On **analytic continuation** from imaginary to real chemical potential in Lattice QCD

Francesco Di Renzo (University of Parma and INFN)

Lattice 2024

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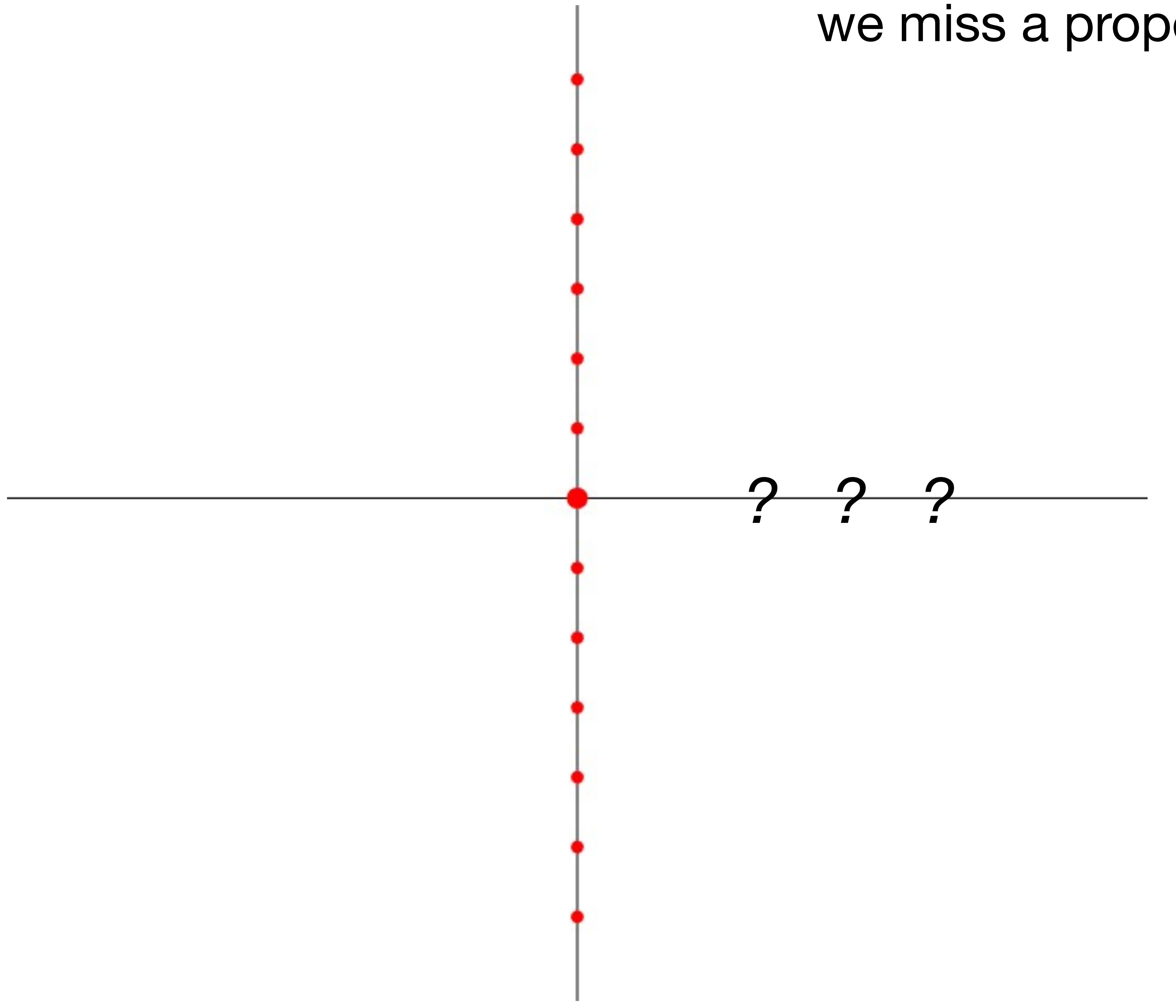
In collaboration with P. Dimopoulos and M. Aliberti (Parma)
Bielefeld Parma Collaboration (… K. Zambello …)

(see talk by C. Schmidt)

SIGN PROBLEM for finite density Lattice QCD:
we miss a properly defined (positive) measure in the path integral! … no MC simulation

(… but everything is fine on the imaginary axis)



Mainly two working solutions:

- Compute Taylor expansions at $\mu_B = 0$
- Compute on the imaginary axis $\mu_B = i\mu_I$

The two solutions are obviously related … and both imply (strictly speaking) an ANALYTIC CONTINUATION

There are tensions in between differente results for Taylor coefficients in the literature…

Agenda

- An invitation (sign problem…)
- Analytic continuation from **multi-point Padé**
- The sign problem as an **inverse problem** …
- … and what you can learn from the latter …
- The goal: **compare different methods on the same data**

A few words on multi-point PADÈ

Suppose you know the values of a function (and of its derivatives) at a number of points

$$\ldots\;,\; f(z_k)\,,\; f'(z_k)\,,\;\ldots,\; f^{(s-1)}(z_k)\,,\;\ldots \qquad\qquad k = 1\ldots N$$

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If you want to approximate the function with a rational function

$$R_n^m(z) = \frac{P_m(z)}{\tilde{Q}_n(z)} = \frac{P_m(z)}{1+Q_n(z)} = \frac{\sum_{i=0}^{m} a_i\, z^i}{1+\sum_{j=1}^{n} b_j\, z^j}$$

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the obvious requirement is that

$$R^{m\,(j)}_n(z_k) = f^{(j)}(z_k) \qquad\qquad k = 1\ldots N, \quad j = 0\ldots s-1$$

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This is the starting point for a ***multi-point Padè approximation***: solve the linear system

$$\begin{aligned} &\ldots \\ P_m(z_k) - f(z_k)Q_n(z_k) &= f(z_k) \\ P'_m(z_k) - f'(z_k)Q_n(z_k) - f(z_k)Q'_n(z_k) &= f'(z_k) \\ &\ldots \end{aligned}$$

from which we want to get the unknown

$$\{a_i \,|\, i = 0\ldots m\} \quad \{b_j \,|\, j = 1\ldots n\} \qquad n + m + 1 = N\, s$$

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In principle you should require that $\nexists\, z_0 \;:\; P_m(z_0) = \tilde{Q}_n(z_0) = 0$

… but we will need to give up with this …

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Yes! LATTICE QCD at IMAGINARY values of the baryonic chemical potential

PHYSICAL REVIEW D **105,** 034513 (2022)

Contribution to understanding the phase structure of strong interaction matter: Lee-Yang edge singularities from lattice QCD

P. Dimopoulos,[1] L. Dini,[2] F. Di Renzo,[1] J. Goswami,[2] G. Nicotra,[2] C. Schmidt,[2] S. Singh,[1,*] K. Zambello,[1] and F. Ziesché[2]

… where we computed and “multi-point Padè approximated”

$$\chi_n^B(T,V,\mu_B) = \left(\frac{\partial}{\partial \hat{\mu}_B}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$

$$= \left(\frac{1}{3}\frac{\partial}{\partial \hat{\mu}_l} + \frac{1}{3}\frac{\partial}{\partial \hat{\mu}_s}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$

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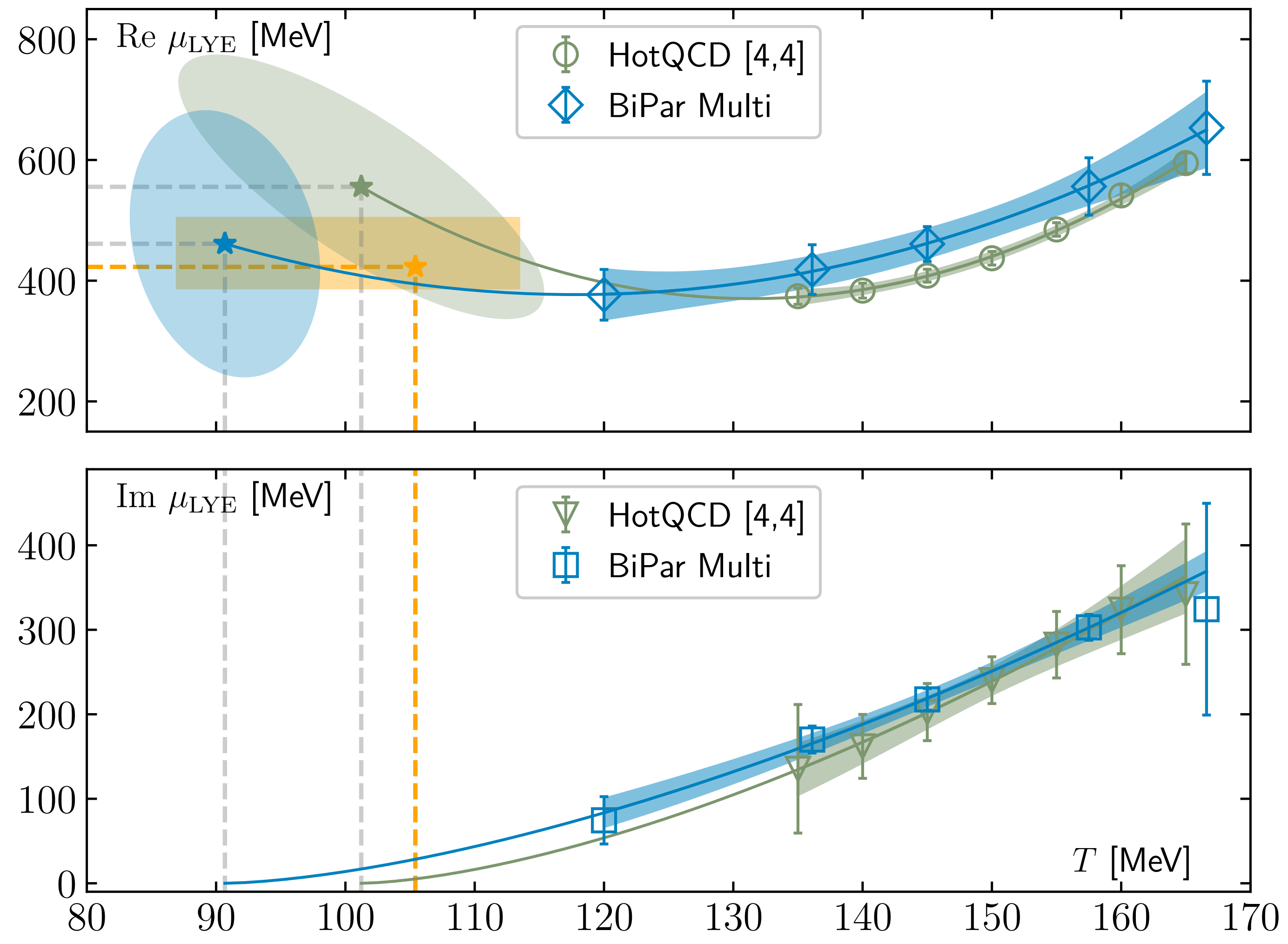

FIG. 4. Scaling fits for the LYE singularities related to the CEP. Green data come from a [4,4] Padé from Ref. [7]. Blue data come from the multi-point Padé. *Top*: Scaling of the real part. *Bottom*: Scaling of the imaginary part. The ellipses shown in the top panel represent the 68% confidence region deduced from the covariance matrix of the fit. The orange box indicates the AIC weighted estimate (6).

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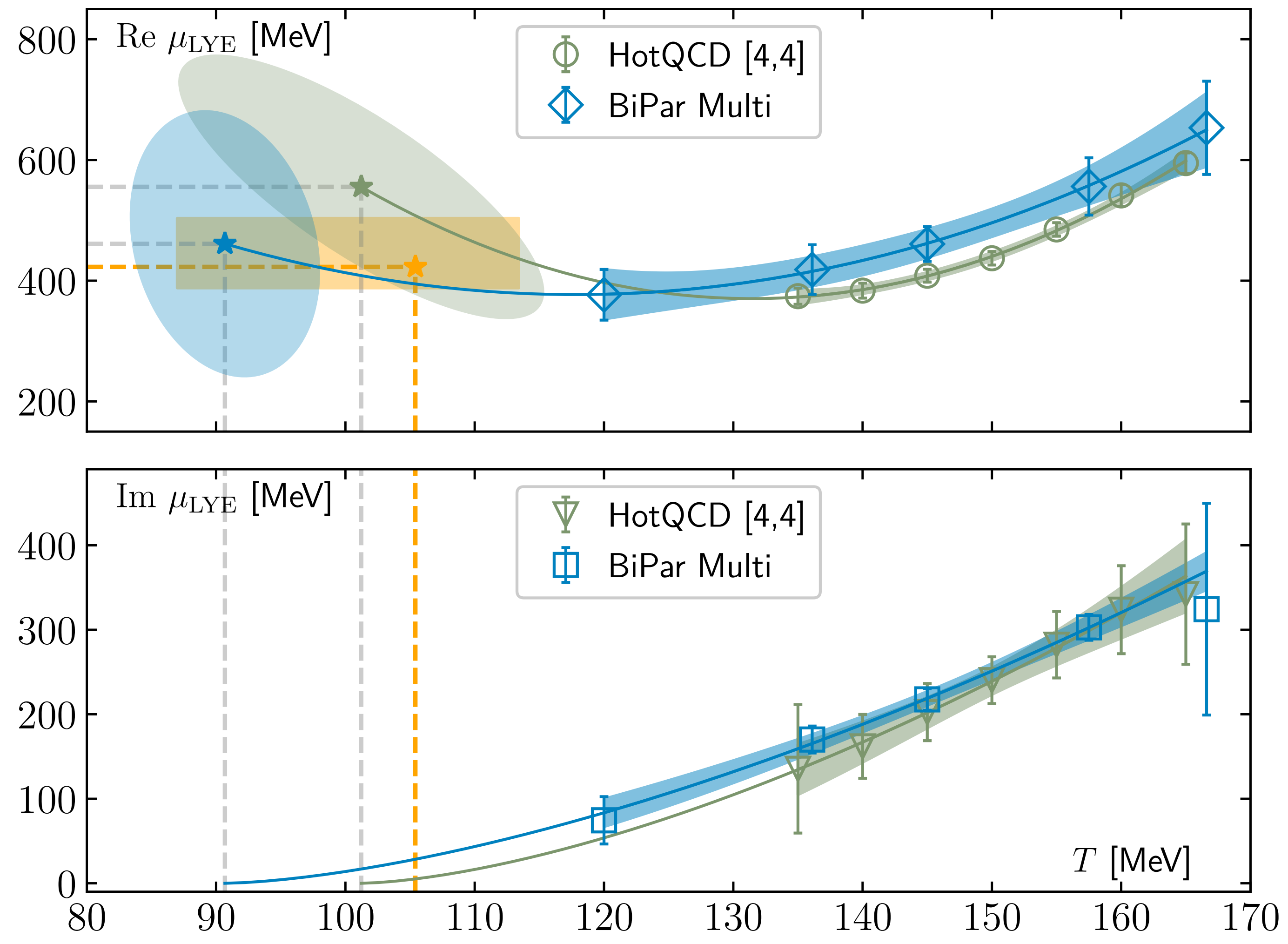

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In the following we will play with a few Bielefeld Parma Collaboration data 2+1 HISQ at physical quarks mass, at fixed cutoff ($N_\tau = 6$)

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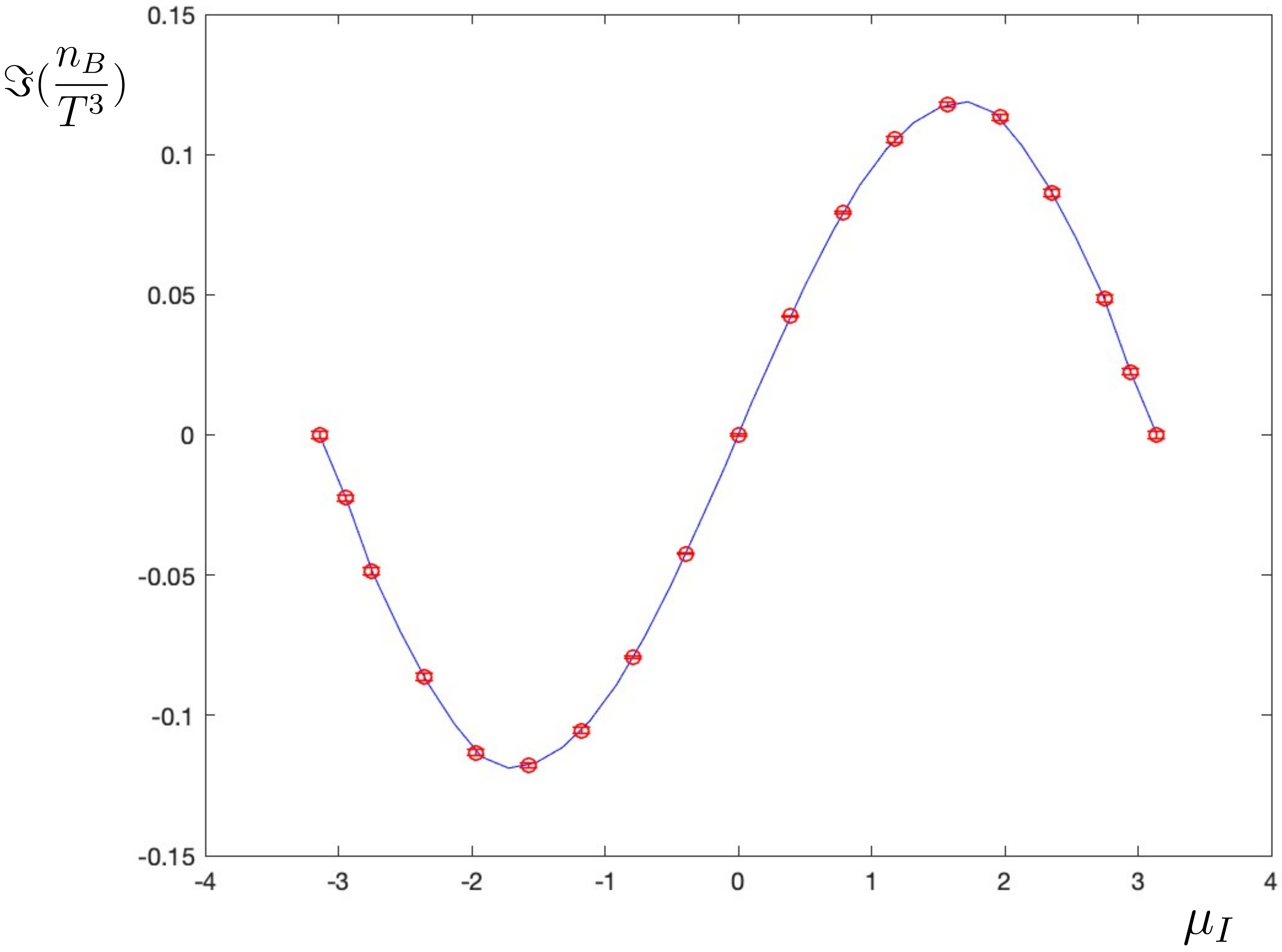
$T = 157.5\ (\sim 155)$ MeV



... which is pretty simple (we will be concerned with the number density):

you take your rational function, which describes very well data at IMAGINARY VALUES of μ_B

CAVEAT: errors on data points are there ... no error shown on the interpolating function (*as for now* ...)

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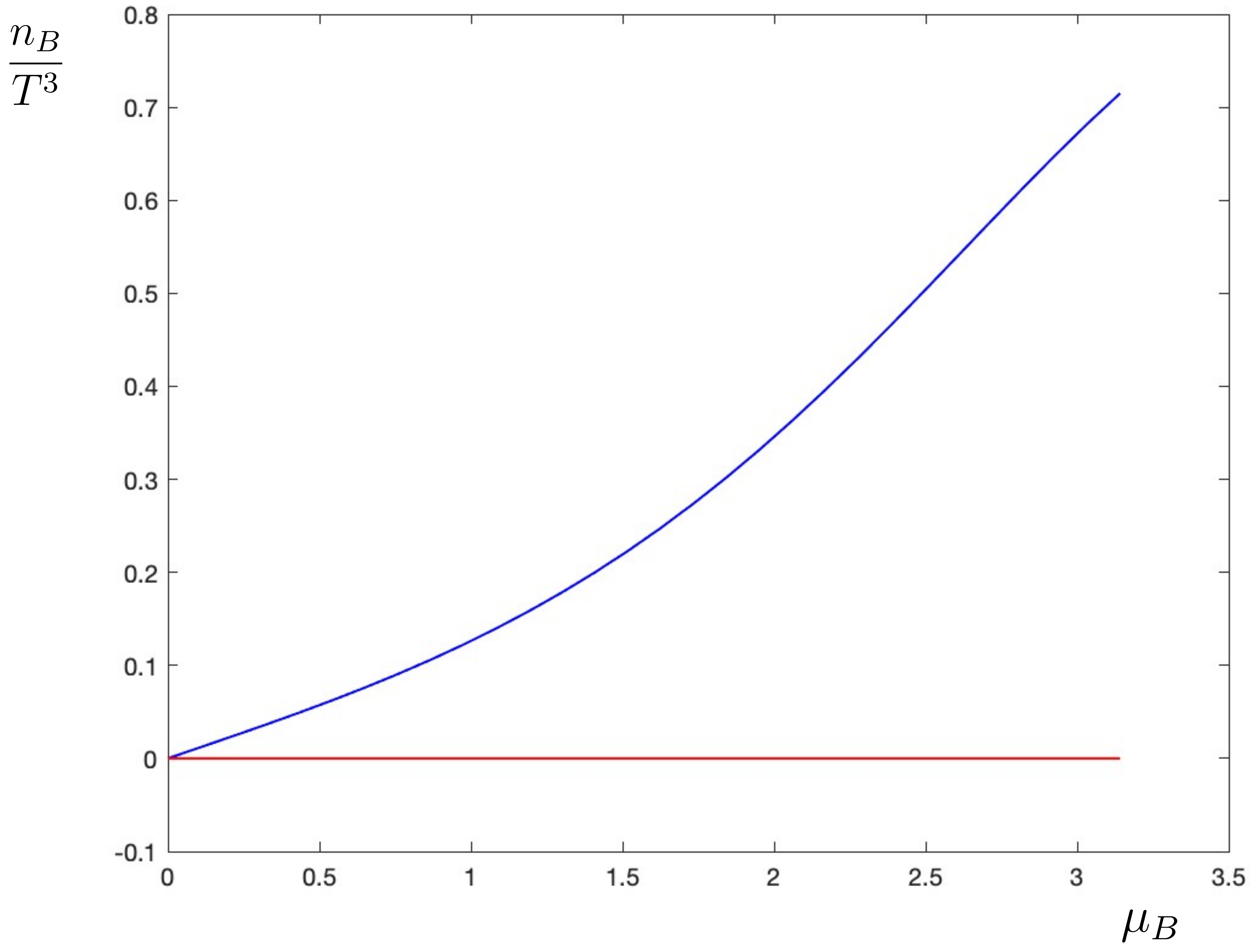

... which is pretty simple (we will be concerned with the number density):

you take your rational function, which describes very well data at IMAGINARY VALUES of μ_B

... and you simply compute it for REAL VALUES of μ_B

CAVEAT: no error shown as for now ... here we are concerned with *trends*... FIXED CUTOFF!

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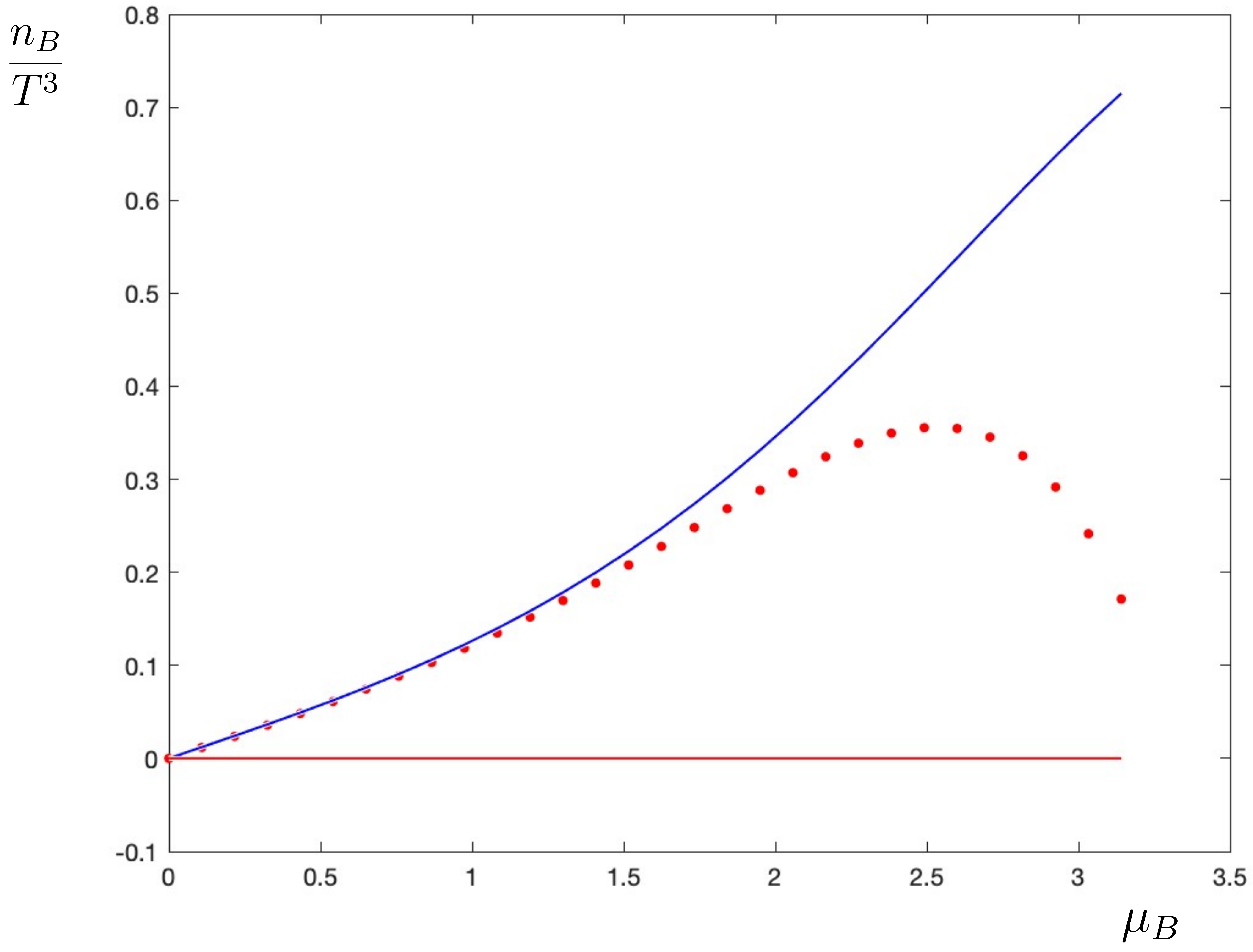

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You can compare the result with HotQCD results

PHYSICAL REVIEW D **105**, 074511 (2022)

Taylor expansions and Padé approximants for cumulants of conserved charge fluctuations at nonvanishing chemical potentials

D. Bollweg,[1] J. Goswami,[2] O. Kaczmarek,[2] F. Karsch,[2] Swagato Mukherjee,[3] P. Petreczky,[3] C. Schmidt,[2] and P. Scior[3]

(HotQCD Collaboration)

CAVEAT: no error shown as for now … here we are concerned with *trends*… FIXED CUTOFF!

Finite density QCD as an inverse problem

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… *aka* How to trade a difficult problem for another (even more?) difficult one …

What does ANALYTICITY mean? … (analytic functions aka olomorphic…)

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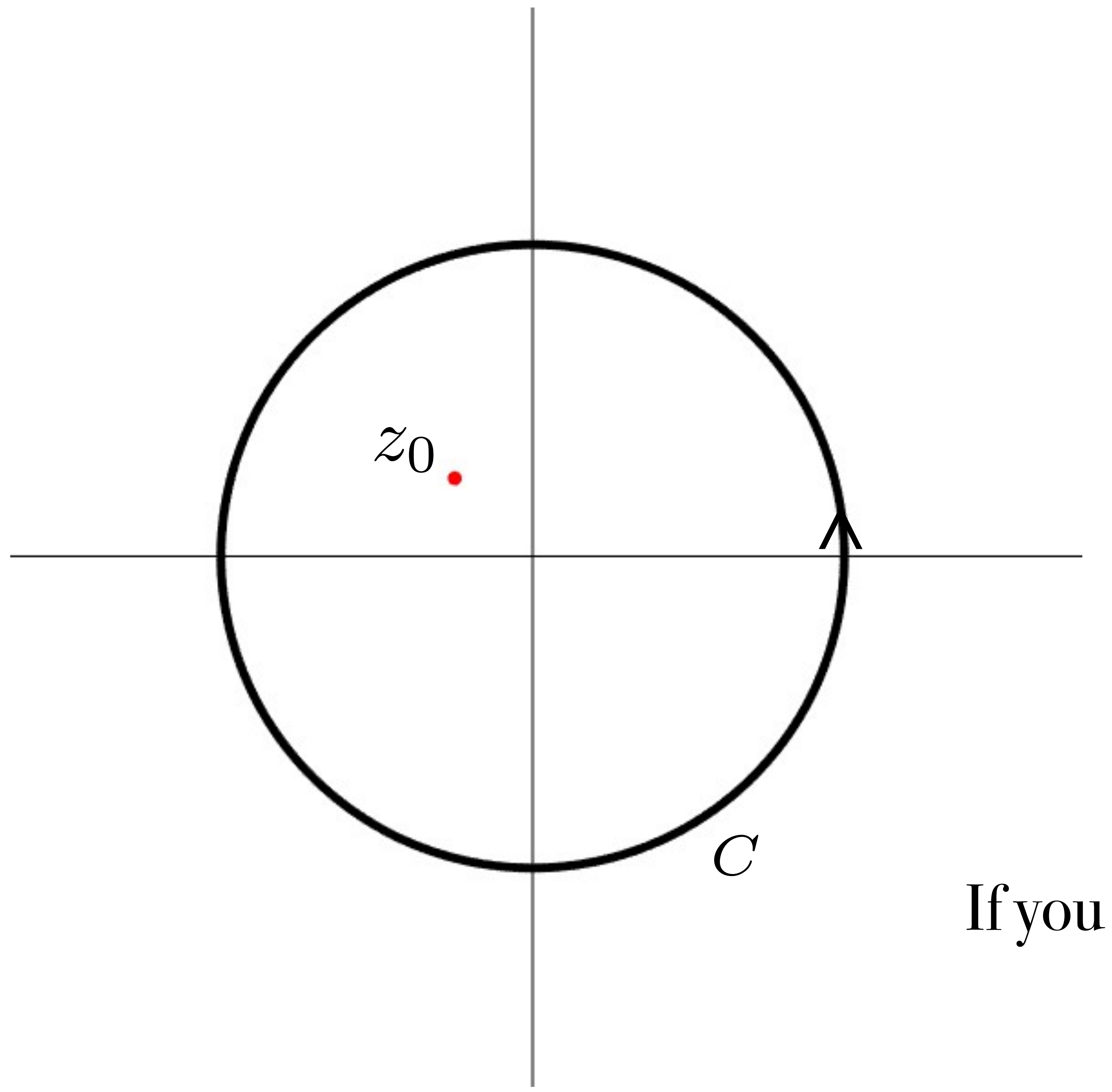
One simple way of thinking of it is that *you can perfectly know such functions from an apparently limited amount of information.*



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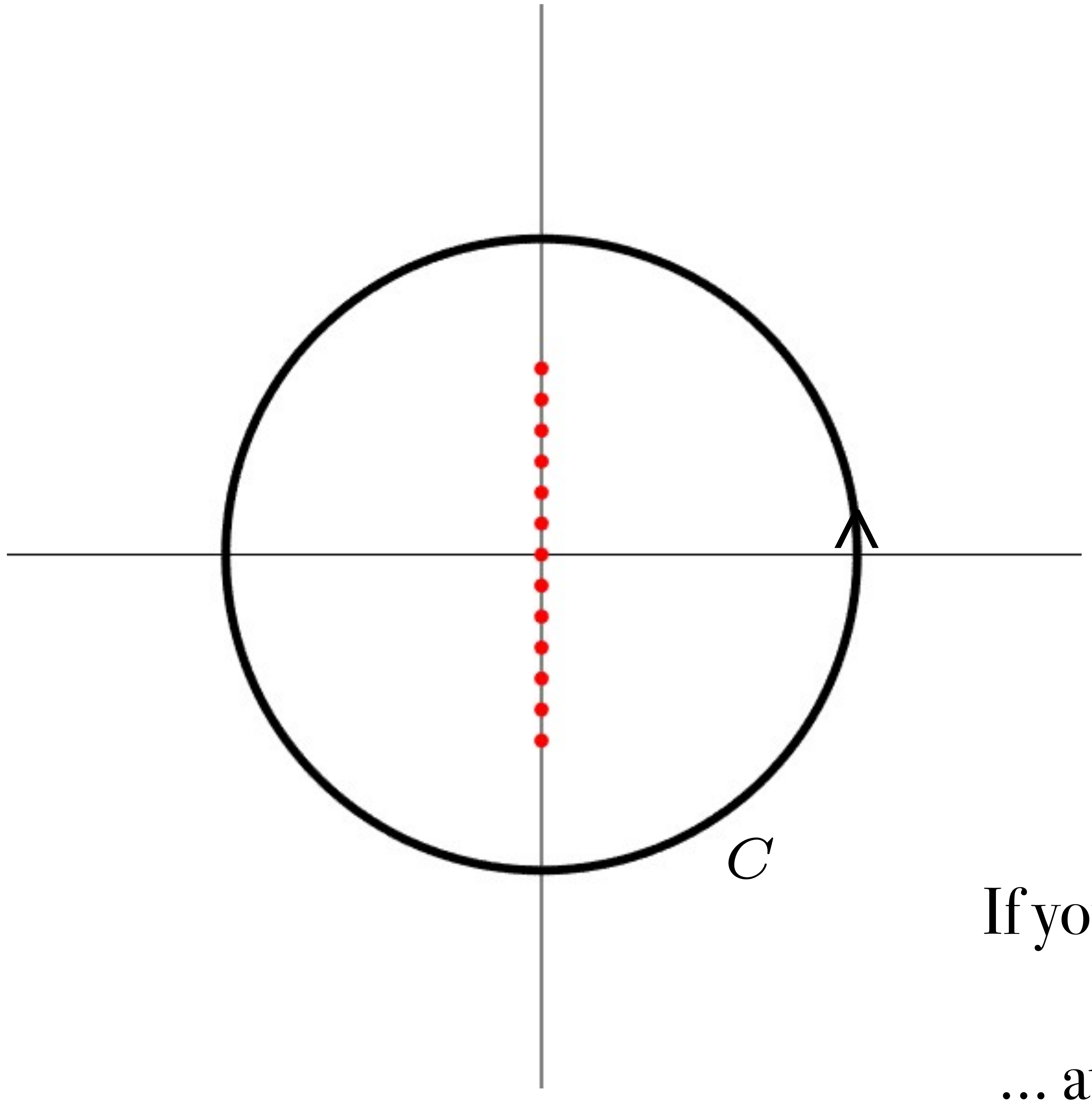
CAUCHY FORMULA

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0}\, dz$$

If you know the function on the contour, you can compute it at any point inside… sounds good!

What does ANALYTICITY mean? ... (analytic functions aka olomorphic...)



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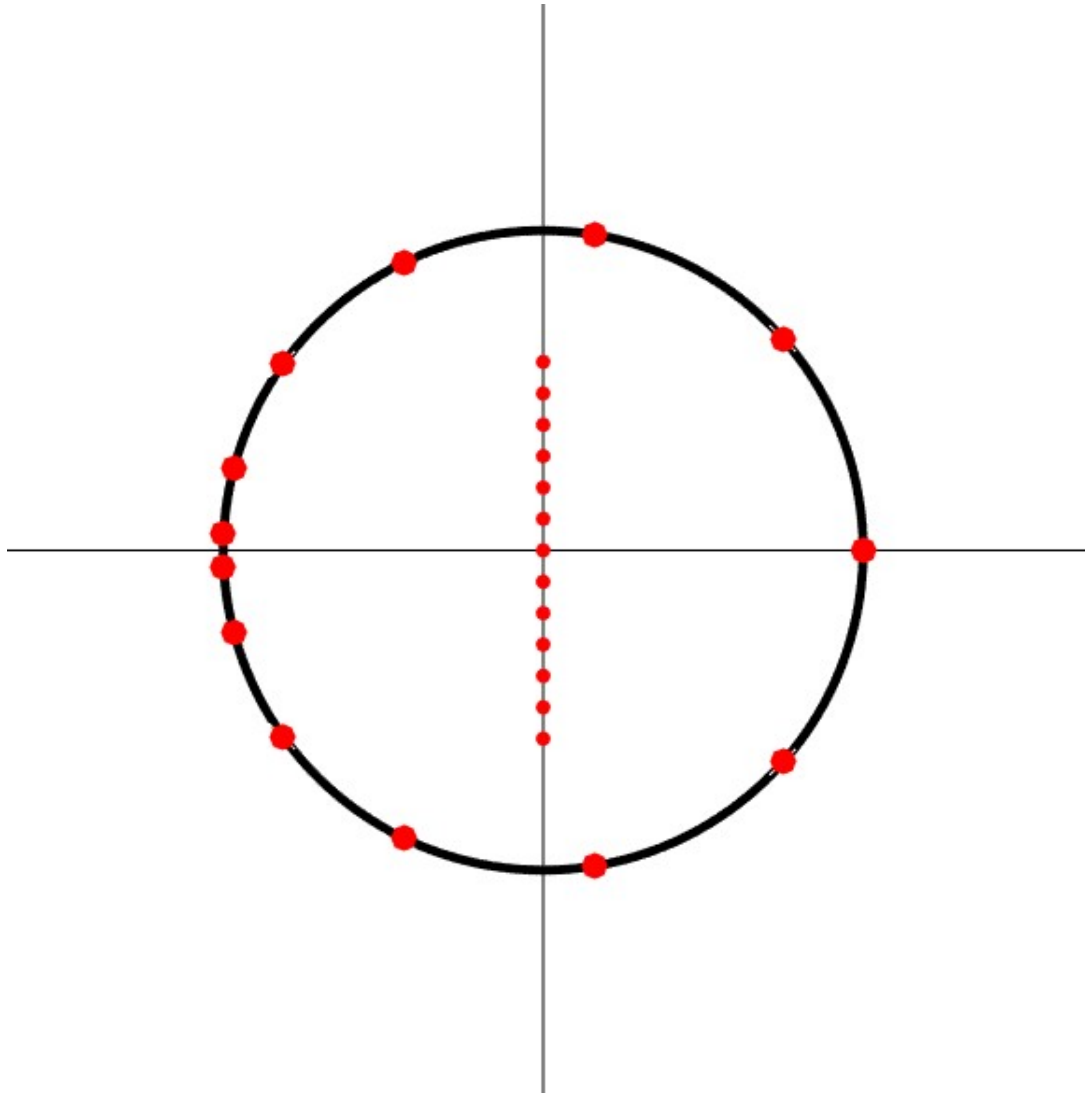
... at any point, including the (only) ones we can compute (on the imaginary axis) in our case...

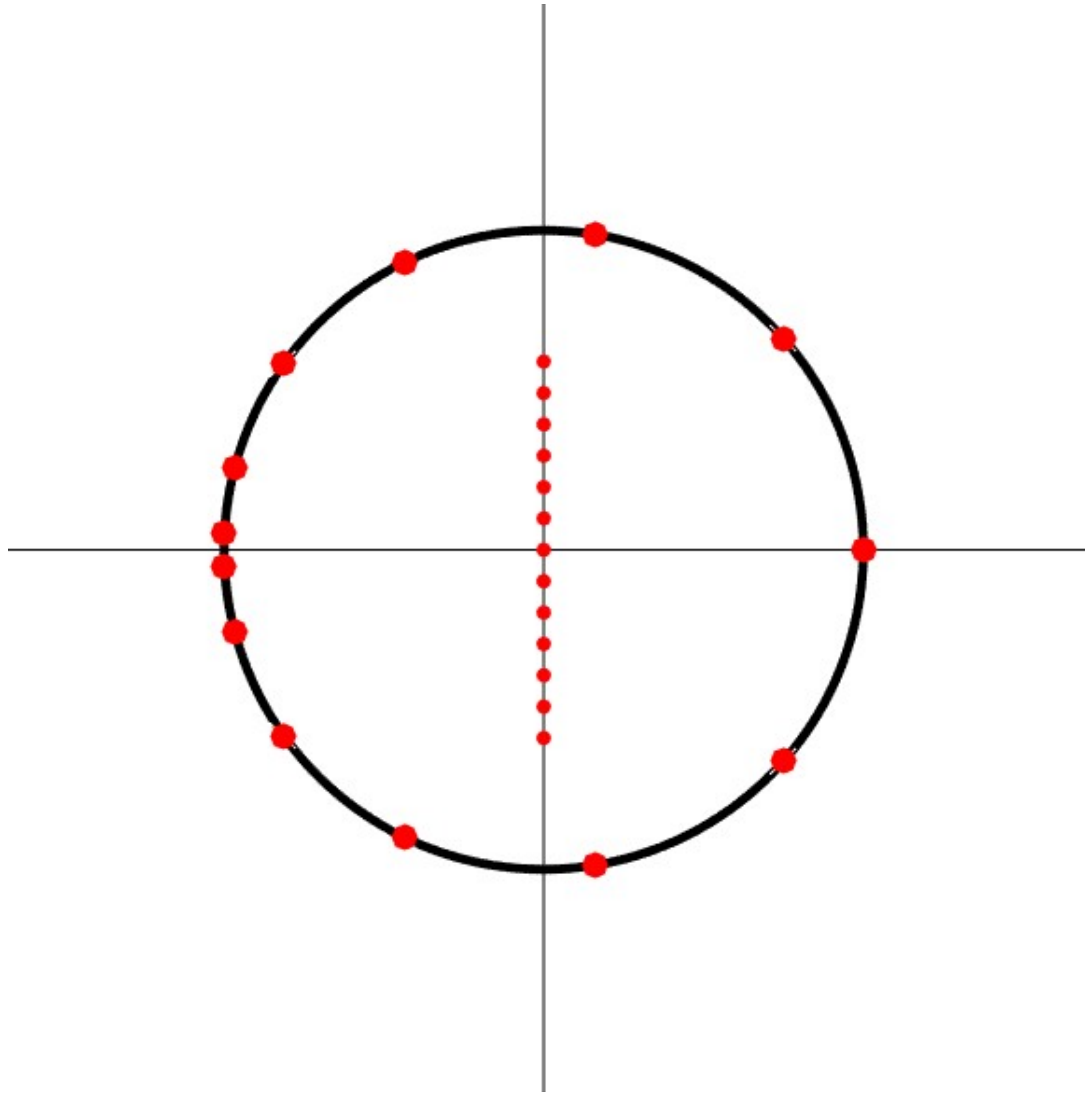


With your favourite QUADRATURE method ... you can go numeric!

