_s is distributed according to some zero-mean density $\hat{p}(\omega_s)$ (independent of gradient orientation).
- Its Fourier transform is given by

$$p(t) \coloneqq \int d\omega \, e^{i\omega t} \, \hat{p}(\omega)$$

$$\boldsymbol{m}_{\nu} = \sum_{\boldsymbol{n} \in \mathbb{Z}^d} e^{i(\omega \tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}} \boldsymbol{x})} \boldsymbol{m}_{\nu}^{(\boldsymbol{n})}$$

Voxel Scale

Susceptibility effects

- In view of the factor $e^{i\omega\tau_{\boldsymbol{n}}}$ in the configuration model, we conclude that damping due to susceptibility effects is fully addressed by a simple multiplication, which depends on the configuration order:

$$m^{(\boldsymbol{n})} \longrightarrow p(\tau_{\boldsymbol{n}}) \cdot m^{(\boldsymbol{n})}$$

- The most common choice for $\hat{p}$ is a Lorentzian and the damping factor assumes the familiar form

$$p(\tau_{\boldsymbol{n}}) = e^{-R_2' \tau_{\boldsymbol{n}}}$$

$$\boxed{\boldsymbol{m}_{\nu} = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_{\nu}^{(\boldsymbol{n})}}$$

Summary

- The microscopic configuration model can be applied to arbitrary sequences or sequence blocks (like RF pulses).
- It is well adapted to imaging, since the configurations $m^{(\boldsymbol{n})}$, which enter the reconstructed image m_{ρ}, are restricted by selective excitation and/or spatial encoding and fully determined by the vector $\boldsymbol{p}_{\boldsymbol{n}}$.
- For the relevant configurations $m^{(\boldsymbol{n})}$, susceptibility effects are easily incorporated by a damping factor, which just depends on $\tau_{\boldsymbol{n}}$.

Summary

$$\boxed{\boldsymbol{m}_\nu = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} e^{i(\omega\tau_{\boldsymbol{n}} - \boldsymbol{p}_{\boldsymbol{n}}\boldsymbol{x})}\, \boldsymbol{m}_\nu^{(\boldsymbol{n})}}$$

- Compared with EPG, the configuration model has a clearer foundation and the multidimensional variant is more flexible, as it can, in principle, be applied to arbitrary sequences.
- In particular, the microscopic approach proved to be essential for the design of crusher gradients and the quantification of susceptibility effects.
- A free CM implementation and more information can be found here: