

# Optimizacija merilnih tuljav pri jedrski kvadrupolni resonanci

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# Uvod

- Jedrska kvadrupolna resonanca (Nuclear Quadrupole Resonance, NQR) je radiofrekvenčna (RF) spektroskopska metoda, ki podobno kot jedrska magnetna resonanca (NMR) meri prehode med energijskimi nivoji atomskih jeder v preiskovani snovi.
- pri NQR resonanco določa interakcija med električnim kvadrupolnim momentom atomskega jedra in gradientom električnega polja bližnjih valenčnih elektronov, zato pri tej metodi niso potrebni veliki in dragi superprevodni magneti za generiranje statičnega magnetnega polja.
- intenziteta izmerjenega signala je sorazmerna številu resonančnih atomskih jeder, kar omogoča kvantitativno analizo vzorcev (maso, razmerja različnih kristaliničnih faz, stopnjo hidratacije, ali pa razmerje med kristalinično in amorfno fazo).
- Na King's College London so npr. potrdili [1], da lahko z NQR meritvami zanesljivo detektirajo vrsto in ugotovijo število tablet v originalno zaprti embalaži zdravila.

[1] J. Barras et al., Analit. Chem. 84, 8070 (2012).

# Uvod

- Pogoji za kvantitativno analizo vzorcev je približno homogeno RF polje na področju vzorca.
- V tem prispevku bomo obravnavali valjaste tuljave, ki jih v prvem približku predpostavimo kot zaporedje krožnih zank, pri končnem izračunu pa jih sestavimo v obliki vijačnice, pri kateri razdalje med ovoji zvezno spreminjamo in optimiziramo tako, da dosežemo čim bolj homogeno polje znotraj tuljave
- Pri tem optimiziramo razdalje tako, da dobimo čim večji delež, kjer polje znotraj tuljave preseže 95% ( $\eta_{95}$ ) ali 99% ( $\eta_{99}$ ) maksimalne vrednosti.
- V dodatku bom pokazal še razširitev na ploščate tuljave, ki jih sestavimo v obliki spirale, kjer oddaljenost med ovoji zvezno spreminjamo in optimiziramo, tako da dosežemo čim bolj homogeno polje na določeni oddaljenosti od tuljave

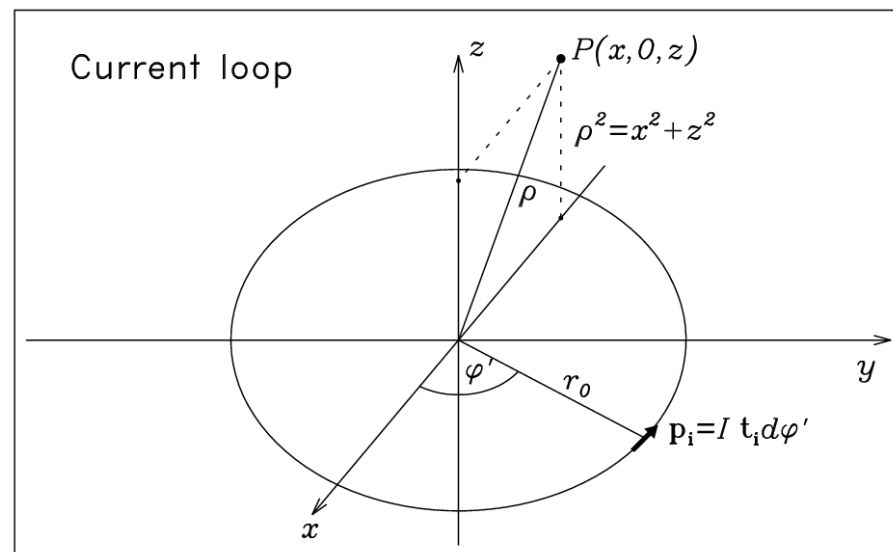
# Izračun polja

Biot-Savart

$$\vec{H}(\vec{r}) = \frac{I}{4\pi} \int_0^{2\pi} \frac{\vec{t}' \times (\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|^3} d\varphi'$$

Izven osi (cilindrično simetrično):

$$H_z = \frac{I r_0^2}{2(z^2 + r_0^2)^{\frac{3}{2}}}$$



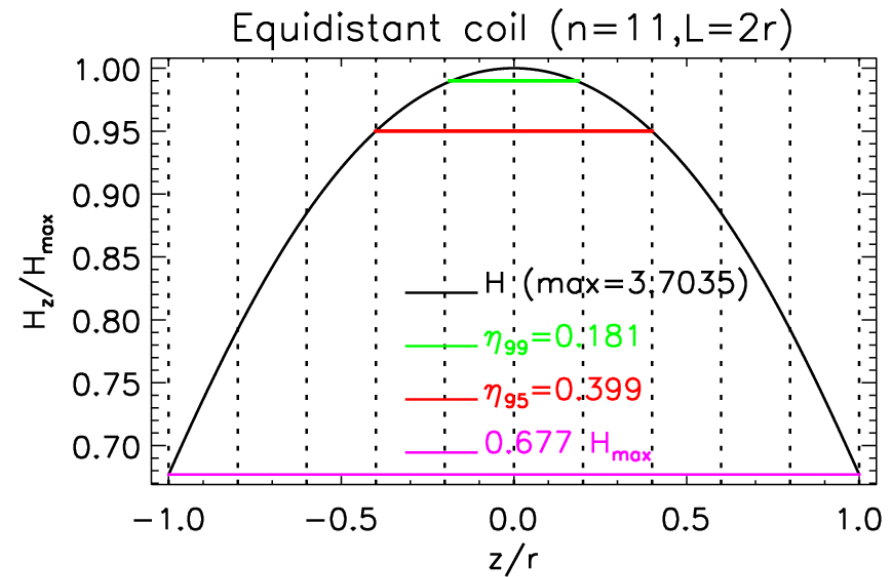
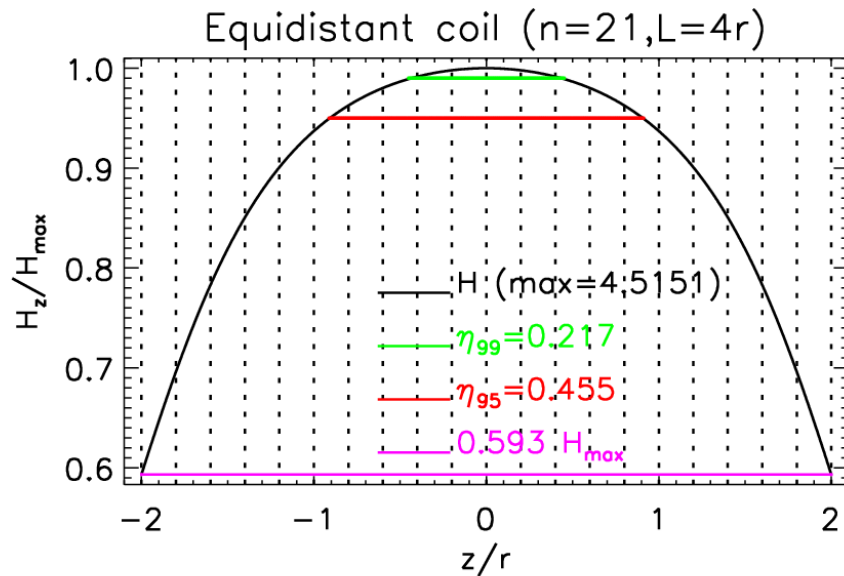
$$(H_\rho, H_\varphi, H_z) = \frac{I}{2\pi \sqrt{z^2 + (\rho + r_0)^2}} \left( \frac{z}{\rho} \left[ \frac{r_0^2 + z^2 + \rho^2}{z^2 + (\rho - r_0)^2} E_2(k) - E_1(k) \right], 0, \left[ \frac{r_0^2 - z^2 - \rho^2}{z^2 + (\rho - r_0)^2} E_2(k) + E_1(k) \right] \right)$$

kjer sta  $E_1(k)$  in  $E_2(k)$  popolna eliptična integrala prvega in drugega reda,  $k^2 = \frac{4r_0}{z^2 + (r_0 + \rho)^2}$  in  $\rho = \sqrt{x^2 + y^2}$ .

$$\vec{H}(\vec{r}) = \frac{1}{4\pi} \sum_{i=1}^{N_d} \frac{\vec{p}_i \times (\vec{r} - \vec{r}_i)}{|\vec{r} - \vec{r}_i|^3}$$

# Valjaste tuljave

Magnetno polje vzdolž osi tuljave, ki je sestavljena iz enakomerno razmaknjenih ovojev



# Valjaste tuljave

Zapis v cilindričnem koordinatnem sistemu:

$$z(\varphi) = \frac{L}{2\pi(n-1)}\varphi, \quad \varphi \in [-n\pi, n\pi] \quad z(\pm(n-1)\pi) = \pm\frac{L}{2}.$$

Poenostavljena oblika:  $\varphi = k\pi$ , kjer  $k = -(n-1) + 2i$ ,  $i = 0, 1, 2, \dots, n-1$

$$z(k) = \frac{L}{2(n-1)}k, \quad k \in [-(n-1), n-1]$$

Brezdimenzijska spremenljivka:  $u = k/(n-1) = \varphi/\pi(n-1)$

$$z(u) = \frac{L}{2}u, \quad u \in [-1, 1] \quad \text{in} \quad z(\pm 1) = \pm\frac{L}{2}.$$

**Model za optimizacijo:**

$$z(u) = \frac{L}{2}[\lambda u + g(u)], \quad g(0) = 0, \quad g(-u) = -g(u), \quad g(\pm 1) = \pm(1 - \lambda).$$

- a) če je  $\lambda = 1$ , potem je ali  $g(u) \equiv 0$  (ekvidistančna rešitev) ali samo  $g(0) = g(\pm 1) = 0$
- b) če je  $\lambda = 0$ , potem je  $z(u) = g(u)$  in
- c) drugače je popravek  $g(u)$  naložen na linearni del z nagibom  $\lambda \frac{L}{2}$ .

# Potenčna funkcija $g(u) = au^p$

$$z(u) = \frac{L}{2} [\lambda u + au^p], \quad z(1) = \frac{L}{2} [\lambda + a] = \frac{L}{2} \implies a = (1 - \lambda) \implies z(u) = \frac{L}{2} [\lambda u + (1 - \lambda)u^p]$$

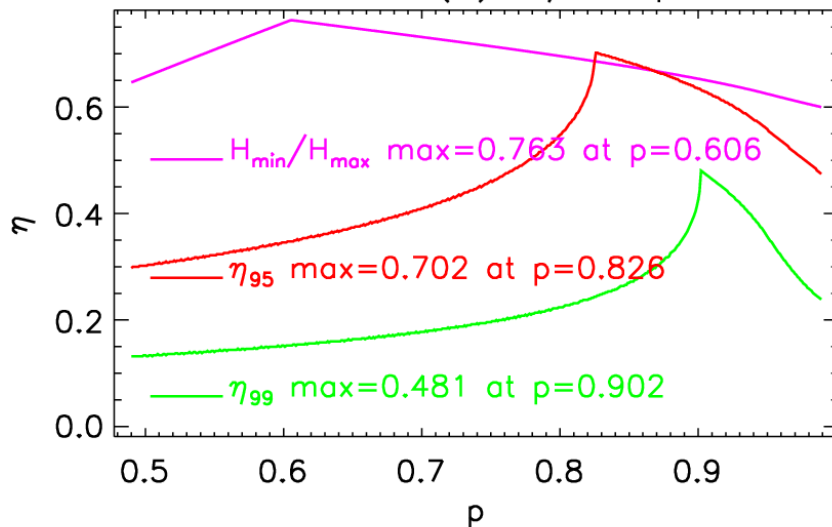
$$\frac{dz}{du} = \frac{L}{2} [\lambda + p(1 - \lambda)u^{p-1}] \geq 0 \implies \lambda + p(1 - \lambda)u^{p-1} \geq 0 \implies \lambda \geq -\frac{pu^{p-1}}{pu^{p-1} - 1}.$$

Na koncu tuljave ( $u=1$ ):  $\lambda + p(1 - \lambda) \geq 0 \implies p \geq \frac{\lambda}{\lambda - 1}, \quad \lambda \geq \frac{p}{p - 1}.$

## Primer $\lambda=0$

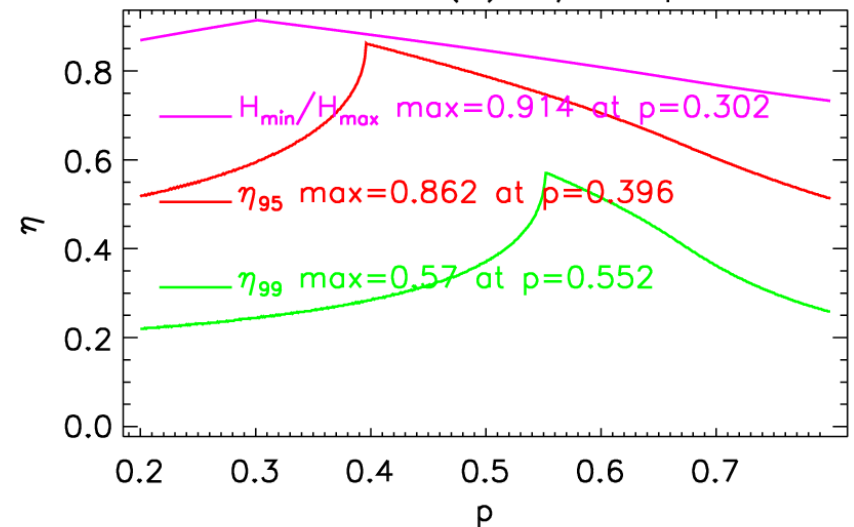
Tuljava ( $n=21, L=4r$ )

Model:  $z(u) = L/2 * u^p$



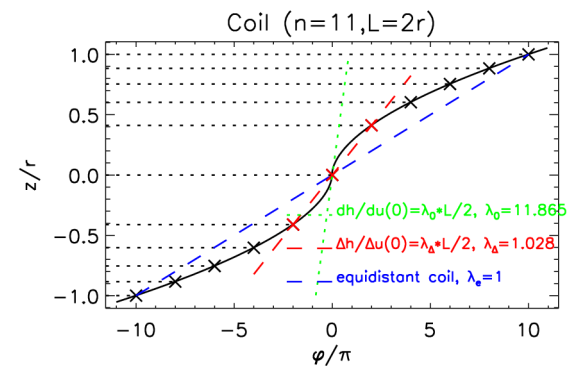
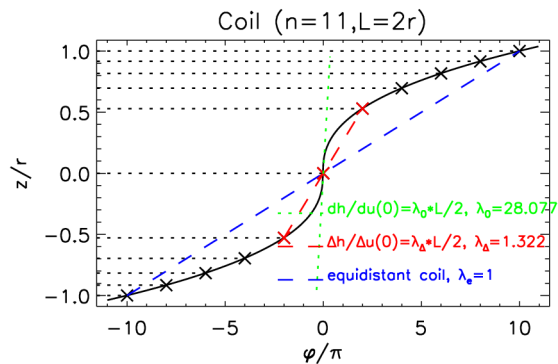
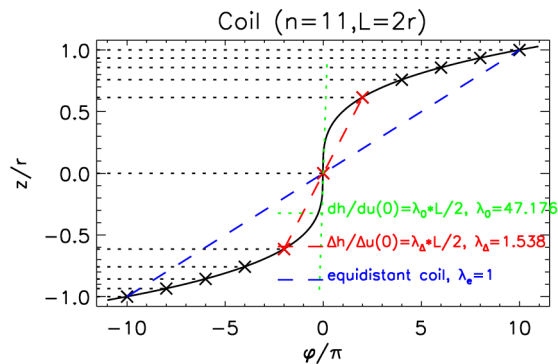
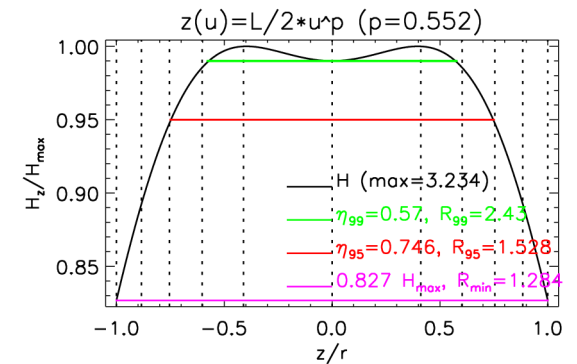
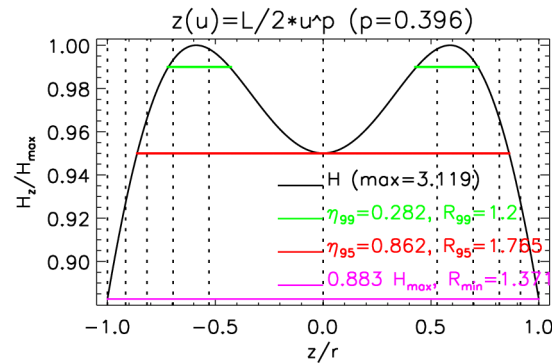
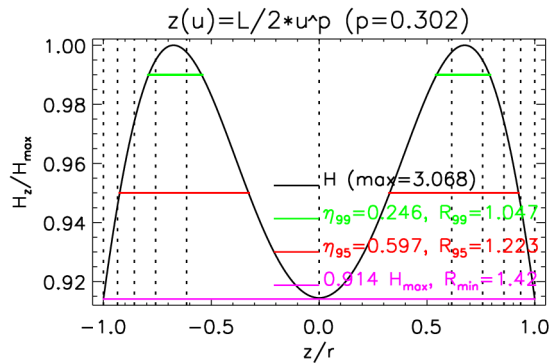
Tuljava ( $n=11, L=2r$ )

Model:  $z(u) = L/2 * u^p$



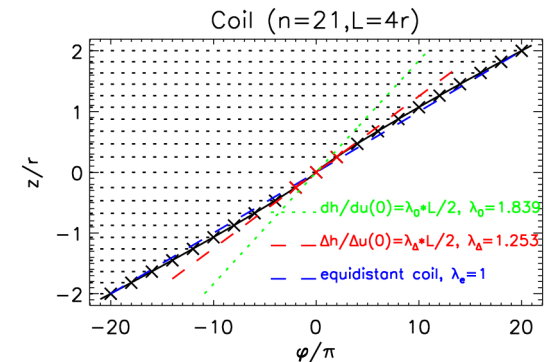
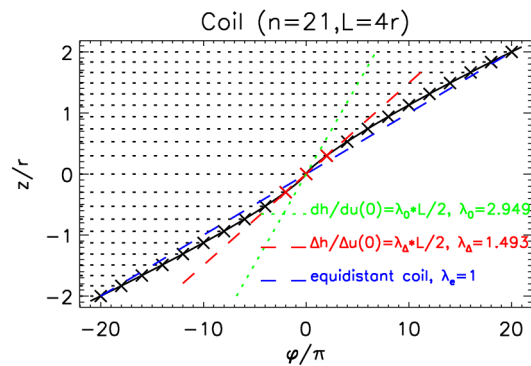
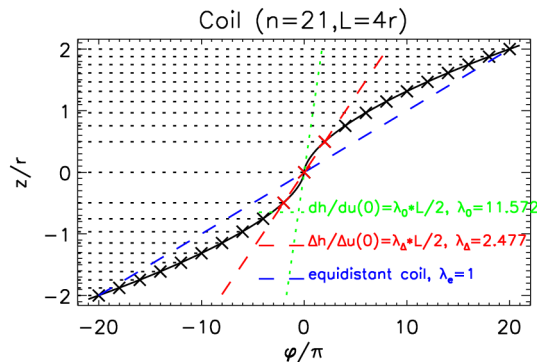
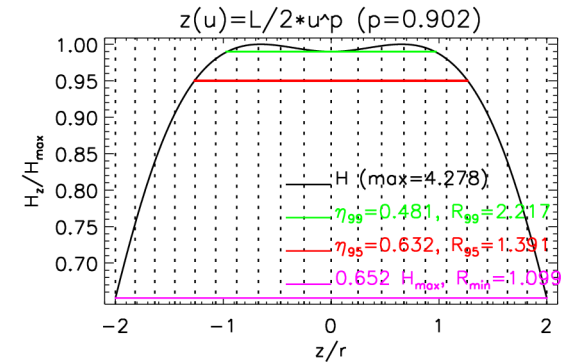
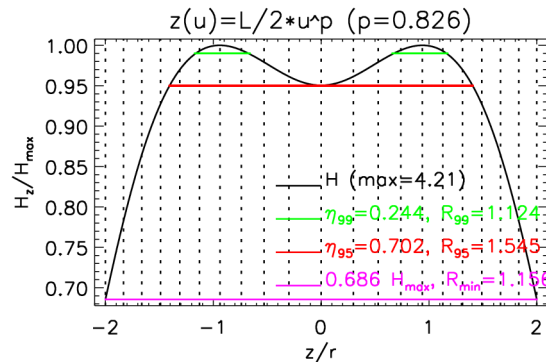
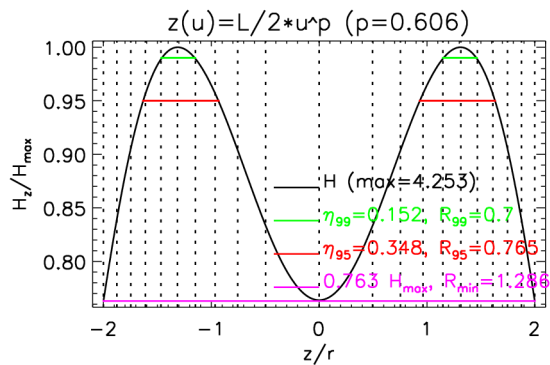
# Potenčna funkcija $g(u) = au^p$

Primer  $\lambda=0$ , tuljava ( $n=11$ ,  $L=2r$ )



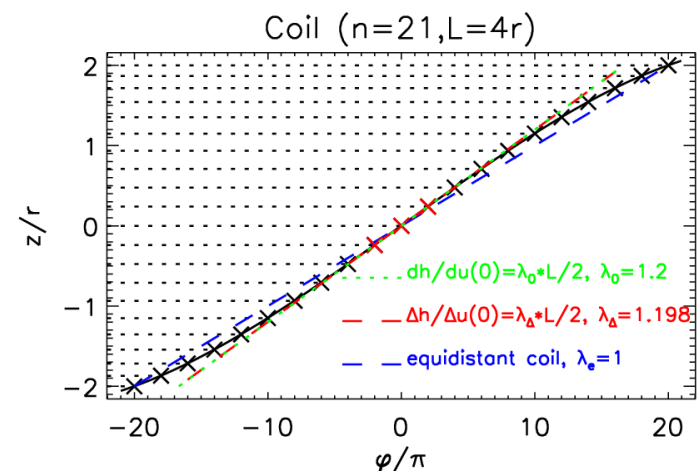
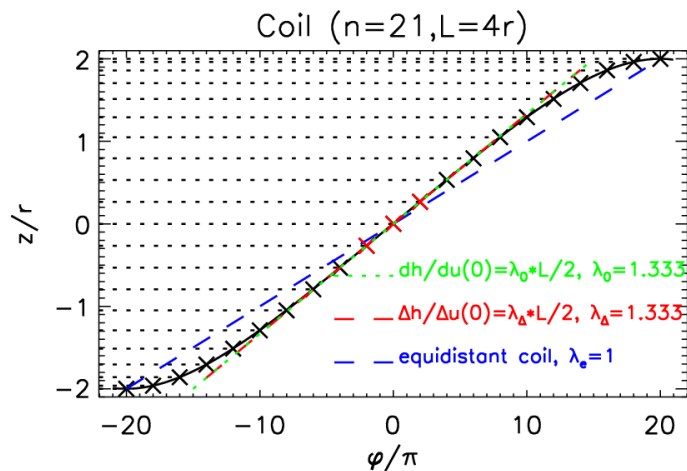
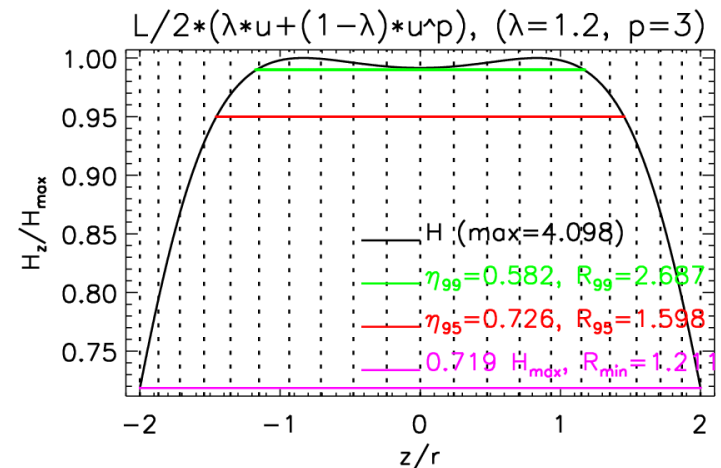
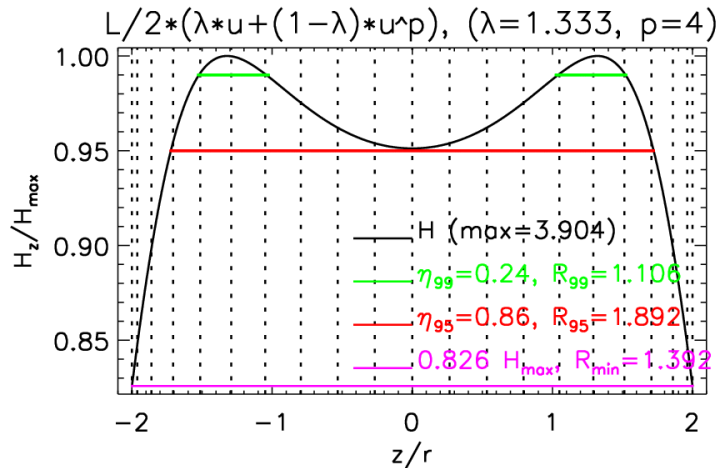
# Potenčna funkcija $g(u) = au^p$

## Primer $\lambda=0$ , tuljava ( $n=21$ , $L=4r$ )



# Potenčna funkcija $g(u) = au^p$

Primer  $\lambda \neq 0$ , tuljava ( $n=21$ ,  $L=4r$ )



# Potencirana sinusna funkcija $g(u) = a_s \sin^p(\alpha u)$

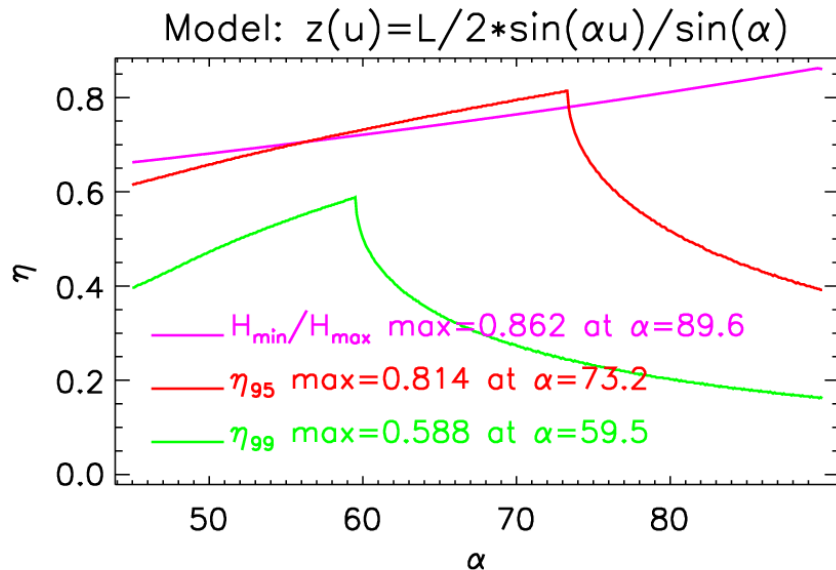
$$z(u) = \frac{L}{2} [\lambda u + a_s \sin^p(\alpha u)], \quad z(1) = \frac{L}{2} \implies a_s = \frac{(1-\lambda)}{\sin^p \alpha} \implies z(u) = \frac{L}{2} \left[ \lambda u + \frac{(1-\lambda)}{\sin^p \alpha} \sin^p(\alpha u) \right]$$

$$\frac{dz}{du} = \frac{L}{2} \left[ \lambda + p\alpha \frac{(1-\lambda)}{\sin^p \alpha} \sin^{p-1}(\alpha u) \cos(\alpha u) \right] \geq 0 \implies \frac{dz}{du}(1) = \frac{L}{2} \left[ \lambda + p\alpha(1-\lambda) \frac{\cos \alpha}{\sin \alpha} \right] \geq 0.$$