De facto, you would like to think of Legendre quadrature

$$f(z_0) = \frac{1}{2\pi}\int_0^{2\pi} \frac{f(R\,e^{i\theta})\,R\,e^{i\theta}}{R\,e^{i\theta} - z_0}\,d\theta \simeq \frac{1}{2\pi}\sum_{k=1}^{n} w_k \,\frac{f(R\,e^{i\theta_k})\,R\,e^{i\theta_k}}{R\,e^{i\theta_k} - z_0}$$

$$y_i = \frac{1}{2\pi}\sum_{k=1}^{n} w_k \,\frac{R\,e^{i\theta_k}}{R\,e^{i\theta_k} - z_i}\,\hat{f}_k\,, \quad i = 1, 2, \ldots, n$$



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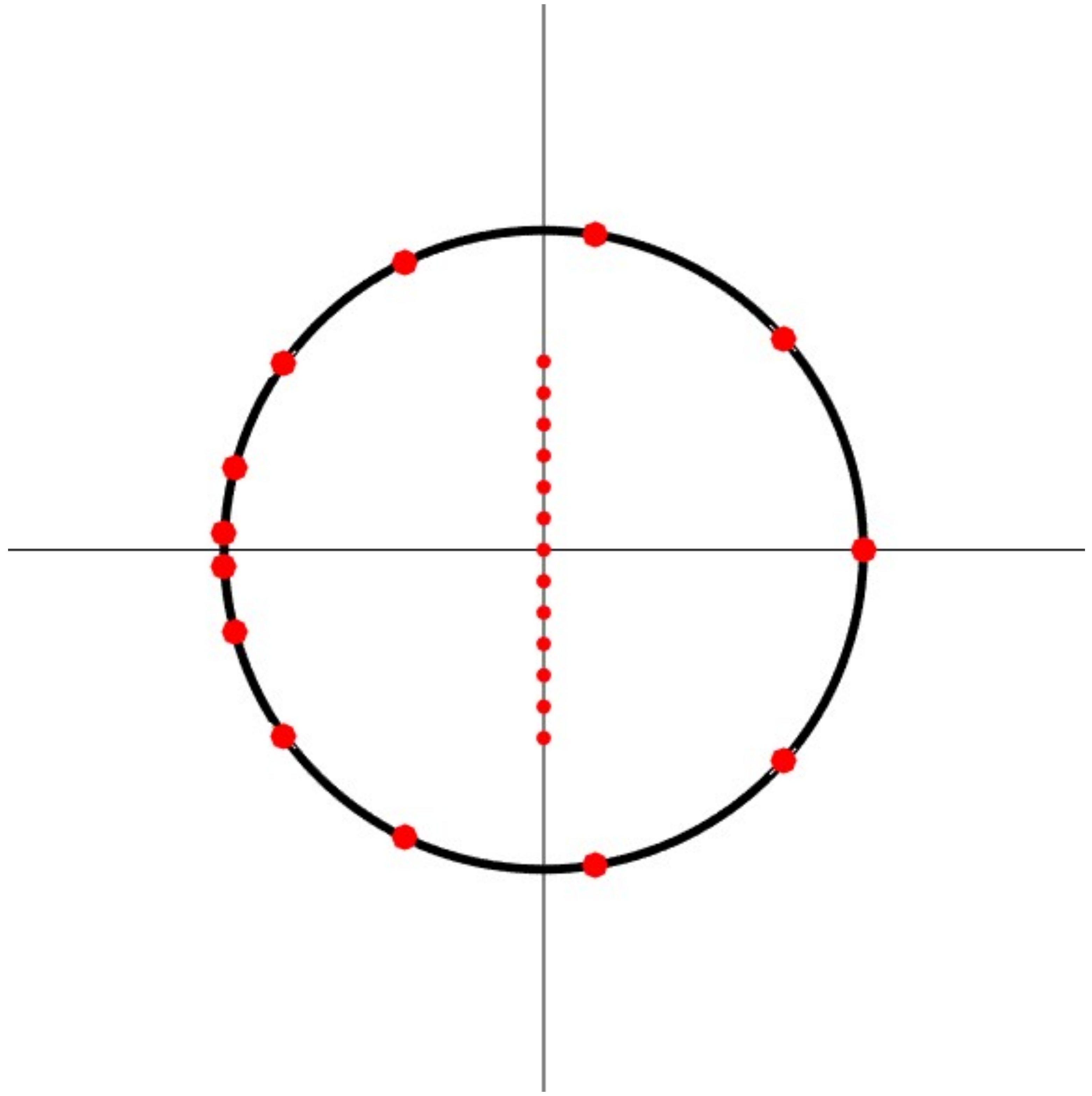
... and then you are ready for your (BRAVE) INVERSE PROBLEM!



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$$A_{ik} = \frac{1}{2\pi}\,w_k\,\frac{R\,e^{i\theta_k}}{R\,e^{i\theta_k} - z_i}$$

$$A\,\mathbf{x} = \mathbf{b}$$

SOLVE for the $\hat{f}_k$!

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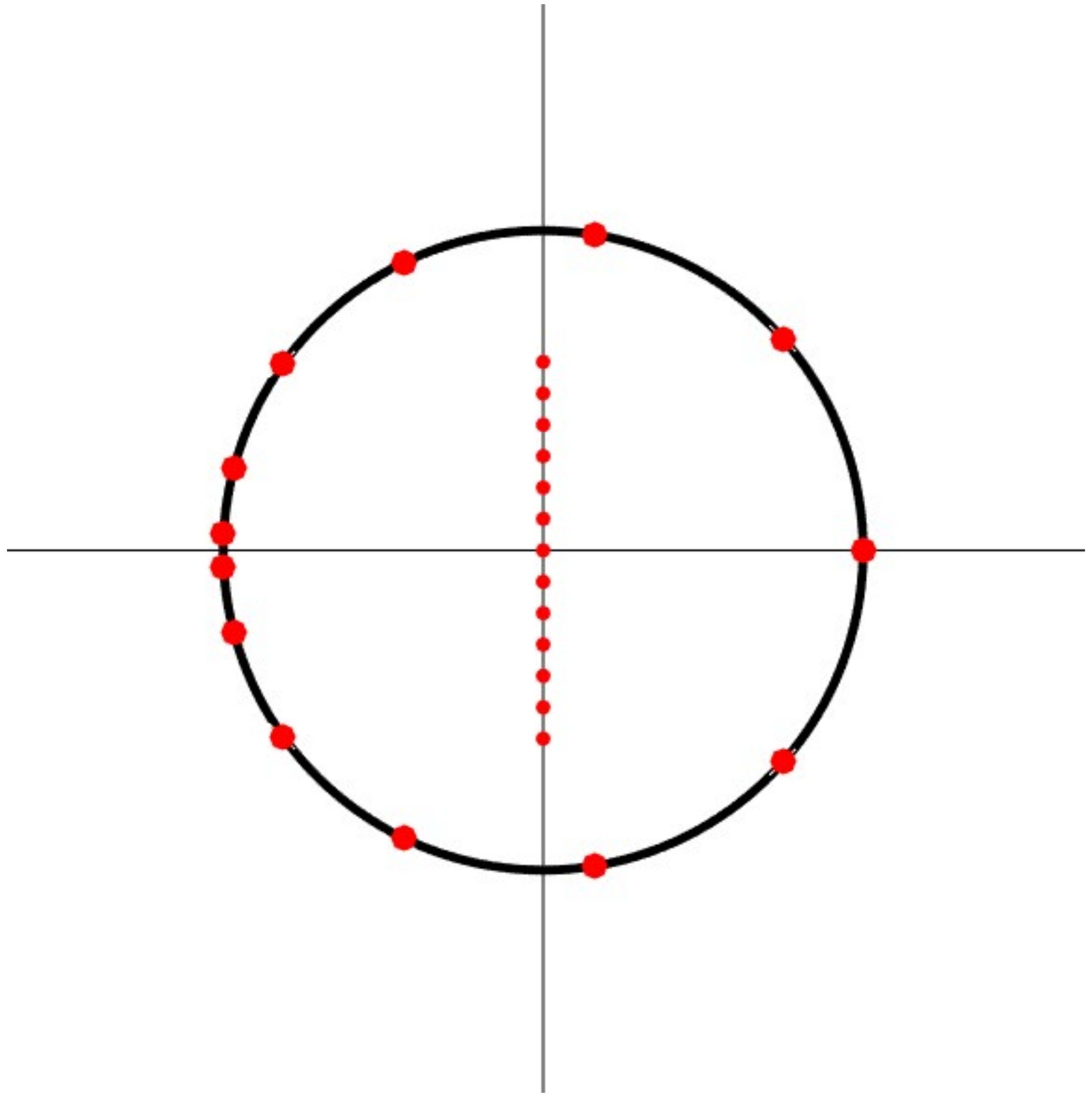

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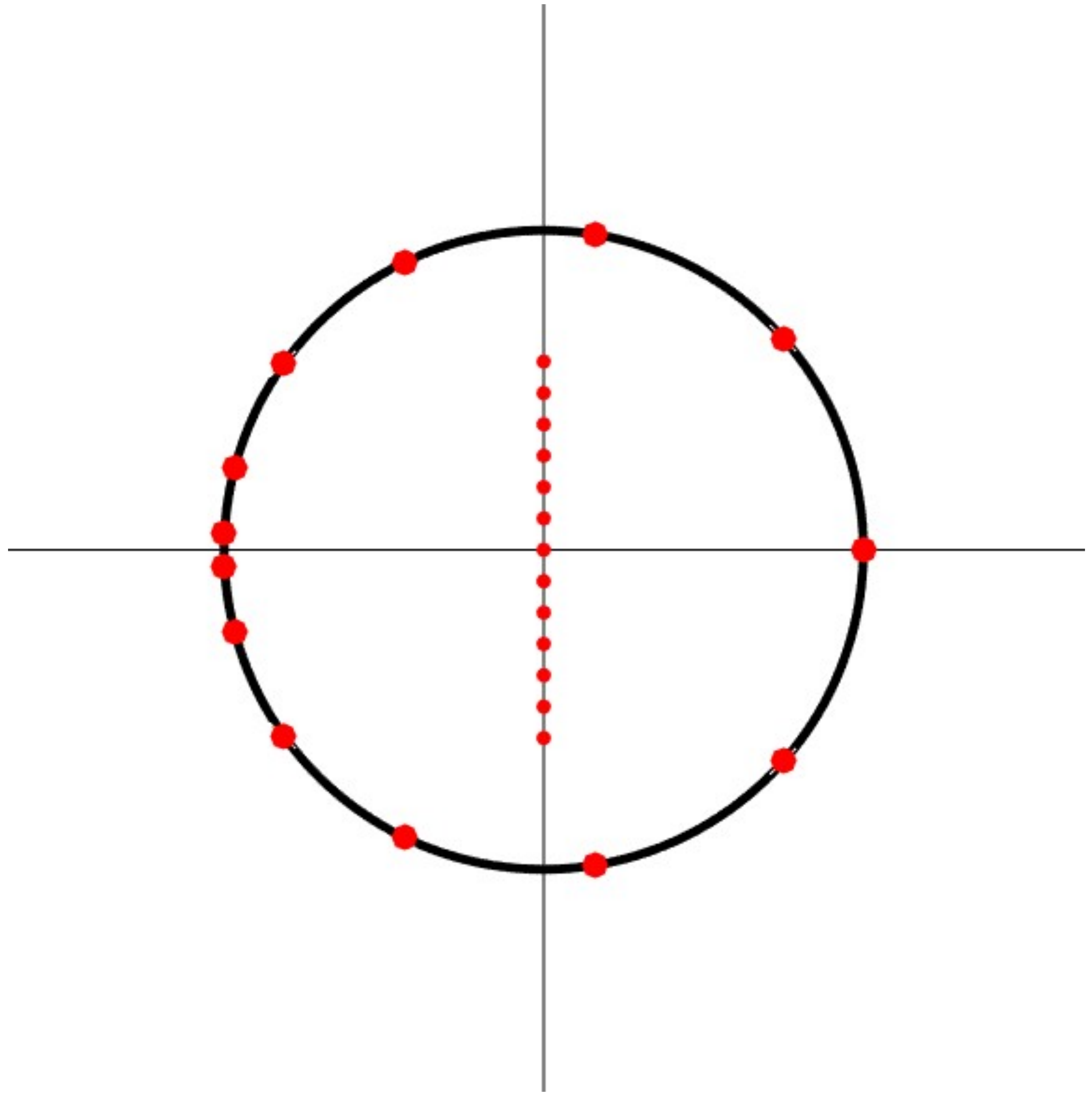
A very SIMPLE idea! ... a NAIVE one ... INVERSE PROBLEM!!!



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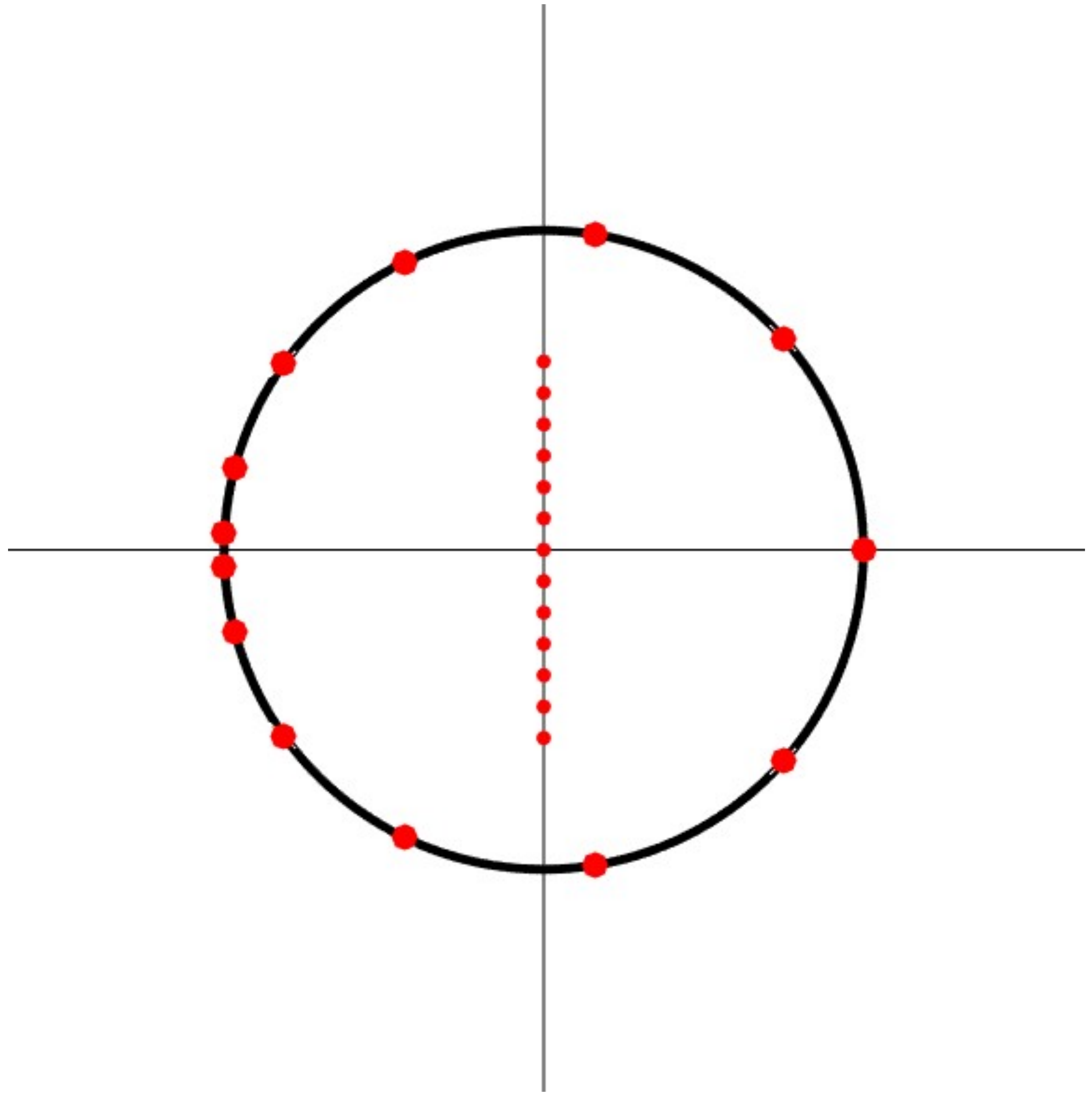
SOLVE for the $\hat{f}_k$!

