A Novel Design Approach to Superconducting Magnet Coil Systems for High-Resolution NMR-Spectroscopy

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Abstract
In high-resolution nuclear magnetic resonance (NMR-) spectroscopy superconducting coils are used to generate magnetic fields with strengths in the range of 5 to 20T (1T=10kG). This paper will present new approaches to the construction of magnetic coil systems that produce sufficient homogeneous magnetic fields. In the past this goal was reached by the combination of several coils of a rectangular cross section. In this paper, the definition of homogeneity is similar to the well-known Helmholtz idea that the curvature radius of the magnetic field is infinite at the origin. It is equivalent if the second derivation vanishes. All described solutions fulfill this condition.

Due to the high costs of the superconducting wire (NbTi or Nb3Sn), compact coils have to be designed with short wire length and small coil diameter. Several new winding techniques are presented using additional support windings between each layer for implementing large winding heights. In order to obtain homogeneous magnetic fields, cross-sections with different current densities are proposed. The new design applies coils of non-rectangular cross section. Here, each coil layer is optimized separately to obtain optimum field homogeneity. The new technology of coil design is best suited for superconducting coil magnet systems of field strength up to approx. 10 T.

Keywords: Superconducting Magnet Coil Systems, Novel Geometric Design, High-Resolution NMR-Spectroscopy

1. Introduction: Review of History and State of the Art Technology
Magnets for NMR-application were built originally as air split iron magnets with well-defined magnetic pole shoes [1]. The magnetic field strength was limited by the saturation of iron at a maximum field strength of 2.12 T.

The first high field SC-magnet system was developed in the early seventies using superconducting wires consisting of NbTi filaments in a copper matrix [2]. Typical system performance achieved for the SC-wire was at 6.36T@4.2K and a current density of 70A/mm². For applications above the critical induction of NbTi (11T) hybrid systems have to be used [2]. An additional inner coil is introduced consisting of NbSn wire. With this technology the maximum induction reaches 20T@4.2K or more if the temperature is lowered to 2K. In 20T magnet systems the proton oscillation frequency is about 1GHz. The wire length in a high resolution NMR spectrum is limited by finite homogeneity of the magnetic induction within the sample volume, and the lack of sufficient stability in time. A good compromise can be achieved with the choice of 10T, 1ppm field inhomogeneity and sovereign time stability in the short circuit mode of the coils. The optimum coil design depends also on the amount of SC-wire length. Milestones in the development of SC-magnet systems for NMR-application are:

1957 [3] (50 years ago) 40MHz-spectrum @ 1T
1973 (34 years ago) 270MHz-spectrum @ 6.35 T
1990 (17 years ago) 5 different high temperature ceramics: T_C > 77 K (80 – 160K)
2007 (today) 1 GHz-NMR-spectrum @25 T

Specification of the best masterpieces:
Total weight: up to 8 t
Free Bore: 50 – 60 mm
Liquid Helium filling: 600 l à 5€ = 3000 €
Liquid Nitrogen filling: 500 l à .1€ = 50 €
Price of NbTi-SL-wire 0.5 mm²: approx. 2 €/m, (2000 €/km)
Price of the complete SC-magnet system: 80000€
2. Fundamentals of Technology

2.1. Winding technique

The simplest winding arrangement is the rectangular cross section. But the implementation causes the most serious problems:

1. The first (lowest) layer of the winding has to be coiled with a maximum of tension, because the forces of the following layers onto the first can loosen the tension.
2. All layers with an odd number are clockwise and all others are counter-clockwise coiled. In the case of an ideal winding the wire cannot fall in the free spaces of the lower layer. Because of the change of the helix gradient the wire tries to follow the gap spaces but then it has to cross the wire below falling in the next gap. This results in a serious elliptic deformation of the winding. But it becomes visible only if about 10 layers are ready. The implementation of an exact circle form makes it necessary to use new coil former or bobbin. But in consequence a bigger amount of SC-wire is necessary because of the larger diameter.

The best qualified winding technique is a filling of the gap spaces with a supporting winding, consisting of a very small diameter of: \( d^0 = D^0/4 \). In case of a 0.5 mm\(^0\) SC-wire the supporting winding measures 0.125 mm\(^0\). In praxis a plastic wire with a diameter of 0.15 mm\(^0\) is preferable. Applying this winding technique even coils with thick windings could be nearly perfectly implemented.