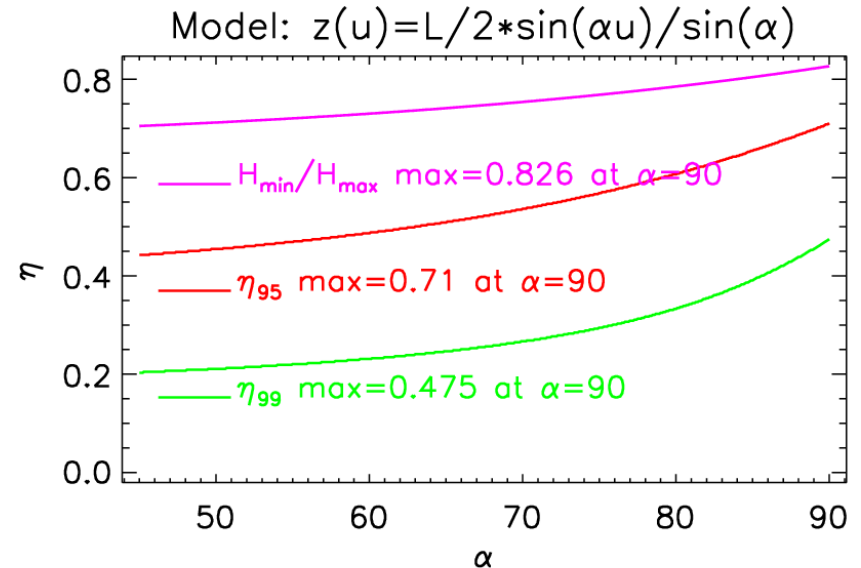
Končna rešitev:  $z(u) = \frac{L}{2} \left[ \lambda u + \frac{(1-\lambda)}{\sin^p \alpha} \sin^p(\alpha u) \right],$  kjer je  $\left( p\alpha \frac{\cos \alpha}{\sin \alpha} \geq \frac{\lambda}{\lambda - 1} \right)$

## Primer $\lambda=0, p=1$

Tuljava (n=21, L=4r)



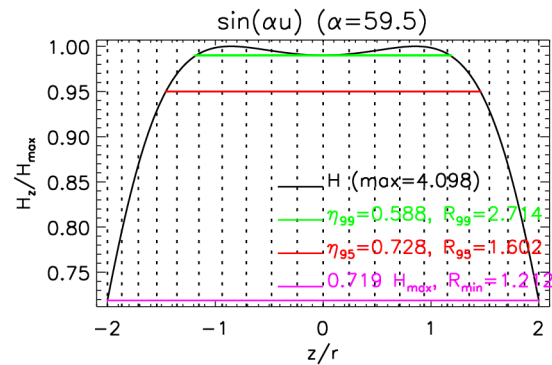
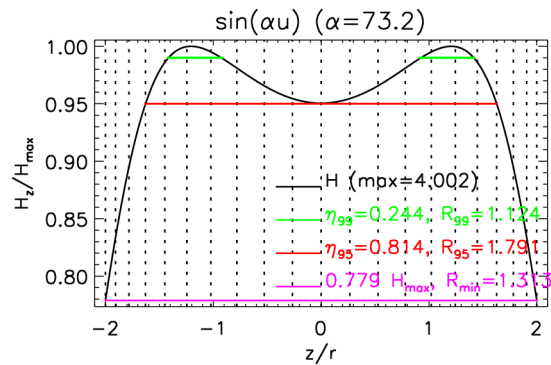
Tuljava (n=11, L=2r)



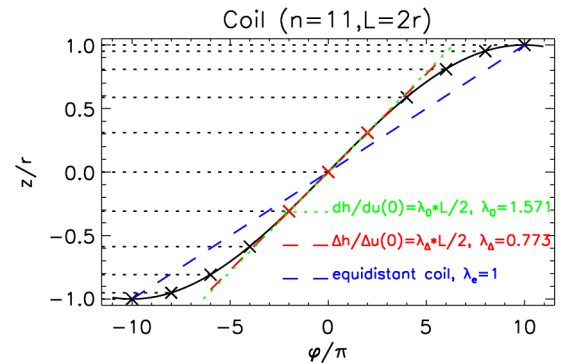
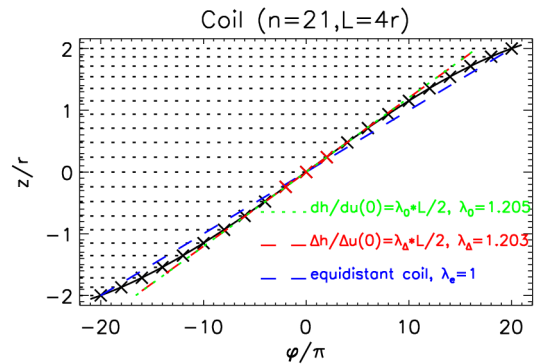
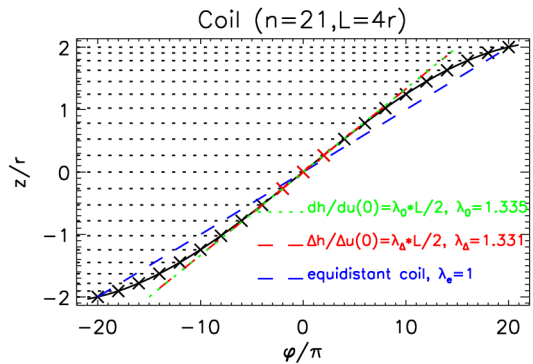
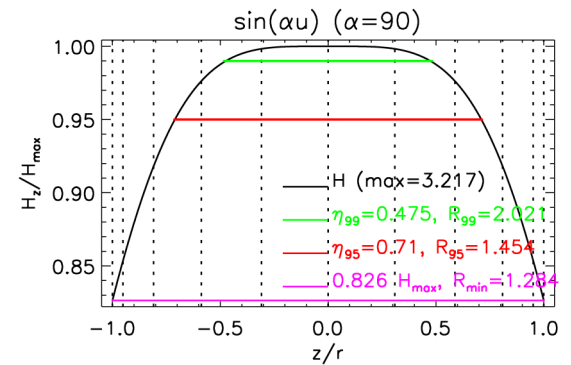
# Potencirana sinusna funkcija $g(u) = a_s \sin^p(\alpha u)$

## Primer $\lambda=0$ , $p=1$

Tuljava ( $n=21$ ,  $L=4r$ )