… but when you have an idea you often get excited … so let's try with the sin function.

Remember: we take our input on the imaginary axis and we want to compute on the real axis!



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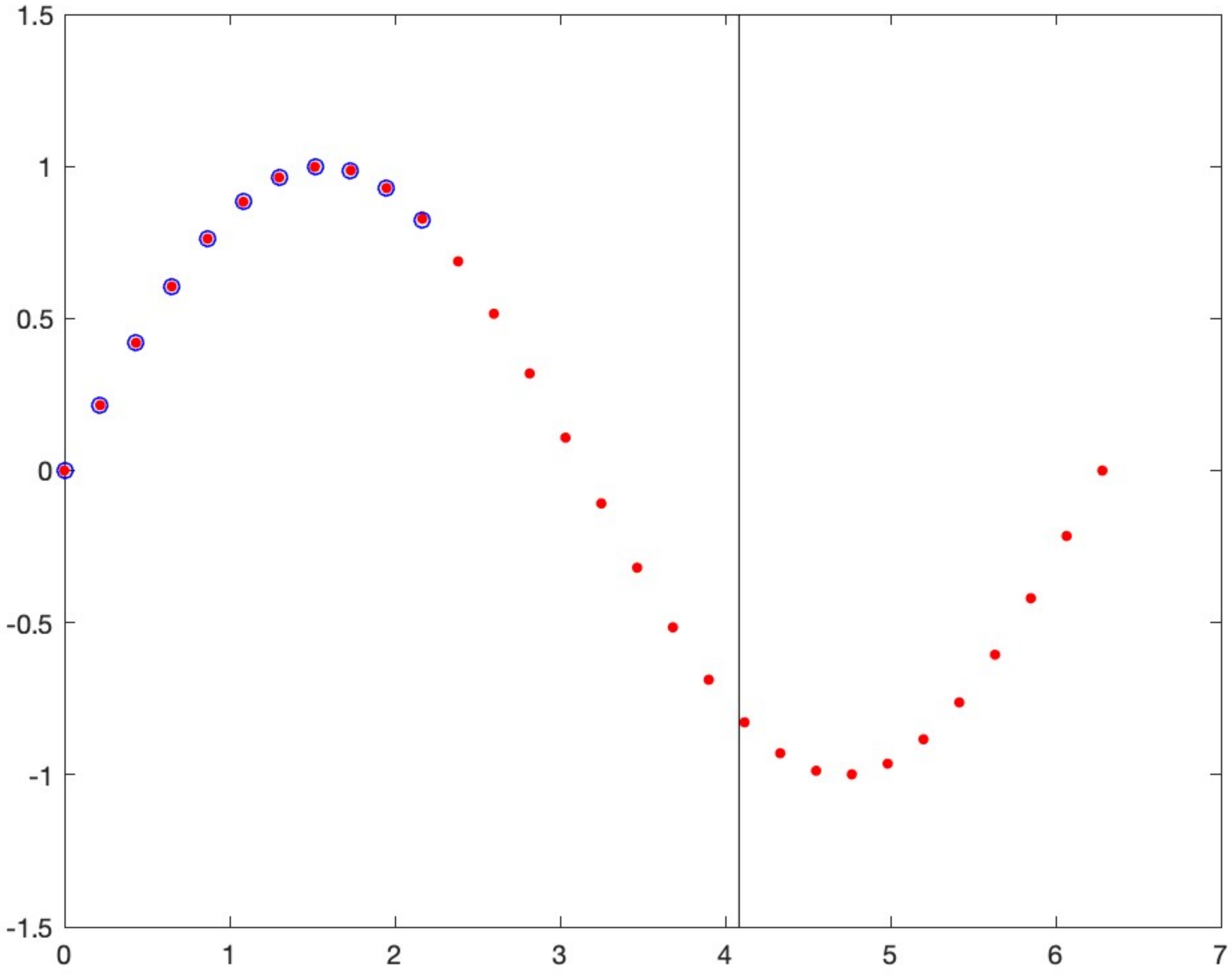
Radius (*ca 4*) and number of points (*13*) chosen having in mind what we have to live with in finite density QCD!

Reconstructing *sin(x)*



It looks like it works … but it should not!

Notice the *barrier* (vertical line) you cannot overcome. For an analytic function, you will get zero if you do…

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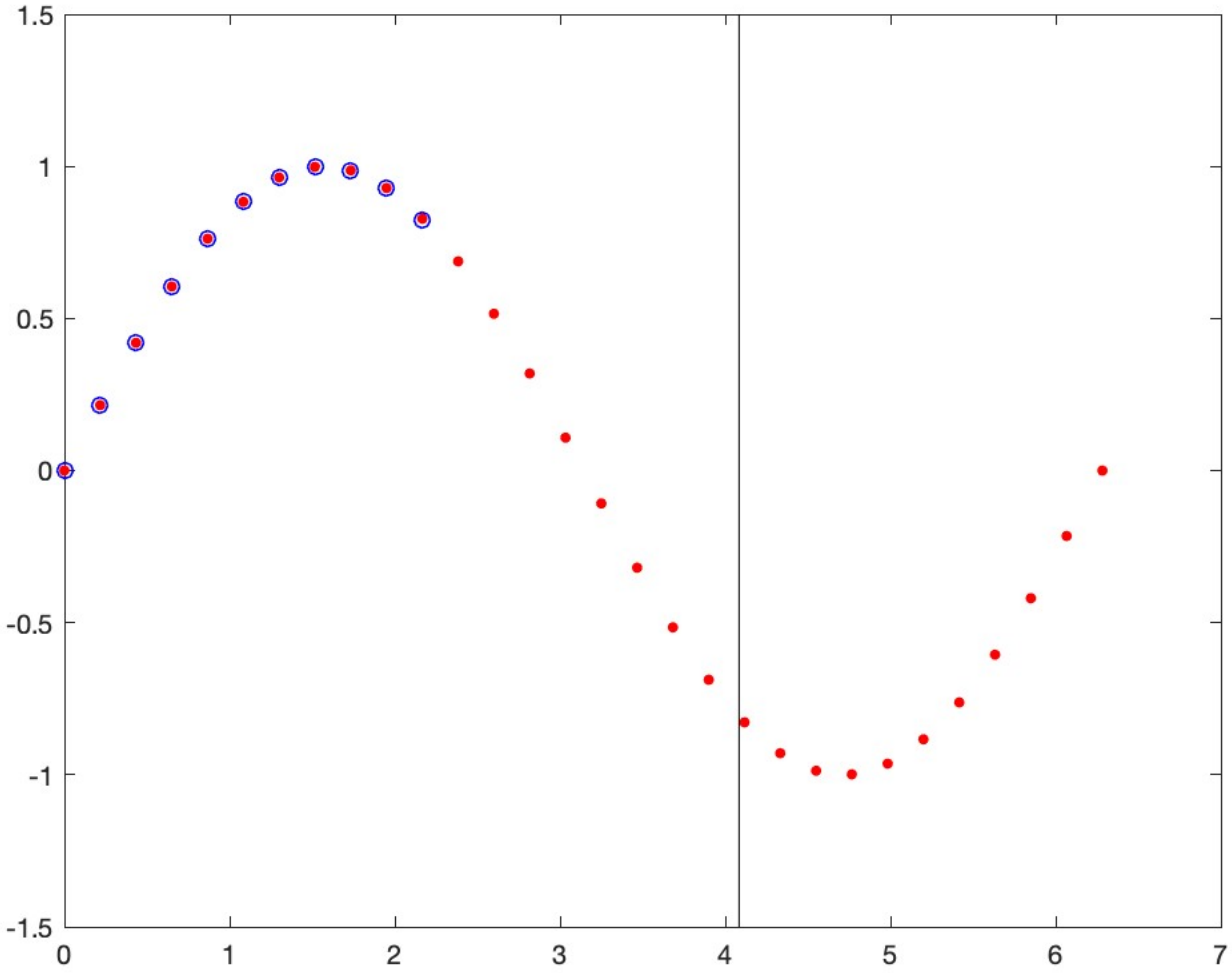

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… and it should not for a combination of
(a) bad condition number of the linear system
(b) the quadrature formula being NOT exact

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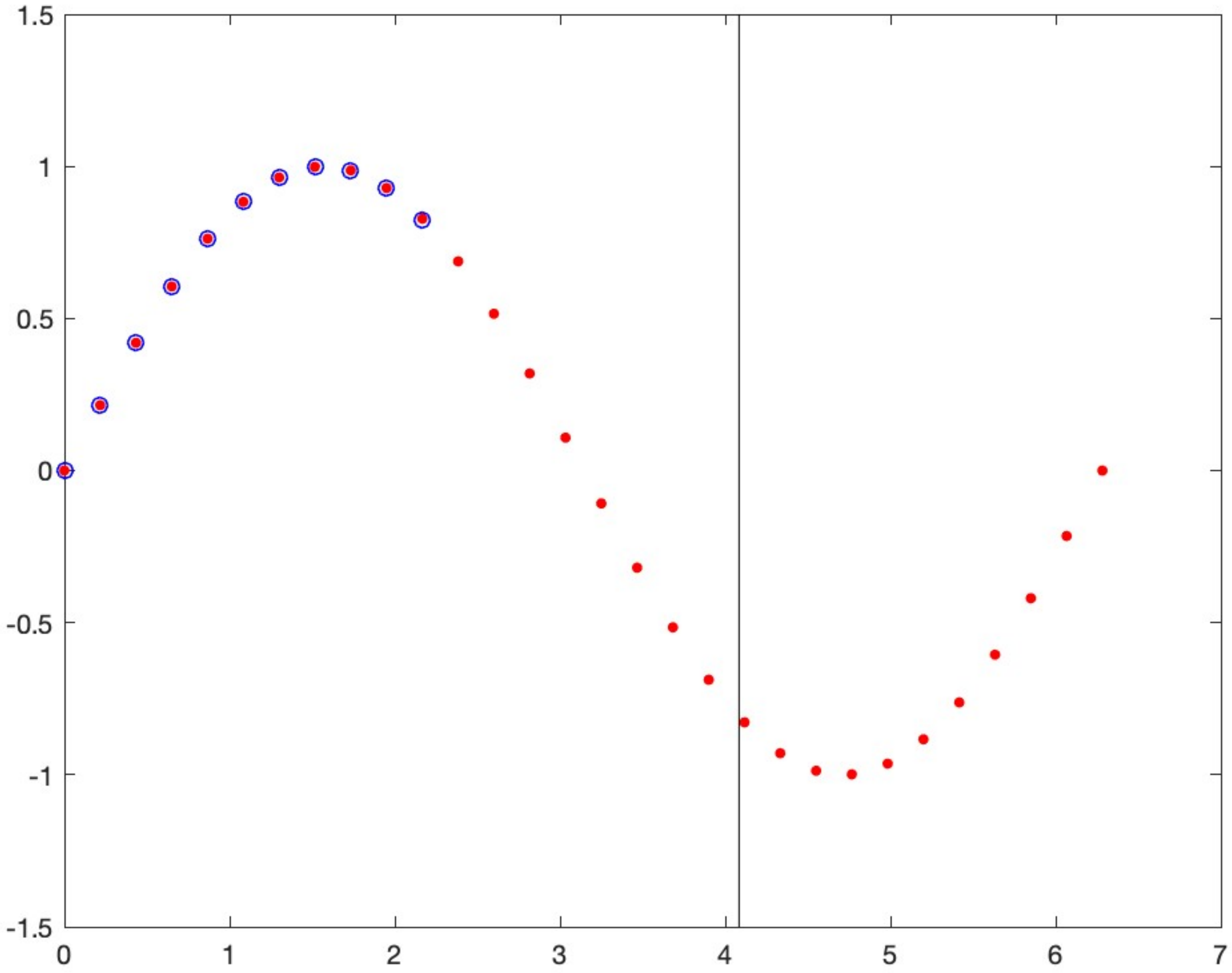

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has *nothing to do with the sin function evaluated at the expected (quadrature) points*

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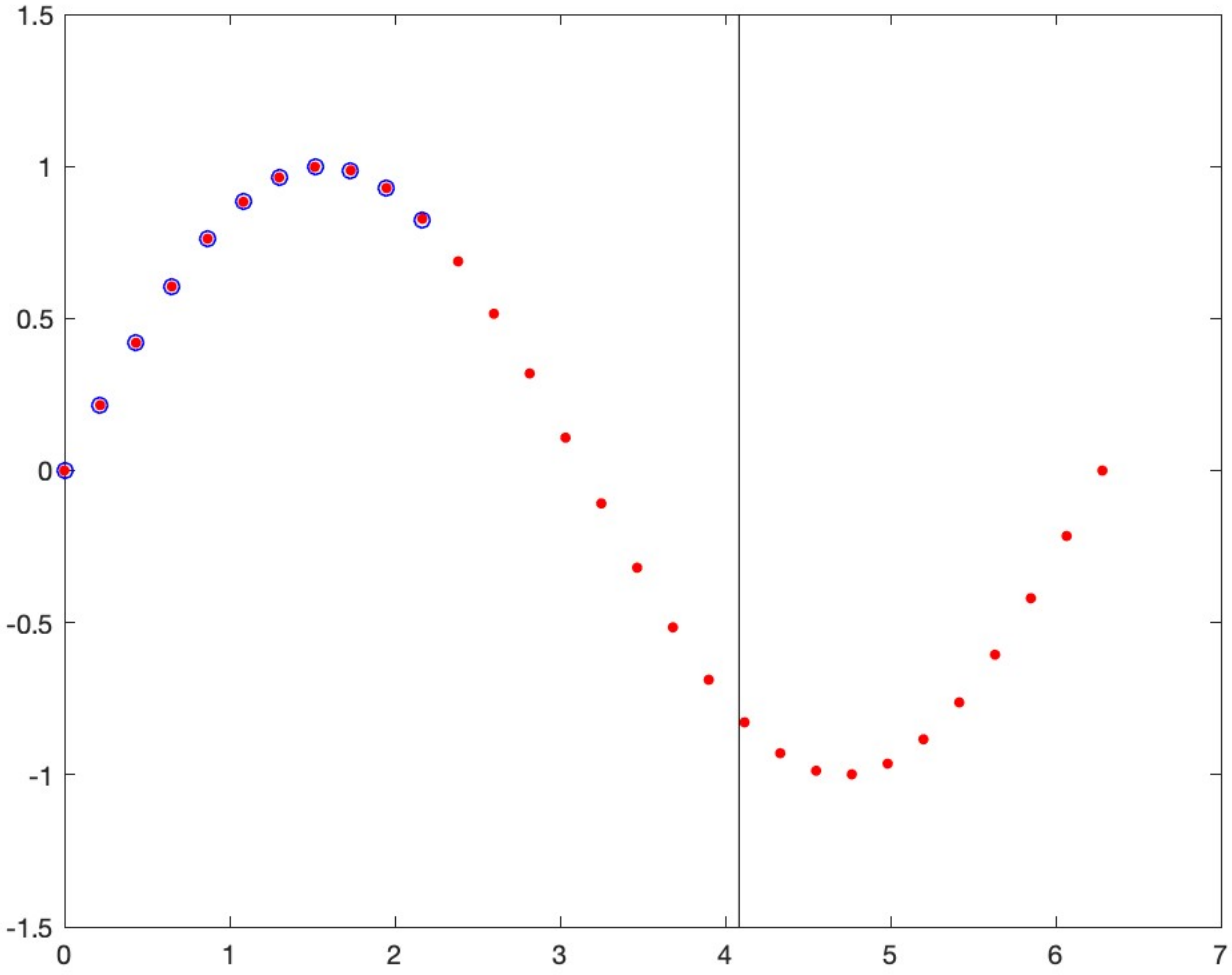

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Nevertheless, you get information out of this machinery,
can this be thought of as an effective formula,
as if you had found a quadrature formula of your own?

