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An Analytical Approach towards Passive Ferromagnetic Shimming Design for a High-Resolution NMR Magnet

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Abstract

This paper presents a warm bore ferromagnetic shimming design for a high resolution NMR magnet based on spherical harmonic coefficient reduction techniques. The passive ferromagnetic shimming along with the active shimming is a critically important step to improve magnetic field homogeneity for an NMR Magnet. Here, the technique is applied to an NMR magnet already designed and built at the MIT's Francis Bitter Magnet Lab. Based on the actual magnetic field measurement data, a total of twenty-two low order spherical harmonic coefficients is derived. Another set of spherical harmonic coefficients was calculated for iron pieces attached to a 54 mm diameter and 72 mm high tube. To improve the homogeneity of the magnet, a multiple objective linear programming method was applied to minimize unwanted spherical harmonic coefficients. A ferromagnetic shimming set with seventy-four iron pieces was presented. Analytical comparisons are made for the expected magnetic field after Ferromagnetic shimming. The theoretically reconstructed magnetic field plot after ferromagnetic shimming has shown that the magnetic field homogeneity was significantly improved.

1. Introduction

As part of an ongoing 1.3 GHz NMR program, a 700 MHz hybrid HTS (High Temperature Superconductor) and LTS (Low Temperature Superconductor) magnet was developed and built at the MIT Francis Bitter Magnet Lab. The magnet assembly consists of one 600 MHz LTS winding and one 100 MHz HTS insert as shown in Fig. 1. Due to the complexity of the coil windings and construction, the measured homogeneity of the magnet was 172 parts per million (ppm), which is not yet NMR quality [1]–[3]. To achieve a high homogeneity field, two methods are typically applied: passive and active shimming. This paper presents a room temperature bore, ferromagnetic shimming design to reduce the spherical harmonic components to a level, such that additional active shimming will be able to achieve the NMR quality homogeneity [4].

Modern NMR spectroscopy requires the magnetic field to be spatially homogeneous in the sample volume. Typical NMR spectroscopy demands the magnetic field should not vary

more than 100 parts per billion (ppb). In order to precisely describe such small magnetic field variations, a series of spherical harmonic expansions are necessary to express the magnetic field variations along the x, y, and z axes [5]–[8]. In a polar coordinate system, for any given point P, the spatial variables are r, ϕ , and θ . The ferromagnetic shimming design, as applied to the 700 MHz magnet involves the following steps:

- Map the magnetic field with a high resolution NMR probe along a cylindrical path on a cylinder of 17 mm diameter and 30 mm high cylinder as shown in Fig. 1b
- Derive twenty-two low-order spherical harmonic coefficients from the magnetic field measurement data
- Calculate the spherical harmonic matrix for all possible locations of the iron pieces
- Develop a linear programming model for the ferro-magnetic shimming to minimize the low-order spherical harmonic coefficients after shimming
- Reconstruct the magnetic field with the spherical harmonic coefficients and evaluate the magnetic field homogeneity

2. Theoretical Background for Spherical Harmonic Coefficients

2.1. Spherical Harmonic Coefficient Derivation from Magnetic Field Mapping Data

For an NMR magnet, the sample volume has no magnetic ux sources: i.e., all magnetic ux lines enter into the sample volume and leave the sample eventually. Based on Maxwell's equation, the curl of the magnetic field in an enclosed space around the NMR sample equals zero. Therefore, the magnetic field at any given point on the spherical surface can be calculated by solving the following Laplace equation [9],

$$\Phi(r, \theta, \phi) = \sum_{n=0}^{\infty} \sum_{m=0}^n r^n P_n^m(\cos\theta) [A_n^m \cos m\phi + B_n^m \sin m\phi] \quad (1)$$

where r, ϕ , θ are the polar coordinates of the field point. n, m are the integer indices, and $P_n^m \cos(\theta)$ is the associated Legendre coefficient. From Eq. (1), an infinite series of orthogonal functions can be introduced to describe the magnetic field distribution for an enclosed space, in this case, a 20-mm diameter spherical volume (DSV).

For the 700 MHz NMR magnet, the only field component of interest is along the z-axis, since typical nuclear spins are aligned along the z-axis only. By taking the derivative with Eq. (1), the z-axis magnetic field component at any given point can be expressed by the sum of an infinite series of terms. However, the contribution of the spherical harmonics becomes smaller and smaller as the index integers n and m increase. Therefore, the magnetic field can be well approximated by a finite series of low order spherical harmonic terms as shown in the following equation,

$$B_z(r, \theta, \phi) = \frac{\partial \Phi(r, \theta, \phi)}{\partial z} \approx \sum_{n=0}^6 \sum_{m=0}^n (n+m+1) r^n P_n^m(\cos\theta) [A_{n+1}^m \cos m\phi + B_{n+1}^m \sin m\phi] \quad (2)$$

Since the magnetic field mapping is performed on a certain cylindrical surface programmed by the positioning system, the spatial variables r , ϕ , and θ are known. The total unknown variables can be solved by multiple magnetic field measurements. The actual magnetic field mapping in this case consists of 256 magnetic field measurement data points. In this paper, only twenty-two data points were used to calculate spherical harmonics, as shown in Table 1. The harmonic coefficients derived from all 256 data points have shown good convergence [2]. It is clearly shown that a few harmonic coefficients are very large, such as the x , y , z , zy , $z2y$, and $z2$ harmonic coefficients.

2.2. Calculating The Magnetic Field with the Magnetized Iron Pieces

The ferromagnetic shimming depends on the superposition of the magnetic field created by the magnetized iron pieces. As shown in Fig. 2, a magnetized iron piece located at point Q acts like a small magnetic dipole, which creates its own magnetic field on a point P.

The magnetic dipole of an iron piece can be expressed as the following,

$$\mathbf{m} = \chi dV H_z \mathbf{K} \quad (3)$$

where χ is the susceptibility of the iron piece, dV is volume of the iron piece, and $\mathbf{k}$ is the unit vector in z -direction. H_z is the magnetic field strength generated by the magnetization of the iron piece. The magnetic dipole moment creates a magnetic scalar potential at point P given by,

$$\Phi = -\frac{\mathbf{m}}{4\pi} \nabla \left(\frac{1}{r_q} \right) \quad (4)$$

r_q is the distance between point Q and origin. The expansion of Green's function ($1/r_q$), for $r < r_q$ in spherical harmonics can be written as,

$$\Phi = -\frac{\chi dV H_z}{4\pi} \frac{1}{r_q^2} \sum_{n=0}^{\infty} \sum_{m=0}^n \epsilon_m \frac{(n-m+1)!}{(n+m)!} P_{n+1}^m(\cos\alpha) \left(\frac{r}{r_q} \right)^n P_n^m(\cos\theta) \cos[m(\phi-\psi)] \quad (5)$$

The magnetic field at point P is the negative gradient of the magnetic scalar potential,

$$\mathbf{B} = -\mu_0 \nabla \Phi(r, \phi, \theta) \quad (6)$$

where μ_0 is permeability of free space. For an NMR magnet, the only effective magnetic field component is on the z -axis: therefore,

$$B_z = -\mu_0 \frac{\partial \Phi(r, \phi, \theta)}{\partial z} \mathbf{z} \quad (7)$$

By converting the Cartesian coordinates to polar coordinates in the derivative format, the magnetic field at point P created by the magnetic dipole moment $\mathbf{m}$ can be expressed as the following approximation with finite series of expansions,

$$\mathbf{B}_z \approx \mu_0 \frac{\chi dV H_z}{4\pi r_q^2} \sum_{n=1}^7 \sum_{m=0}^{n-1} \varepsilon \frac{1}{r_q^n} \frac{(n+m+1)!}{(n+m)!} P_{n+1}^m(\cos\alpha) r^{n-1} (n+m P_{n-1}^m(\cos\theta) \cos m(\phi-\psi)) \mathbf{z} \quad (8)$$

where B_z is the magnetic field at point P generated by the magnetic dipole moment at point Q. χ is the susceptibility, dV is the volume of the iron piece, and r, ϕ, θ are the polar coordinates for the point P. The iron pieces are made out of sheet steel with a saturation field of approximately 1.8 Tesla. So, in this study, the iron piece was assumed to have constant magnetic field during the steady state operations of the NMR magnet.

3. Ferromagnetic Shimming Design

3.1. Overall Spherical Harmonic Coefficients Calculation

The objective of ferromagnetic shimming is to arrange iron pieces in the room temperature bore of the magnet to cancel out unwanted spherical harmonics. In our approach, a thin-walled shimming tube with a 54 mm diameter and 72 mm height is used to attach a maximum of 480 iron pieces, as shown in Fig. 3. Each iron piece is 3 mm wide and 8 mm high with twenty different possible thicknesses. The iron pieces will be located and secured with epoxy to a phenolic holder. The superposition principle applies to magnetic fields, and spherical harmonics are linear expansion terms of the magnetic fields. Therefore, the superposition principle applies to the spherical harmonic coefficients as well. The overall spherical harmonic coefficients after the iron pieces are in place can be calculated as following,

$$SH_n^m = SHm_n^m + SHi_n^m \quad (9)$$

where the SH_n^m is the set overall or after ferromagnetic shimming spherical harmonic coefficients. SHm_n^m is the set of spherical harmonic coefficients before shimming and SHi_n^m is the set of spherical harmonic coefficients induced by the iron pieces.