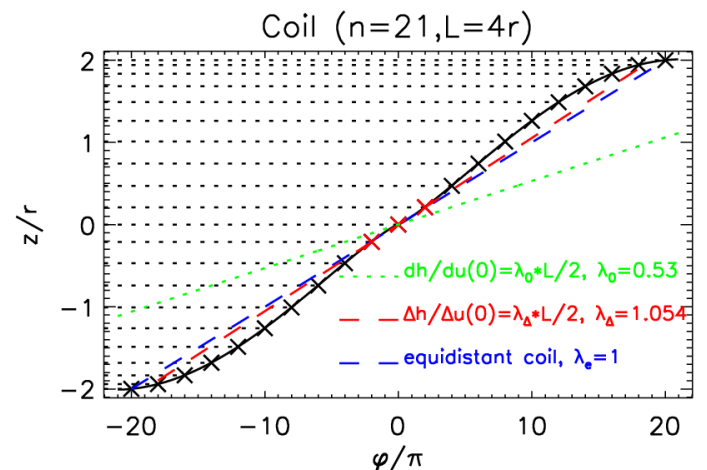
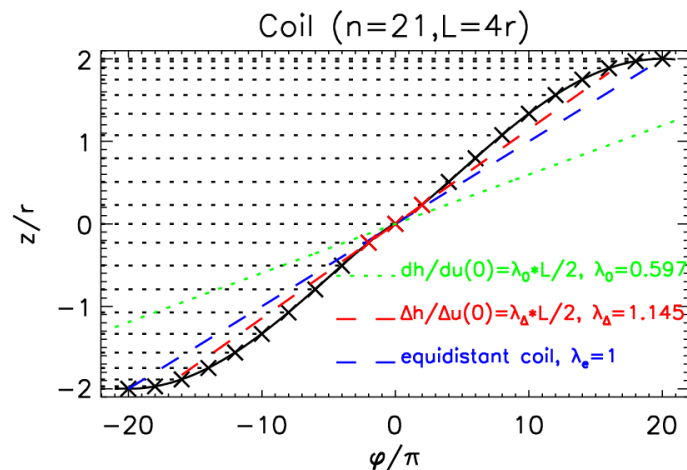
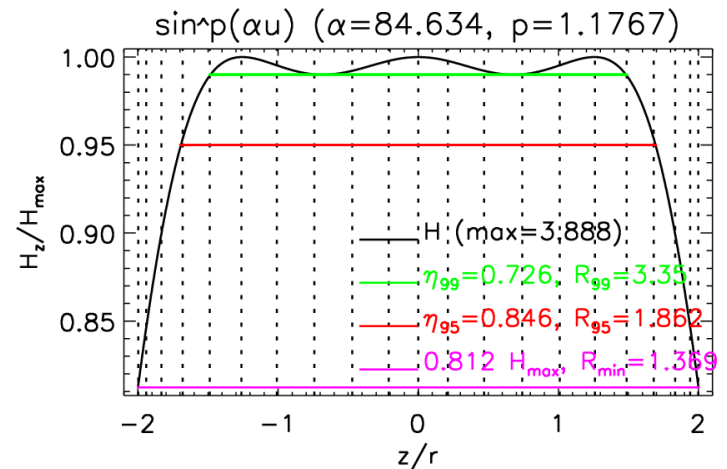
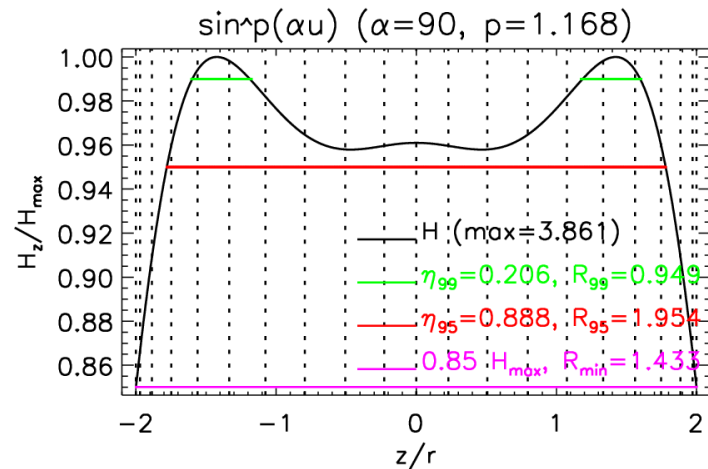


Tuljava ( $n=11$ ,  $L=2r$ )



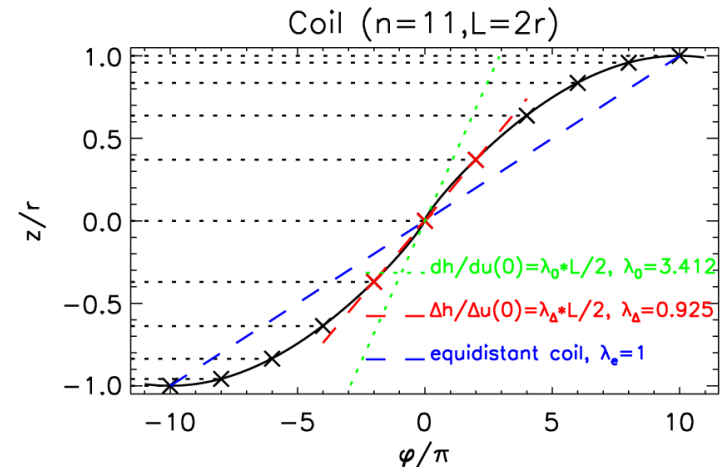
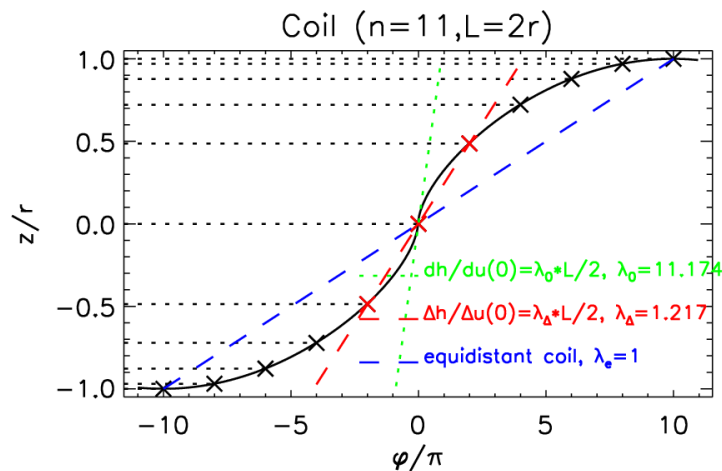
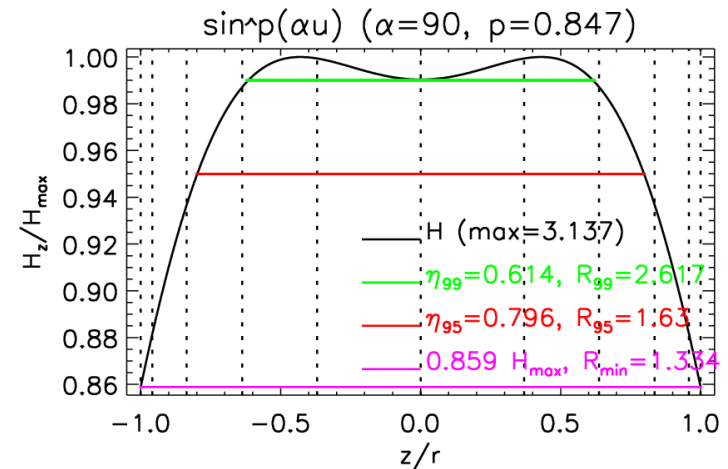
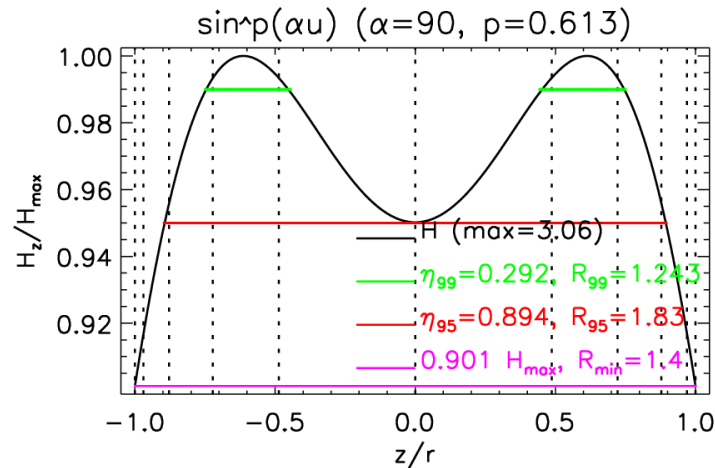
# Potencirana sinusna funkcija $g(u) = a_s \sin^p(\alpha u)$

Primer  $\lambda=0$ ,  $p \neq 1$ , tuljava ( $n=21$ ,  $L=4r$ )



# Potencirana sinusna funkcija $g(u) = a_s \sin^p(\alpha u)$

Primer  $\lambda=0$ ,  $p \neq 1$ , tuljava ( $n=11$ ,  $L=2r$ )