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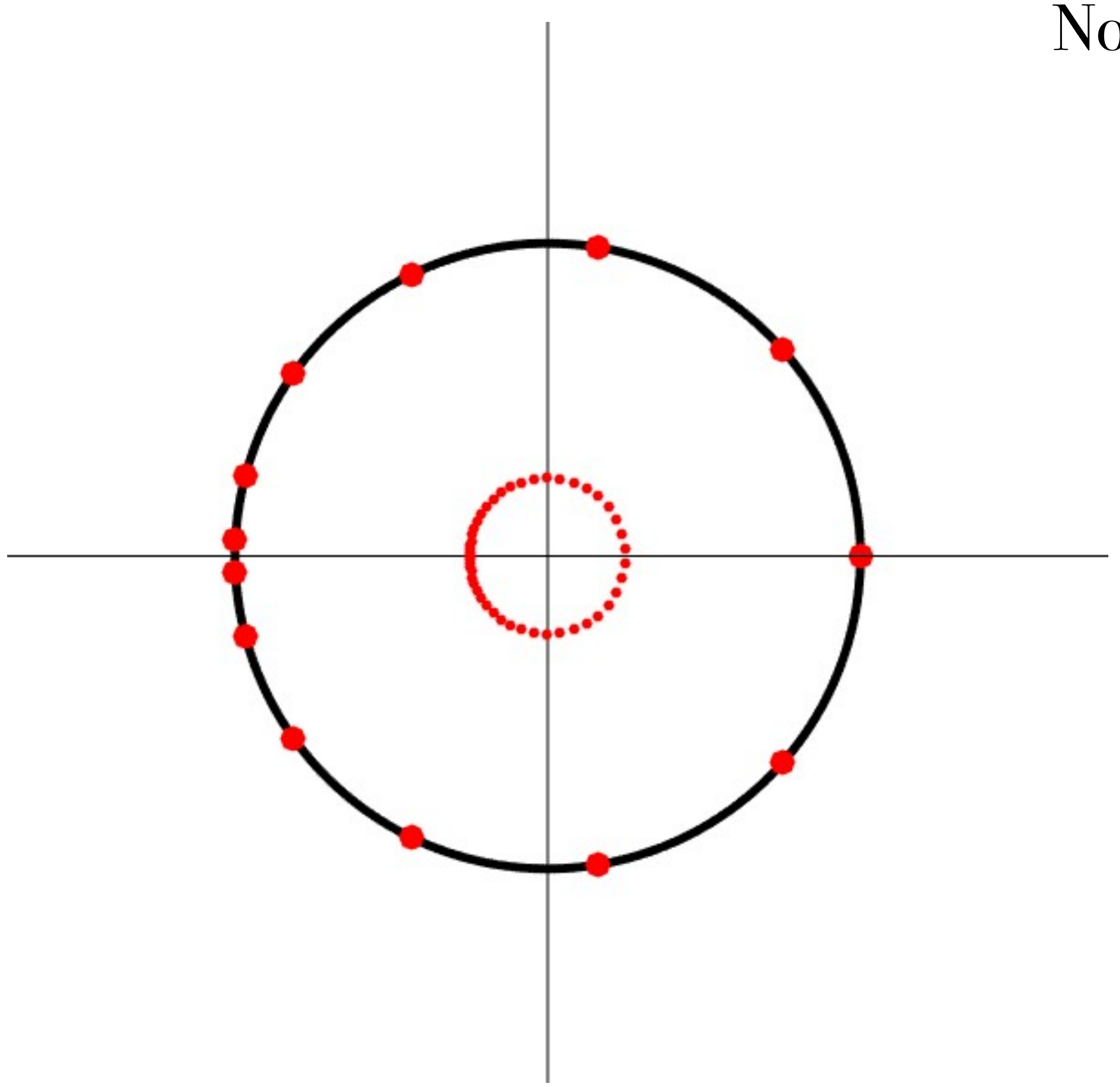
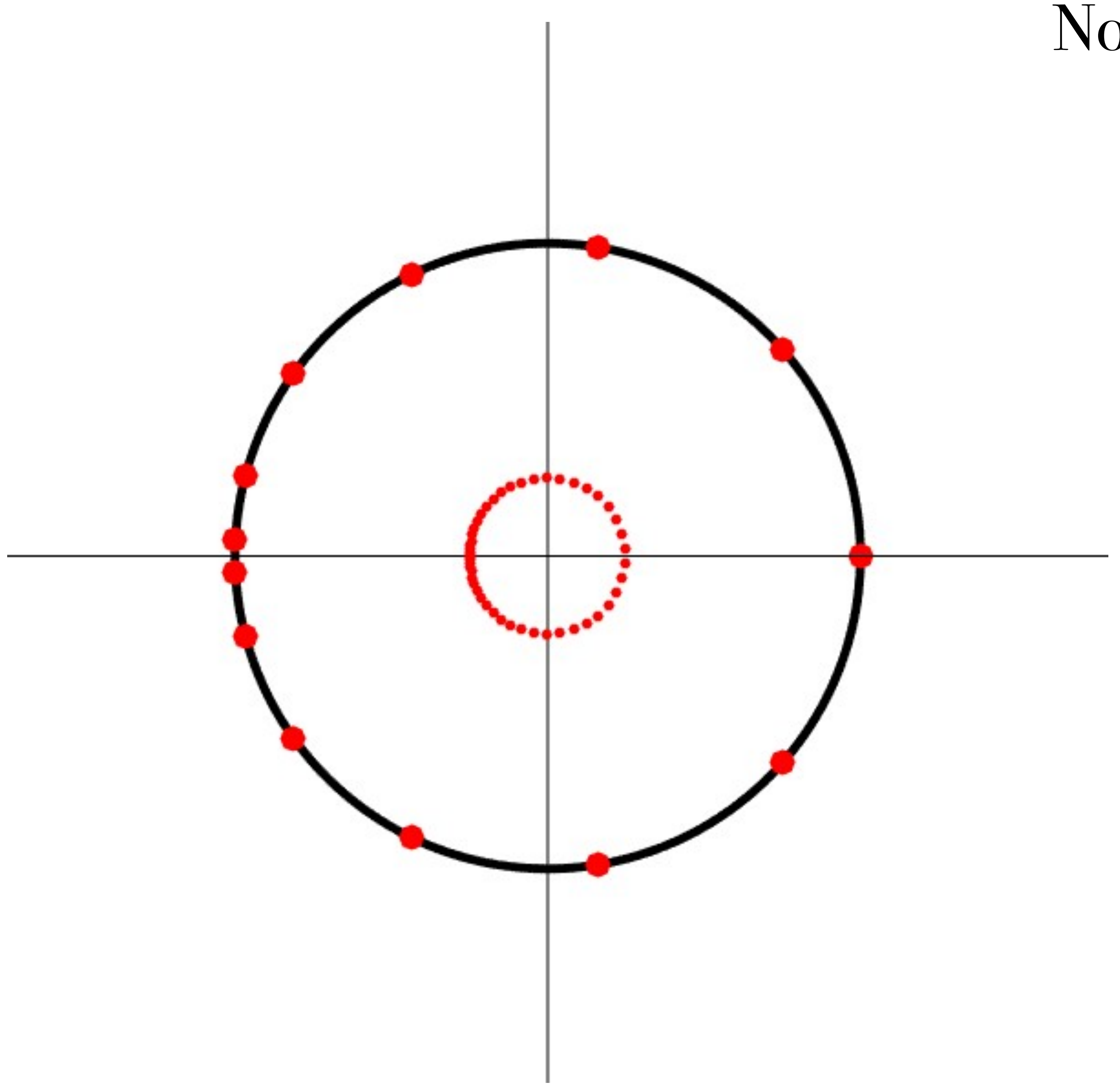


Now, forget about the inverse problem, and remember Cauchy formula for derivatives

$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_C \frac{f(z)}{(z-z_0)^{n+1}}\, dz = \frac{n!}{2\pi i} \int_0^{2\pi} \frac{f(R\,\exp(i\theta))\; R\,\exp(i\theta)}{(R\,\exp i\theta - z_0)^{n+1}}\, d\theta$$



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$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}}\, dz = \frac{n!}{2\pi i} \int_0^{2\pi} \frac{f(R\,\exp(i\theta))\, R\,\exp(i\theta)}{(R\,\exp i\theta - z_0)^{n+1}}\, d\theta$$

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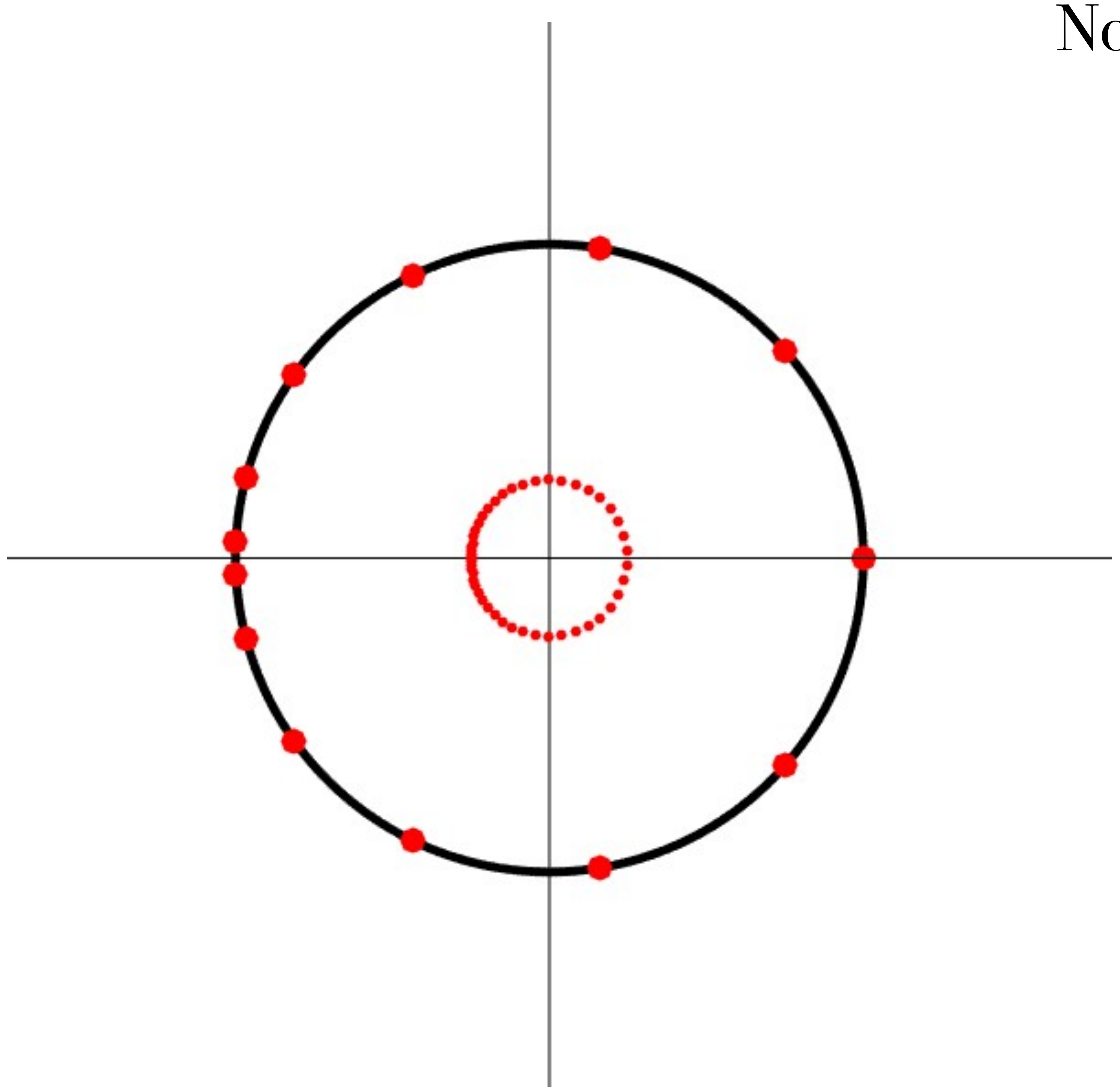

