Supporting Information. How to increase further the resolving power of the ultra-high magnetic field FT ICR instruments? The new concept of FT ICR cell – the open dynamically harmonized cell as a part of the vacuum system wall

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The analytical solution for best k

The supplementary materials for article "How to increase further the resolving power of the ultra-high magnetic field FT ICR instruments? The new concept of FT ICR cell – the open dynamically harmonized cell as a part of the vacuum system wall" by E. Nikolaev and A. Lioznov

To approximately find the best k, that makes the electric potential inside the working region of Zig-Zag cell analytically, firstly we must solve the following sub-problem: to find the potential distribution on the axis of the conductive infinitely-long hollow grounded cylinder with a ring with a voltage in the region near $z = 0$. From the point of view of mathematical physics, the problem can be formulated as follows: to find $\phi(\rho, z)|_{\rho=0}$ where

$$\Delta\phi(\rho, z) = \frac{\partial^2\phi}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\phi}{\partial\rho} + \frac{\partial^2\phi}{\partial z^2} = 0, \qquad \phi(R, z) = \begin{cases} \phi_0, |z| \leq l \\ 0, else \end{cases} \tag{1}$$

The procedure of solving such equations is pretty standard. By separating the variables $\phi(\rho, z) = A(z) \cdot B(\rho)$ we get two equations:

$$\frac{d^2A}{dz^2} + \lambda^2 A = 0; \qquad \frac{d^2B}{d\rho^2} + \frac{1}{\rho}\frac{dB}{d\rho} - \lambda^2 B = 0 \tag{2}$$

The solution of the equations are

$$A(z) = \cos\lambda z; \qquad B(\rho) = I_0(\lambda\rho) \tag{3}$$

Where I_0 is the modified Bessel function of the first kind and zero order. Because the problem has symmetry on z, the $\sin\lambda z$ term disappears from $A(z)$.

The general solution of the equation would be presented in form

$$\phi(\rho, z) = \int_{-\infty}^{+\infty} c(\lambda)\cos(\lambda z) I_0(\lambda\rho) d\lambda \tag{4}$$

where $c(\lambda)$ is the coefficient of decomposition.

The boundary conditions may be presented as the Fourier integral:

$$\int_{-\infty}^{+\infty} a(\lambda)\cos(\lambda z) d\lambda = \phi(R, z) \tag{5}$$

where

$$a(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \cos(\lambda z)\phi(R, z)dz = \frac{1}{2\pi}\int_{-l}^{+l} \cos(\lambda z)\phi_0 dz = \frac{\phi_0}{\pi}\frac{\sin\lambda l}{\lambda} \tag{6}$$

Knowing $a(\lambda)$ we can find $c(\lambda)$ and, finally, get

$$\phi(\rho, z) = \frac{\phi_0}{\pi} \int_{-\infty}^{+\infty} \frac{\sin \lambda l}{\lambda} \frac{\cos(\lambda z) I_0(\lambda \rho)}{I_0(\lambda R)} d\lambda \tag{7}$$

This equation may be simplified. Firstly, we are interesting only in $\rho = 0$, thus $I_0(\lambda\rho)|_{\rho=0} \equiv 1$. Secondly, we'll integrate on l, so suppose $l \ll 1$. Thus, $\sin(\lambda l)/\lambda|_{l \ll 1} = l$. Finally, we can use variable substitution $\lambda R \to \lambda$. With all these manipulations, the eq. (7) transforms into:

$$\phi_{impulse}(\phi_0, z) = \frac{\phi_0}{\pi R} l \int_{-\infty}^{+\infty} \frac{\cos(\lambda z/R)}{I_0(\lambda)} d\lambda \equiv \frac{\phi_0}{\pi R} l \cdot I(z/R) \tag{8}$$

Numerical integration shows, that when $z/R \gg 1$ the integral $I(z/R)$ is approximately equal to $\exp(\gamma z/R + \delta)$, where $\gamma < 0$ and δ are some constants. Using python's scipy.integrate.quad we get $\gamma \simeq -2.4$, $\delta \simeq 2.5$.

$$\phi_{impulse}(\phi_0, z)|_{z/R \gg 1} = \frac{\phi_0}{\pi R} l e^{\gamma z/R} e^{\delta} \tag{9}$$

Now we can return to the main task. We'll suppose that the best k coefficient is such, that the mean difference on the cell axis of the real potential distribution inside zig-zag cell $\phi_{real}(k, z, \rho)$ from the ideal potential $\phi_{ideal}(z, \rho) \sim 2z^2 - \rho^2$ is zero.

In other words

$$k_{opt} = argmin_k |\phi_{real}(k, \rho = 0, \theta, z) - \phi_{ideal}(\rho = 0, \theta, z)| \tag{10}$$

We can introduce $\phi_\Delta(k, \rho, \theta, z) \equiv \phi_{ideal}(\rho, \theta, z) - \phi_{real}(k, \rho, \theta, z)$. It can be found from the Laplace equation with the boundary conditions $\phi_\Delta(k, R, \theta, z)$, which will be the difference between the boundary conditions of the ideal and real potentials $\phi_{ideal}(R, \theta, z) - \phi_{real}(k, R, \theta, z)$, where the boundary conditions of ϕ_{ideal} were described in eq. (**??**), while the boundary conditions of ϕ_{real} were described in eq. (**??**). For the analytical solution we would assume that the cylinder is infinite ($z_{full} = +\infty$).