# Vsota dveh potenc $g(u) = au^{p_1} + bu^{p_2}$

$$z(u) = \frac{L}{2} [\lambda u + au^{p_1} + bu^{p_2}] \implies z(1) = \frac{L}{2} [\lambda + a + b] = \frac{L}{2} \implies a + b = (1 - \lambda).$$

$$\frac{dz}{du}(1) = \frac{L}{2} [\lambda + ap_1 + bp_2] = 0 \implies \lambda + ap_1 + bp_2 = 0 \implies ap_1 + bp_2 = -\lambda.$$

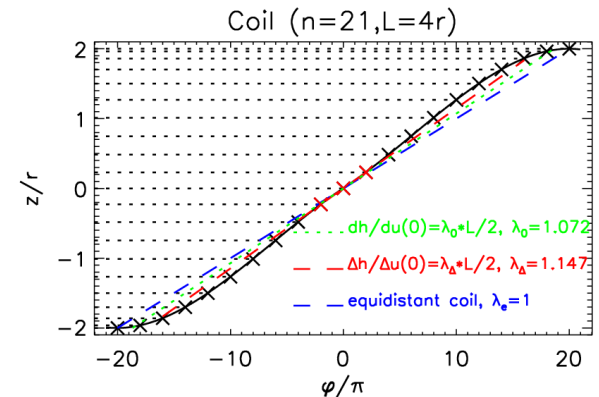
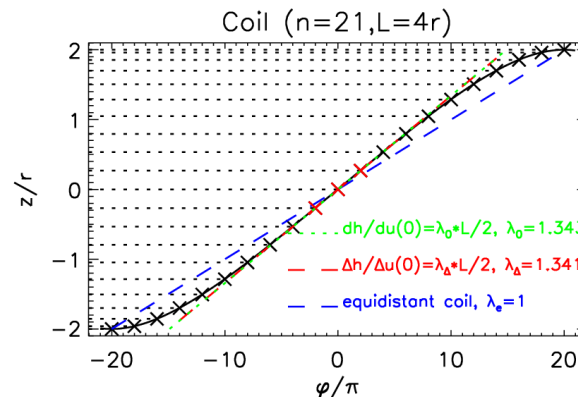
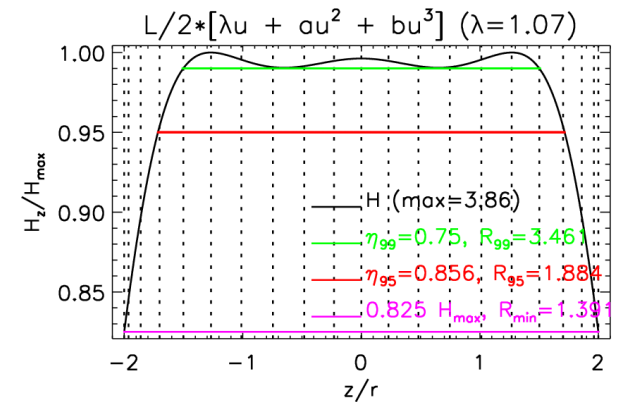
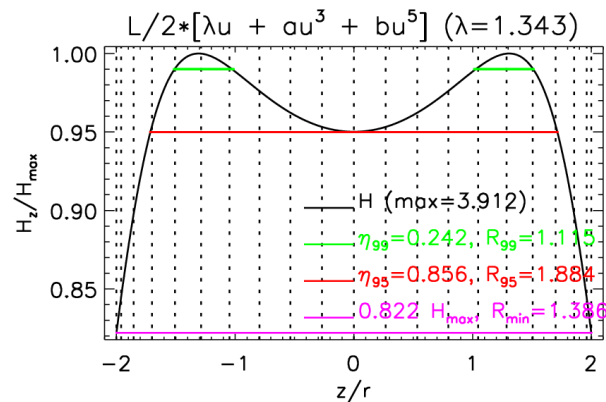
$$a = \frac{\lambda - p_2(\lambda - 1)}{(p_2 - p_1)}, \quad b = \frac{p_1(\lambda - 1) - \lambda}{(p_2 - p_1)} \implies z(u) = \frac{L}{2} \left[ \lambda u + \frac{\lambda - p_2(\lambda - 1)}{(p_2 - p_1)} u^{p_1} + \frac{p_1(\lambda - 1) - \lambda}{(p_2 - p_1)} u^{p_2} \right]$$

Primer

(n=21, L=4r)

p1=konst

p2=konst.



# Povzetek rezultatov za valjaste tuljave

| modelska funkcija<br>$(2/L) * z(u)$ | Tuljava $n=21, L=4r$                  |                                         |                                        |
|-------------------------------------|---------------------------------------|-----------------------------------------|----------------------------------------|
|                                     | $\eta_{99}$                           | $\eta_{95}$                             | $H_{\min}/H_{\max}$                    |
| $u$                                 | <b>0.218</b>                          | <b>0.455</b>                            | <b>0.593</b>                           |
| $au^p$                              | 0.481 ( $p=0.727$ )                   | 0.702 ( $p=0.860$ )                     | 0.765 ( $p=0.606$ )                    |
| $\lambda u + au^p$                  | 0.481 ( $\lambda = 1.2, p=3$ )        | 0.702 ( $\lambda = 1.333, p=4$ )        | 0.826 ( $\lambda = 1.333, p=4$ )       |
| $a_s \sin(\alpha u)$                | 0.588 ( $\alpha=59.5$ )               | 0.814 ( $\alpha=73.2$ )                 | 0.862 ( $\alpha=89.6$ )                |
| $a_s \sin^p(\alpha u)$              | 0.726 ( $\alpha=84.634, p=1.1767$ )   | 0.888 ( $\alpha=90, p=1.168$ )          | 0.850 ( $\alpha=90, p=1.168$ )         |
| $\lambda u + au^{p_1} + bu^{p_2}$   | 0.75 ( $p_1=2, p_2=3, \lambda=1.07$ ) | 0.856 ( $p_1=3, p_2=5, \lambda=1.343$ ) | 0.825 ( $p_1=2, p_2=3, \lambda=1.07$ ) |
| modelska funkcija<br>$(2/L) * z(u)$ | Tuljava $n=11, L=2r$                  |                                         |                                        |
|                                     | $\eta_{99}$                           | $\eta_{95}$                             | $H_{\min}/H_{\max}$                    |
| $u$                                 | <b>0.182</b>                          | <b>0.399</b>                            | <b>0.677</b>                           |
| $au^p$                              | 0.570 ( $p=0.552$ )                   | 0.862 ( $p=0.396$ )                     | 0.914 ( $p=0.392$ )                    |
| $a_s \sin(\alpha u)$                | 0.475 ( $\alpha=90$ )                 | 0.710 ( $\alpha=90$ )                   | 0.826 ( $\alpha=90$ )                  |
| $a_s \sin^p(\alpha u)$              | 0.614 ( $\alpha=90, p=0.847$ )        | 0.894 ( $\alpha=90, p=0.613$ )          | 0.901 ( $\alpha=90, p=0.613$ )         |

# Dodatek: ploščate tuljave

V prvem približku sestavimo ploščato tuljavo s srednjim radijem  $r_0$  in širino  $2w$  iz koncentričnih krožnih zank.