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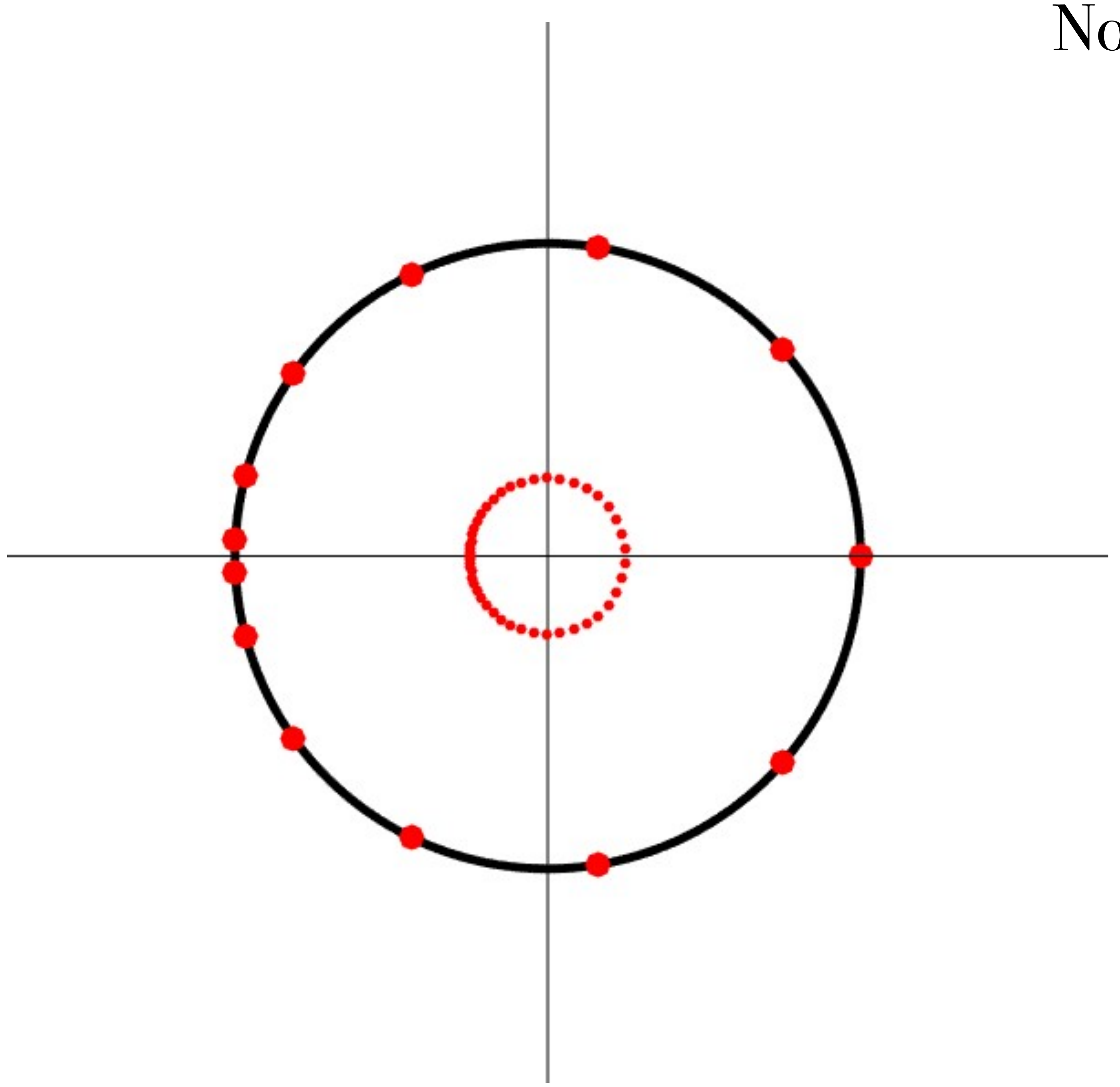

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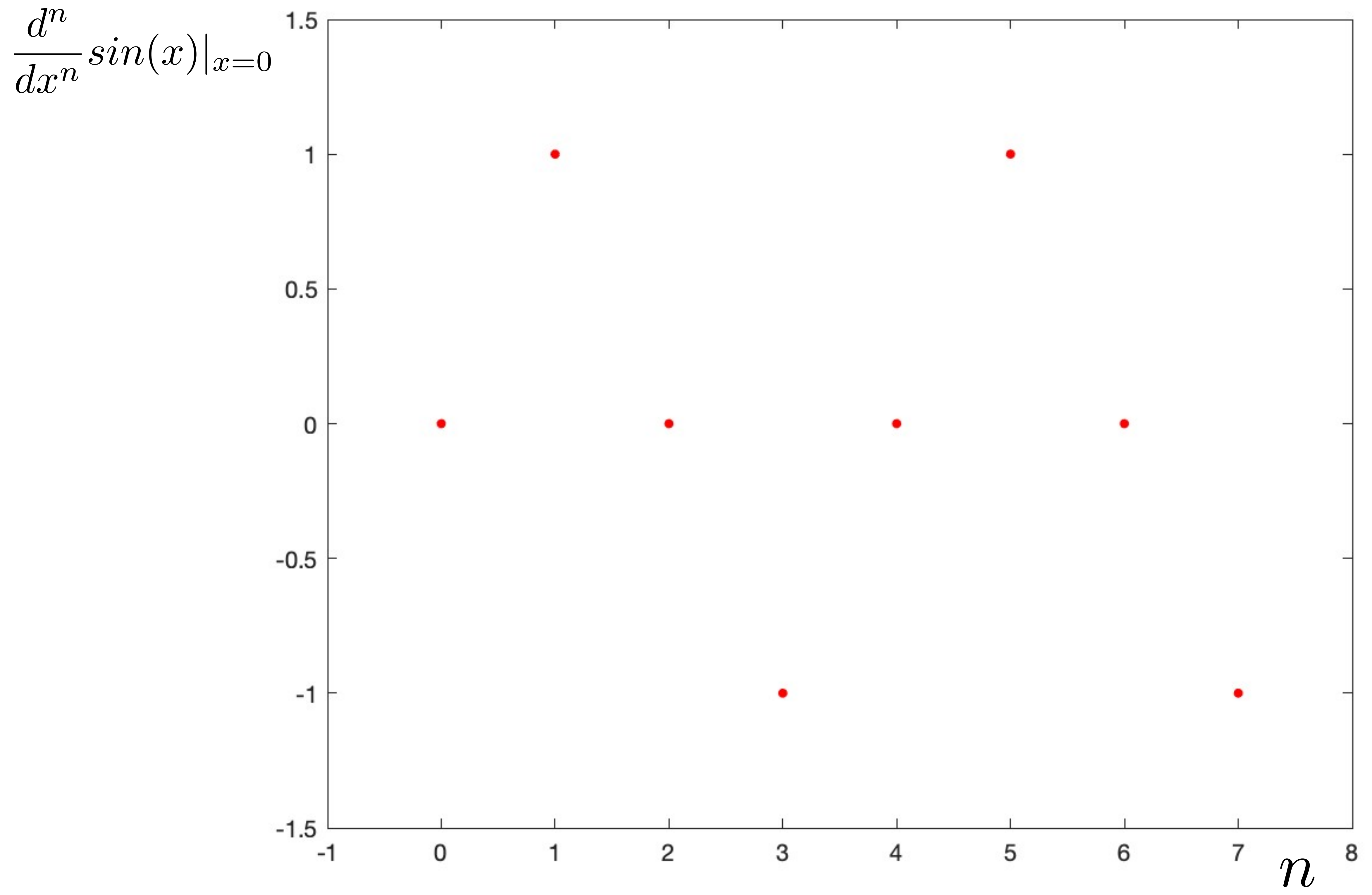

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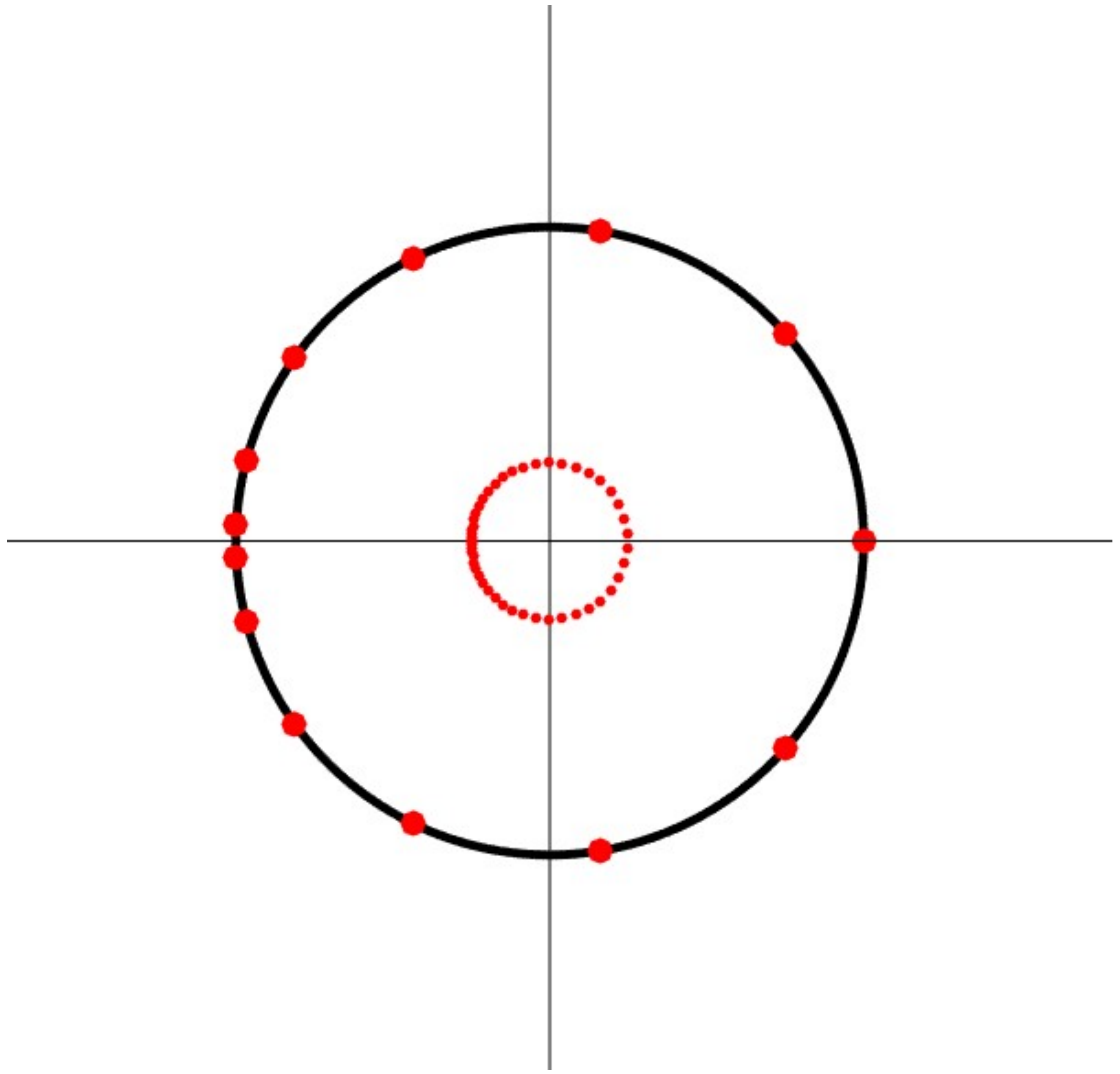
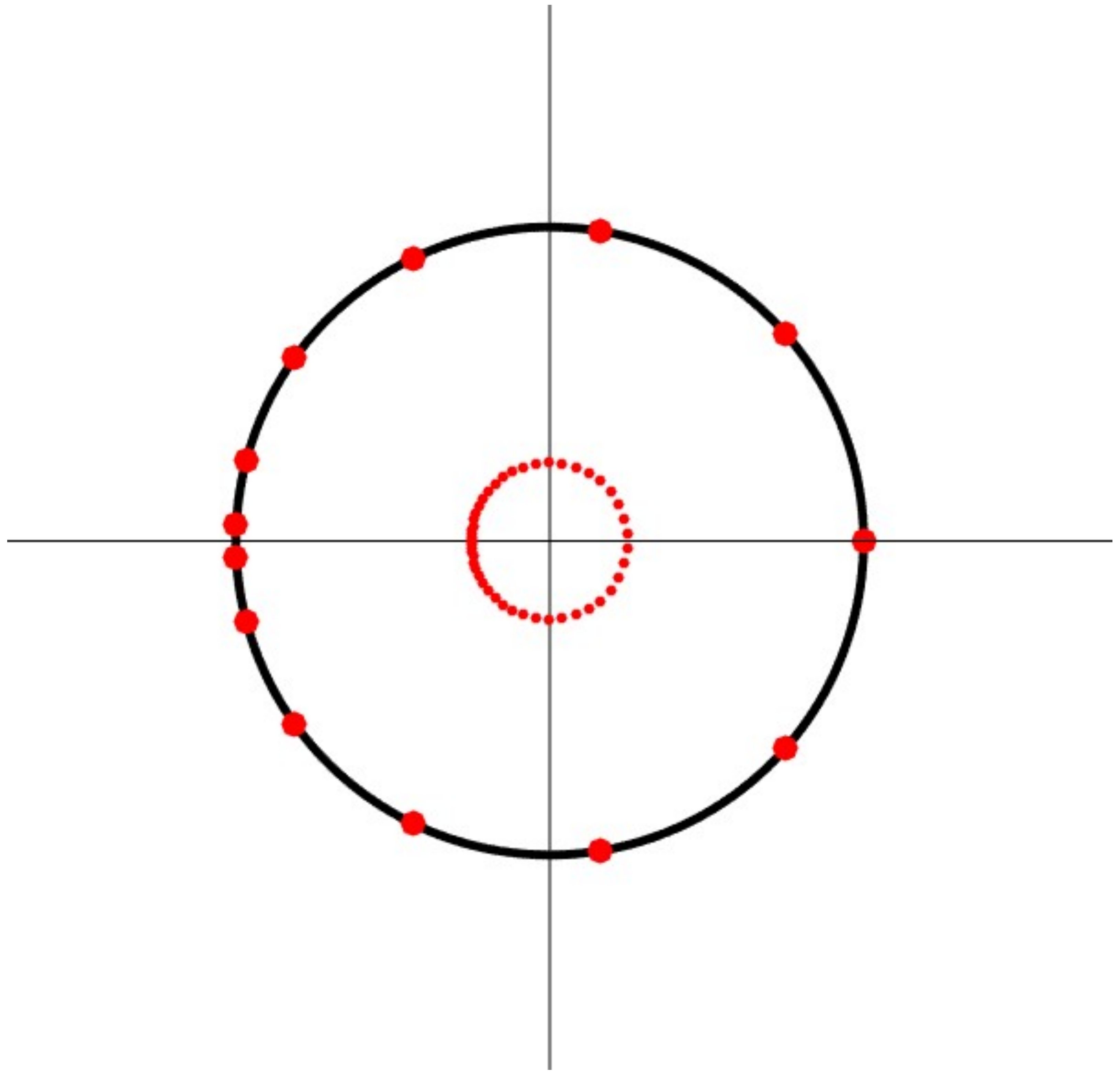


Now, I do something different: I use our inverse problem solution (our *effective quadrature formula*, as we called it) to evaluate our function at the quadrature points on the smaller contour.

Does it work?