From Eq. (8), the magnetic field is linearly proportional to the volume of the iron piece. Each iron piece creates its own magnetic field, which corresponds to a set of spherical harmonics. Assuming the thickness of the iron piece is 25.4 μm , a matrix of 480×22 spherical harmonics can be calculated based on the location of the iron pieces. The problem now becomes to determine which iron piece will be attached to the shimming tube and the thickness of the iron piece. One solution is to calculate the spherical harmonics for all possible locations and thicknesses of the iron pieces.

3.2. Multiple Objective Linear Programming Optimization

If the iron pieces have 20 different thicknesses, the number of possible solutions is the factorial of 9600, which is infinity for most 32-bit calculators. It would take a supercomputer to calculate all possible solutions and then find the optimal solution. However, the objective of the ferromagnetic shimming can be achieved by linear programming [10]–[12]. A set of 480 decision variables are defined in the range of 0 to 20. Each decision variable corresponds to one location on the shimming tube. If the decision variable is zero, then the location will be empty without iron pieces. Otherwise, the value of

the decision variable represents the thickness of the iron pieces. The objective of the linear programming is now to minimize the sum of SH_n^m . The output of the linear programming software is shown in Fig. 4, which provides the information of iron piece thicknesses.

4. Ferromagnetic Shimming Set and Simulation Results

4.1. 3-D Rendering of the Ferromagnetic Shimming Set

By using the linear programming approach, seventy-four iron pieces are required to achieve optimal solutions. The location of the iron pieces can be determined by the ψ angle and the z-axis coordinate. The detailed location and thickness information is shown in Table 2.

To better illustrate the location and relative thickness of the iron pieces, a 3D rendering of all seventy-four iron pieces is shown in Fig. 5. The thickness of the iron pieces is scaled by a factor of 3 to better show the differences between all iron piece.

4.2. The Spherical Harmonics After Ferromagnetic Shimming

After calculating the spherical harmonic coefficients created by the seventy-four iron pieces, the reduced spherical harmonic coefficients are shown in Table 3. The low order harmonics, x, y, z, zy, z2y, and z2, have been reduced significantly.

4.3. The Magnetic Field Comparisons Before and After Ferromagnetic Shimming

To illustrate homogeneity differences of the magnetic fields before and after the ferromagnetic shimming, the spherical harmonic coefficients in both Table 1 and 2 were used to reconstruct the magnetic field plots, as shown in Fig. 6. If the homogeneity were 0 ppm, the main magnetic field plot would be a vertical line at 700 MHz, which is 0 Hz in Fig. 6. For a 30 mm high and 17 mm diameter cylinder, the magnetic field before shimming is 112 kHz, which is approximately 160 ppm. The frequency width after shimming is around 13 kHz; therefore, the homogeneity is approximately 18 ppm. From the magnetic field plot comparison, the ferromagnetic shimming indeed improves the magnetic field homogeneity significantly.

5. Conclusion

A passive ferromagnetic shimming set was designed for a high resolution NMR magnet using a linear programming model. The analysis has shown that the passive shimming set was able to theoretically increase the homogeneity of the magnet to less than 20 ppm. The shimming set will be built to test the effectiveness of the shimming set in the near future. This paper is just the first step for the realization of the actual magnet shimming design. The same design approach will be extended and applied to the design of the final 1.3 GHz NMR magnet. The linear programming and spherical harmonic co-efficient reduction techniques allow us to find optimal solutions quicker. Many iterations of magnetic field mapping and shimming will be carried out before a passive shimming set can be finalized.

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Figure 1.

(a) An NMR magnet with 600 MHz LTS (L600) and 100 HTS (H100) insert. Note: the drawing is not in scale. ; (b) Polar coordinate system for the magnetic field mapping path

Figure 2.
Polar coordinate system schematic for a sphere and magnetic dipole moment

Figure 3. Polar coordinate system for a magnetic dipole moment m and any given points on a sphere surface.

The figure consists of four screenshots of a linear programming software interface, each displaying a list of decision variables and their corresponding values. The windows are titled 'file:///C:/Users/YSU/D...'. The data is as follows:

Decision Variable	Value
decision_181	0
decision_182	0
decision_183	0
decision_184	0
decision_185	0
decision_186	0
decision_187	0
decision_188	20
decision_189	20
decision_190	0
decision_191	20
decision_192	20
decision_193	0
decision_194	20
decision_195	20
decision_196	20
decision_197	20
decision_198	20
decision_199	20
decision_200	0
decision_201	20
decision_202	0
decision_203	0
decision_204	0
decision_205	0
decision_204	0
decision_205	0
decision_206	0
decision_207	0
decision_208	0
decision_209	0
decision_210	0
decision_211	20
decision_212	0
decision_213	20
decision_214	20
decision_215	20
decision_216	20
decision_217	18.9
decision_218	20
decision_219	20
decision_220	17
decision_221	7
decision_222	0
decision_223	20
decision_224	0
decision_225	0
decision_226	0
decision_227	0
decision_228	0
decision_277	20
decision_278	20
decision_279	20
decision_280	0
decision_281	20
decision_282	20
decision_283	0
decision_284	0
decision_285	0
decision_286	0
decision_287	0
decision_288	0
decision_289	0
decision_290	0
decision_291	0
decision_292	0
decision_293	0
decision_294	0
decision_295	20
decision_296	0
decision_297	0
decision_298	20
decision_299	20
decision_300	20
decision_301	20
decision_456	20
decision_457	20
decision_458	20
decision_459	20
decision_460	20
decision_461	0
decision_462	0
decision_463	20
decision_464	0
decision_465	0
decision_466	0
decision_467	0
decision_468	0
decision_469	0
decision_470	20
decision_471	20
decision_472	0
decision_473	20
decision_474	20
decision_475	20
decision_476	20
decision_477	20
decision_478	20
decision_479	20

Figure 4.
Screen shot of the linear programming software showing partial 480 decisions

Figure 5.

(a) 3-D rendering of the ferromagnetic shimming set, (b) Rotated 90° along z-axis, (c) Rotated -90° along z-axis,

Figure 6.
Reconstructed magnetic field plots based on the spherical harmonic coefficients

Table 1

Spherical Harmonic Coefficients Before Ferro-magnetic Shimming

	1	x	y	c2	c3	s2	s3
1		10672 ^a	19149 ^a	-3541 ^b	372 ^c	-1924 ^b	101 ^c
Z	18554 ^a	222 ^b	28769 ^b	-1105 ^c	454 ^d	-25 ^c	-445 ^d
z2	5612 ^b	-391 ^c	-7830 ^c	1343 ^d		1352 ^d	
z3	-426 ^c	989 ^d	-2943 ^d				
z4	222 ^d						

Note: The units of the spherical harmonic Coefficients are [Hz/cm]^a,

[Hz/cm²]^b,

[Hz/cm³]^c,

[Hz/cm⁴]^d,

Table 2

Location and Thickness of Iron Pieces in the Ferromagnetic Shimming Set

ψ Deg	Height cm	Thickness mil	ψ Deg	Height cm	Thickness mil	ψ Deg	Height cm	Thickness mil
0	-3.5	20	90	3.5	20	216	3.5	20
0	-0.5	6	108	-3.5	20	234	-0.5	16
0	0.4	19	108	-2.9	20	234	0.4	20
0	2.9	20	108	3.5	20	234	1.1	20
0	3.5	20	126	-3.5	20	234	1.7	20
18	2.9	20	126	-2.9	20	234	2.9	20
18	3.2	20	126	-1.4	19	234	3.5	20
18	3.5	20	126	-0.8	20	252	1.1	20
36	-1.4	20	126	-0.5	3	252	3.5	20
36	0.4	20	126	3.5	15	270	-3.5	20
36	2.9	20	144	-3.5	20	270	-0.2	20
36	3.2	20	144	1.4	4	270	1.1	7
36	3.5	20	162	-3.5	20	270	1.7	10
54	-1.4	20	162	-0.2	15	288	-3.5	20
54	2.9	20	162	1.4	20	288	-0.5	8
54	3.2	20	162	3.5	20	288	-0.2	12
54	3.5	20	180	-3.5	20	288	1.1	17
72	-1.4	16	180	3.5	20	288	1.7	10
72	0.7	11	198	2.3	20	306	-3.5	20
72	2.9	20	198	2.9	20	306	1.1	16
72	3.2	20	198	3.2	7	324	-3.5	20
72	3.5	20	198	3.5	20	324	1.7	20
90	-3.5	20	216	0.4	6	342	-3.5	20
90	2.9	20	216	2.3	20	342	1.7	20
90	3.2	17	216	2.9	20			

Table 3

Spherical Harmonic Coefficients After Ferro-magnetic Shimming

	1	x	y	c2	c3	s2	s3
1		-286 ^a	-8 ^a	-78 ^b	647 ^c	-76 ^b	339 ^c
z	-140 ^a	317 ^b	-109 ^b	-12 ^c	9 ^d	-41 ^c	-53 ^d
z2	-15 ^b	172 ^c	-33 ^c	31 ^d		-21 ^d	
z3	115 ^c	-747 ^d	-10 ^d				
z4	-277 ^d						

Note: The units of the spherical harmonic Coefficients are [Hz/cm]^a,

[Hz/cm²]^b,

[Hz/cm³]^c,

[Hz/cm⁴]^d,