## Arhimedova spirala

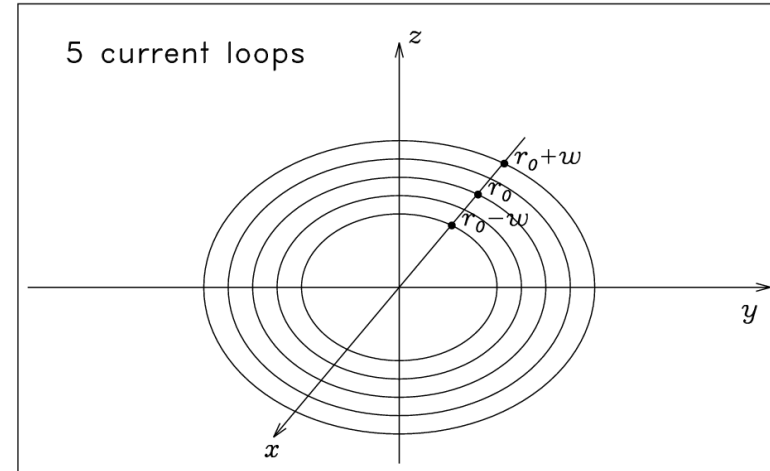
$$r(\varphi) = a'\varphi + b = \frac{a}{2\pi}\varphi + b$$

$$\Delta r = r(\varphi + 2\pi) - r(\varphi) = 2\pi a' = a$$

$$r(\varphi) = a \frac{\varphi + \varphi_0}{2\pi} + b, \text{ kjer sta } a = \frac{2w}{n-1} \text{ in } b = r_0 - w - \frac{w\varphi_0}{(n-1)\pi}$$

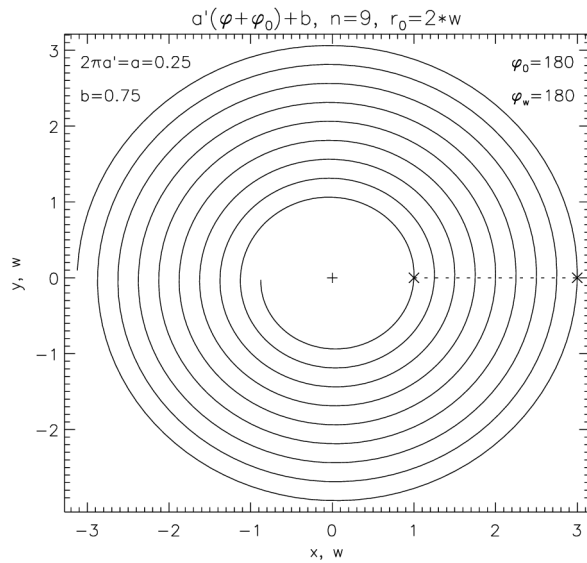
## Optimizacija: potencirana Arhimedova spirala

$$r'(\varphi) = (a'\varphi)^p + b$$

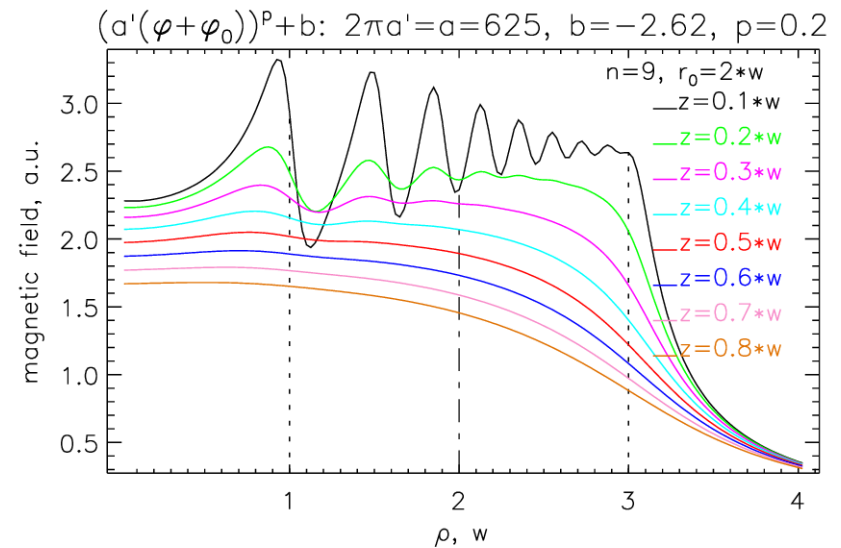
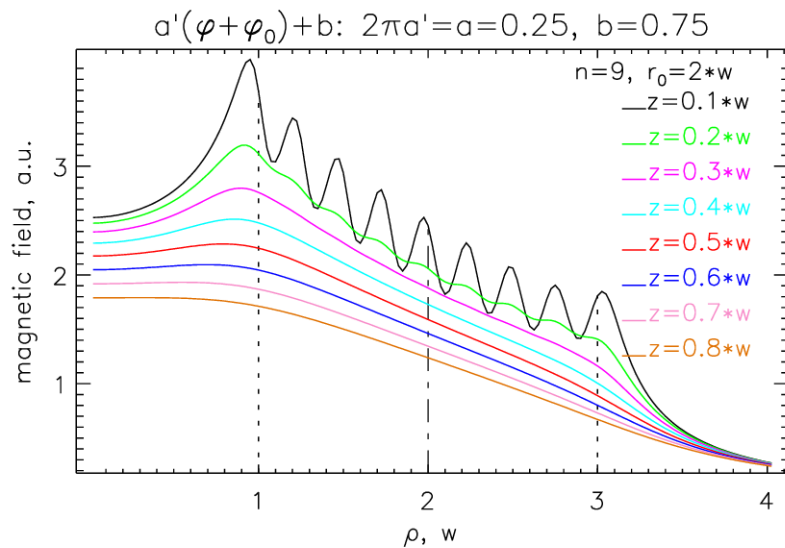
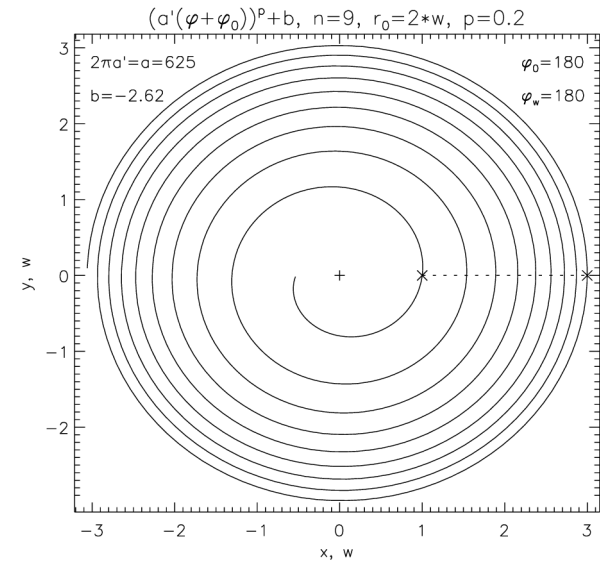


$$r_1 = r_0 - w \text{ do } r_2 = r_0 + w$$

# Arhimedova spirala



# Potencirana spirala



# Zaključki

- S preprostim matematičnim modelom smo optimizirali razdalje med sosednjimi ovoji, tako da smo dobili čim bolj homogeno velikost polja znotraj valjaste tuljave in na določeni oddaljenosti od ploščate tuljave.
- Pri valjastih tuljavah smo tako že z optimizacijo enega do dveh parametrov dosegli znatno povečanje prostornine, v kateri je polje večje od neke želene vrednosti.
- Prostornino, kjer polje preseže 95% maksimalne vrednosti, smo z manj kot manj kot 50% povečali na več kot 80% celotne prostornine tuljave.
- Še večje je povečanje prostornine, kjer polje preseže 99% maksimalne vrednosti, saj se to iz okoli  $1/5$  poveča na okoli  $2/3$  celotne prostornine tuljave.

Hvala za pozornost