3. There are several methods for realizing uniform magnetic fields. The best-known is the usage of so-called „notch-coils“. Two additional outer coils prevent the decay of the magnetic field on the central axis. This solution requires a considerable amount of SC-wire. In this contribution a better known method is the usage of the double-ring arrangement of Helmholtz [5] (distance = radius of the ring-coils), fulfilling the condition \( k(0) = 0 \) @ \( z=0 \). The curvature \( k \) is given by:

\[
k = \frac{d^2 B(z)}{dz^2} \cdot \left( 1 + \left( \frac{d}{dz} B(z) \right)^2 \right)^{-3/2}
\]

Today more sophisticated demands are known taking into account the different sizes of sample volumes. In the field of analytic chemistry (NMR) volumes from 1 mm\(^3\) up to 1 cm\(^3\) are used. In the region of nuclear magnetic tomography (MRT) the volumes are much higher (> 100 dm\(^3\)). In both cases the main magnetic field should have an inhomogeneity of 1 ppm in the sample volumes. That is sufficient in MRT. In NMR, additional shim-coils are used to trim the magnetic field so that the resolution of the spectrum is about a factor 1000 higher compared to MRT.

2.2. Methods of field homogenization

2.2.1. Definition of field homogeneity

A very famous solution is the double-ring arrangement of Helmholtz [5] (distance = radius of the ring-coils), fulfilling the condition \( k(0) = 0 \) @ \( z=0 \). The curvature \( k \) is given by:

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2.2.2. Computation of magnet systems with homogeneous fields

2.2.2.1 Optimized Solution for High-Field magnet systems

The main field coil of a magnetic system is a solenoid-coil consisting of multiple layers. A maximum of field strength using a minimum of SC-wire-length is achievable if the windings are as close as possible, beginning on the smallest diameter. To fulfill the condition of homogeneous magnetic fields it is necessary to reduce the current density to half by using a blind winding in addition over a computed correction length. (Ref. Fig.1)

The axial magnetic induction of a multi-layer cylindrical coil can be computed by:

\[
B_\alpha(z,L,R_a,R_i) = \frac{1}{2} \frac{N I \mu g(z,L,R_a,R_i)}{L (R_a - R_i)}
\]

For the geometric factor \( g(z,L,R_a,R_i) \) is equal to:
This field will be superimposed by the correcting field:

\[ B_{h,k}(z) = \frac{1}{2L_k} \sum_{i}^N I_k * \mu \cdot g_k(z) \]

The correcting current:

\[ I_k = \frac{-1}{2} \]

Corresponding for the geometric factor \( g_k \) follows:

\[ g_k(z, L_k, R_i, R_a) = g(z, L_k, R_i, R_a) \]

The total field induction must have the curvature zero @ \( z=0 \). That means that the second derivation of the total field \( B(z) \) vanishes:

\[ \frac{d^2}{dz^2} \left[ B_s(z) + B_{h,k}(z) \right] \bigg|_{z=0} = 0 \]

From this condition the correction length \( L_k \) can be calculated. The following results can be found with MATLAB™ for a realistic case of a 56 layer coil. Note: The problem has two solutions:

**Solution 1 (Fig. 2)**

Given: Internal radius: \( R_i = 40 \text{ mm} \), External radius: \( R_a = 70 \text{ mm} \) (number of layers = 56), Length: \( L = 200 \text{ mm} \)

Diameter of the SC-wire: \( \text{DM} = 0.54 \text{ mm} \), \( \mu_0 = 4 \pi \times 10^{-7} \text{ G} / (\text{A} \cdot \text{cm}) \)

Current density: \( I/\text{DM}^2 = 191 \text{ A/mm}^2 \), Correcting Current density: \( I_k/\text{DM}^2 = 95.5 \text{ A/mm}^2 \)

Calculated optimum: correcting length: \( L_{k1} = 8.88 \text{ mm} \), Conversions factor = 0.1078 T/1A

(That means 6.35T @ 58.9A), Field homogeneity: \( 10^{-5} \) within 1 cm (on z-axis) and <10^{-6} within 0.5 cm.

**Solution 2 (Fig. 3)**

Given: Internal radius: \( R_i = 40 \text{ mm} \), External radius: \( R_a = 70 \text{ mm} \) (number of layers = 56), Length: \( L = 200 \text{ mm} \)

Calculated optimum: correcting length: \( L_{k2} = 152.359 \text{ mm} \), Conversions factor = 0.06077 T/1A

(That means 6.35T @ 104.5A), Field homogeneity: \( 8.5 \times 10^{-8} \) within 1 cm (on z-axis) and <10^{-8} within 0.6 cm.