On the axis the real potential is the same as the averaged one. So, since we are only interested in the potential distribution along $\rho = 0$, we can simplify the boundary conditions by averaging them over the polar angle. Thus, we can write the following conditions for $\phi_\Delta(R, z)$:

$$\phi_0(k,z) \equiv \phi_\Delta(k,z,R) = \begin{cases} 0, & |z| \leq z_0 \\ (2-k)\beta\left(\frac{z^2}{z_0^2} - 1\right)\phi_0, & z_0 < |z| \leq z_1 \\ \left(1 - k + \beta\left(\frac{z^2}{z_0^2} - 1\right)\right)\phi_0, & z_1 < |z| \end{cases} \tag{11}$$

Now we can find the potential ϕ_Δ along $\rho = 0$ from the equation

$$\phi_\Delta(k,z,\rho=0) = \int d\phi_{impulse}(\phi_0(k,z_1), |z - z_1|)dz_1 \tag{12}$$

or

$$\phi_\Delta(k,z,\rho=0) = \int_{-\infty}^{+\infty} dz' \frac{\phi_0(k,z')}{2\pi R} \int_{-\infty}^{+\infty} d\lambda \frac{\cos(\lambda|z-z'|/R)}{I_0(\lambda)} \tag{13}$$

For $|z| < z_0$ $\phi_0(k,z) = 0$, therefore the integral $\int_{-\infty}^{+\infty} dz'$ splits into two integrals: $\int_{-\infty}^{-z_0} dz' + \int_{+z_0}^{+\infty} dz'$. We are only interesting in the electric potential distribution inside the working volume ($|z| < 0.5z_0$). Simulation shows, that for such z for all $|z'| \geq z_0$ we can use approximation $|z - z'|/R \gg 1$ for $\phi_{impulse}$ (eq. 9). Thus, the previous equation can be simplified as

$$\phi_\Delta(k,z,\rho=0) = \frac{e^\delta}{2\pi R}\left(\int_{-\infty}^{-z_0} dz' e^{\frac{\gamma}{R}(z-z')}\phi_0(k,z') + \int_{z_0}^{+\infty} dz' e^{\frac{\gamma}{R}(z'-z)}\phi_0(k,z')\right) \tag{14}$$

because $\phi_0(z) = \phi_0(-z)$ and $\exp(z) + \exp(-z) = 2\cosh(z)$ we get

$$\phi_\Delta(k,z,\rho=0) = \frac{e^\delta}{2\pi R} 2\cosh(z \cdot \gamma/R) \int_{z_0}^{+\infty} dz' e^{\frac{\gamma}{R}z'}\phi_0(k,z') \tag{15}$$

The integral is divided to sub-integrals with borders $z_0 ... z_1$ and $z_1 ... \infty$ with simple integrands.

If we define (from $\int \exp z \cdot (z^2 - 1) dz$ with some coefficients)

$$I_{z^2}(z) \equiv \exp(\gamma z/R) \left[\frac{(\gamma z/R)^2 - 2(\gamma z/R) + 2}{(\gamma z_0/R)^2} - 1 \right] \tag{16}$$

the ϕ_Δ can be expressed through

$$i_0 = \beta I_{z^2}(z_1) - 2\beta I_{z^2}(z_0) - e^{\gamma z_1/R} \tag{17}$$

$$i_1 = \beta I_{z^2}(z_0) - \beta I_{z^2}(z_1) + e^{\gamma z_1/R} \tag{18}$$

as

$$\phi_\Delta(k, z, \rho = 0) = \frac{e^\delta \phi_0}{\pi R} \cdot R/\gamma \cdot (i_1 k + i_0) \cdot \cosh(\gamma z/R) \tag{19}$$

And the mean value on z potential in the working volume (when $|z| < 0.5 z_0$)

$$< \phi_\Delta(k) >_z = \frac{1}{0.5 z_0} \frac{e^\delta \phi_0}{\pi R} \cdot R/\gamma \cdot (i_1 k + i_0) \cdot \sinh(\gamma \cdot 0.5 z_0/R) \tag{20}$$

From this equation[1] the best k coefficient can be find. In this approximation the best coefficient k is

$$k_{opt} = -i_0/i_1 = \frac{2\beta I_{z^2}(z_0) - \beta I_{z^2}(z_1) + e^{\gamma z_1/R}}{\beta I_{z^2}(z_0) - \beta I_{z^2}(z_1) + e^{\gamma z_1/R}} \tag{21}$$

where $I_{z^2}(z)$ is defined in eq. (16). For $\beta = 0.9, z_0/R = 2$ we get $k = 2.18$.

[1]you may notice, that the best k may also be found from eq. (19). But we are still using the equation (20), because it is the solution of the equation (10), that was used to initially formulate the problem