Both solutions fulfill the Helmholtz condition that the central curvature of the magnetic induction is zero: \( k(0) = 0 \). The magnet system corresponding to 2.2.2.1 is more compact, needs a larger wire length, and generates a higher field strength by a factor of 1.774 compared to the system in 2.2.2.2 if the currents are equal. To reach the same field strength (perhaps 6.35T = 3-fold iron saturation) the design of 2.2.2.1 needs 58.9, respectively 104.5A in the design of 2.2.2.2. The critical current for NbTi@4.2K is 111.7A [6]. So the design of 2.2.2.1 guarantees a stable operation, the design of 2.2.2.2 is more on the critical edge. Consequently the first design is recommended for high field applications, the second for high homogeneous fields (\( 10^{-8} \) within 1 cm).

**3. New magnet design: Optimization of each winding layer**

On the regarded systems several disadvantages can be observed. First disadvantage is the fact that the SC-wire must have a certain calculated value. It is impossible to utilize the fully delivered length which is – as a rule- larger than the ordered one. To avoid any shortening of the expensive SC-wire the design of a magnet system is can only be regarded as superb, if the total length of the available wire will be used. Then the stability of the magnet will increase to become a very robust system.
A second disadvantage of rectangular-crossed systems is the lack of uniformity of the current density. Due to the use of interlayer foils the distances between single turns in z-direction are often shorter than in radial expansion. The design of systems with geometrical optimization of each layer dimension has many advantages. The total field strength results from superposition of all single values.

The computation of single-layer magnet systems is relative simple:

$$B_s(z, L, R) = \frac{1}{2} N \frac{I}{L} \mu g(z, L, R)$$

For the geometric factor $g(z, L, R)$ follows:

$$g(z, L, R) = \frac{z + \frac{L}{2}}{\sqrt{R^2 + \left(z + \frac{L}{2}\right)^2}} - \frac{z - \frac{L}{2}}{\sqrt{R^2 + \left(z - \frac{L}{2}\right)^2}}$$

In addition, the correcting field with the half current density is equal to:

$$B_{aK}(z, L_K, R) = \frac{1}{2} \frac{N}{L_K} \frac{I_K}{L} \mu \mu g_{K}(z, L_K, R)$$

The correcting current:

$$I_K = \frac{I}{2}$$

Corresponding, for the geometric factor $g_{K}$ follows:

$$g_{K}(z, L_K, R) = g(z, L, R) \text{ with } L = L_K$$

The total field induction must have the curvature zero @ z=0. Now the correction length $L_K$ can be calculated. As we had seen earlier: the design of multilayer systems has two solutions, too.

**Solutions (Fig. 4 and Fig. 5)**

Given: Internal radius: $R_i = 40 \text{ mm}$, External radius: $R_a = \text{variable}$, Length: $L = 200 \text{ mm}$

Diameter of the SC-wire: $D_M = 0.54 \text{ mm}$

Current density: $I/L = 0.5 \text{ A/mm}$,

Correcting Current density: $I_K/L_K = 0.25 \text{ A/mm}$

Calculated optimum: correcting length: Fig. 6 and Fig. 9.

**Fig. 4:** High-field Coil with concentric correction: each layer optimization (design approach)

**Fig. 5:** System for large sample volumes with outer correction: each layer optimization (design approach)

**Homogeneous high field magnet system for small sample volumes (with concentric correction)**

In Fig. 6 the size of the correcting length of each layer is given.

**Fig. 6:** Ordinal number of single layer over the exact correcting length (in mm) (with concentric correction)

**Homogeneous magnet system for large sample volumes (with outer correction)**

In Fig. 9 the size of the correcting length of each layer is given.

**Fig. 7:** Total magnetic induction (in G) over the ordinal number of the single layer (with concentric correction)
The comparison between the two non-rectangular cross-section solutions can be summarized:

1. Both designs are comparable with regards to mechanical efforts in implementing the magnetic systems.
2. The solutions are suitable for different applications:
   2.1. The high-field system is applicable to achieve a large chemical shift in NMR-spectrum
   2.2. The system with large uniform field volume is preferred to explore super-fine resolution spectra. This system also shows an excellent stability in time.

4. Conclusion

Starting with an outlook of the history of magnets for NMR-spectroscopy, this contribution concentrates on the best possible cross-section for high and homogeneous magnetic fields. Field homogeneity for different current densities can be achieved by a special winding technique. Best results can be found using non-rectangular cross-sections. In principle there are two best solutions: one for generating high fields, one for achieving high homogeneity. The given example designs are optimal for field strength of 8T up to 10T. The method itself is universal.

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6. References