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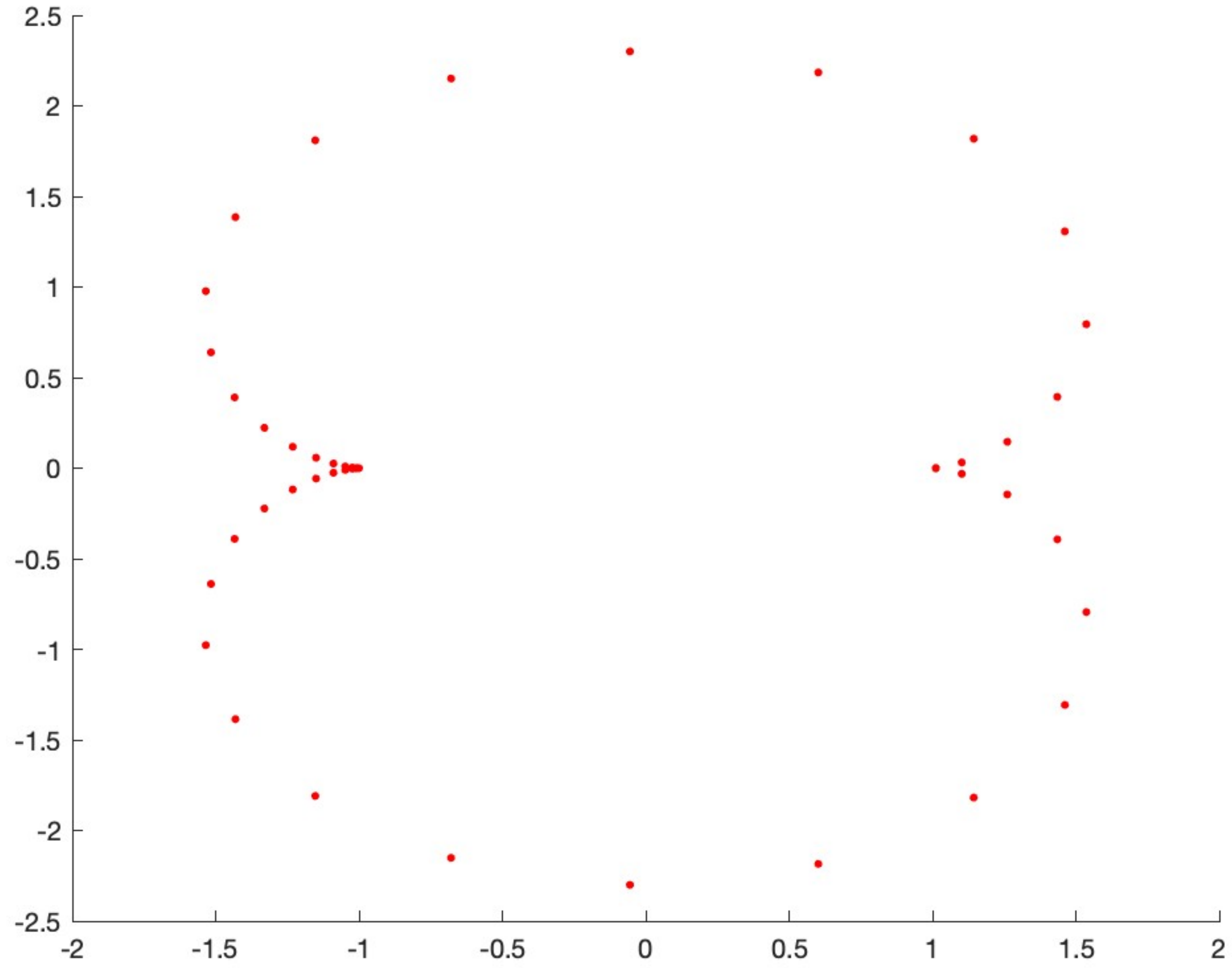
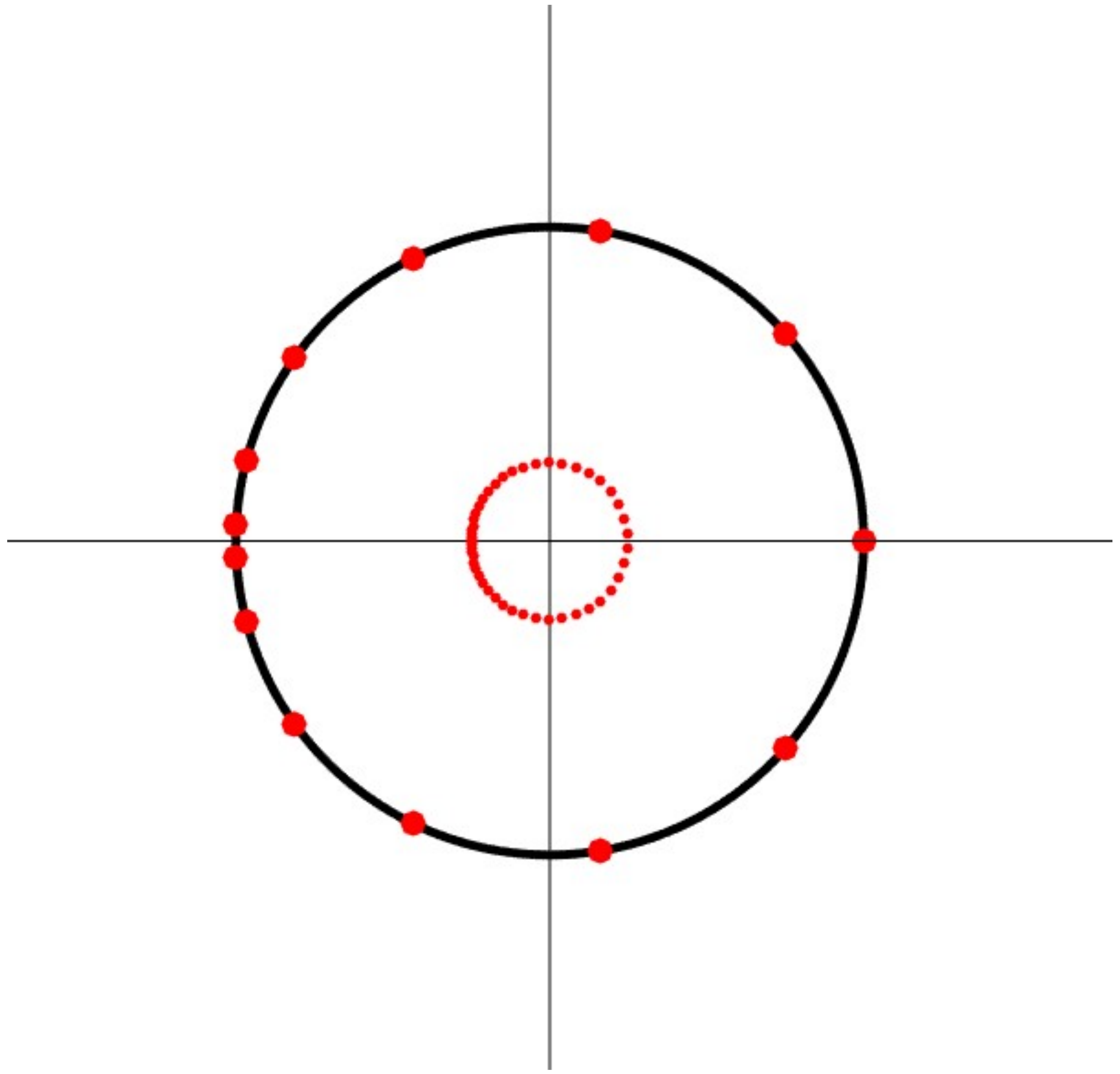
Let me plot (on the complex plane) the values I have to get





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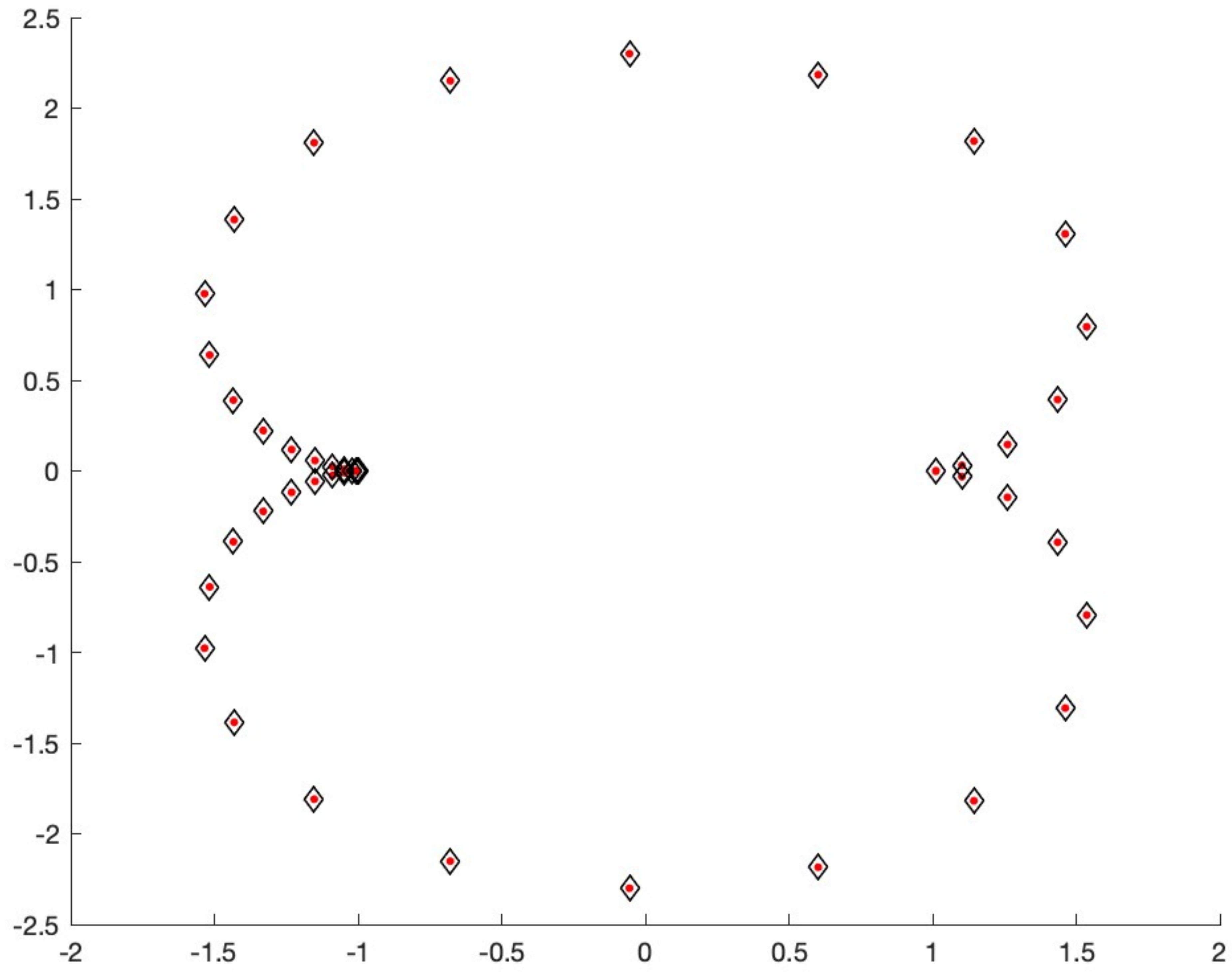
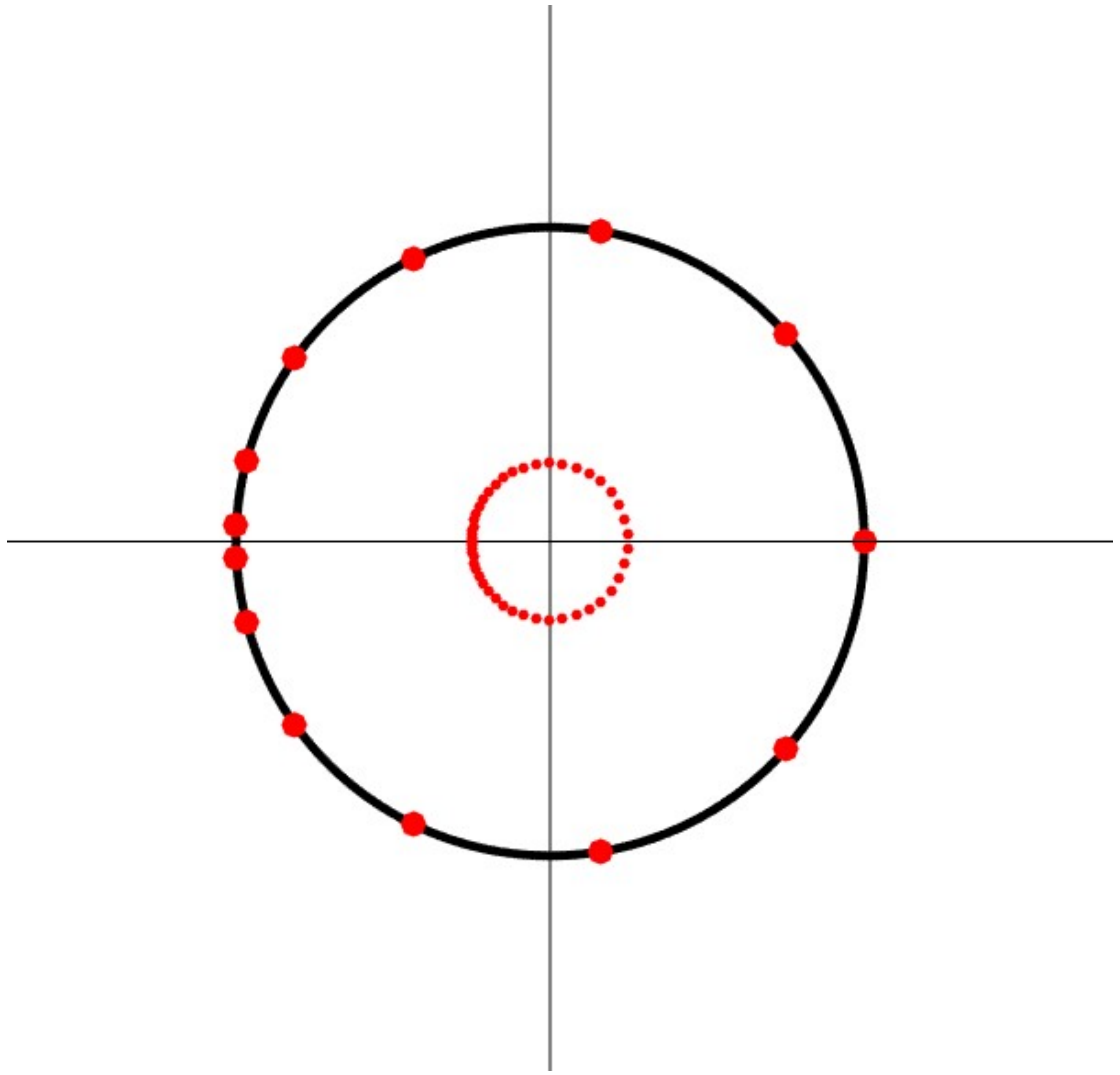
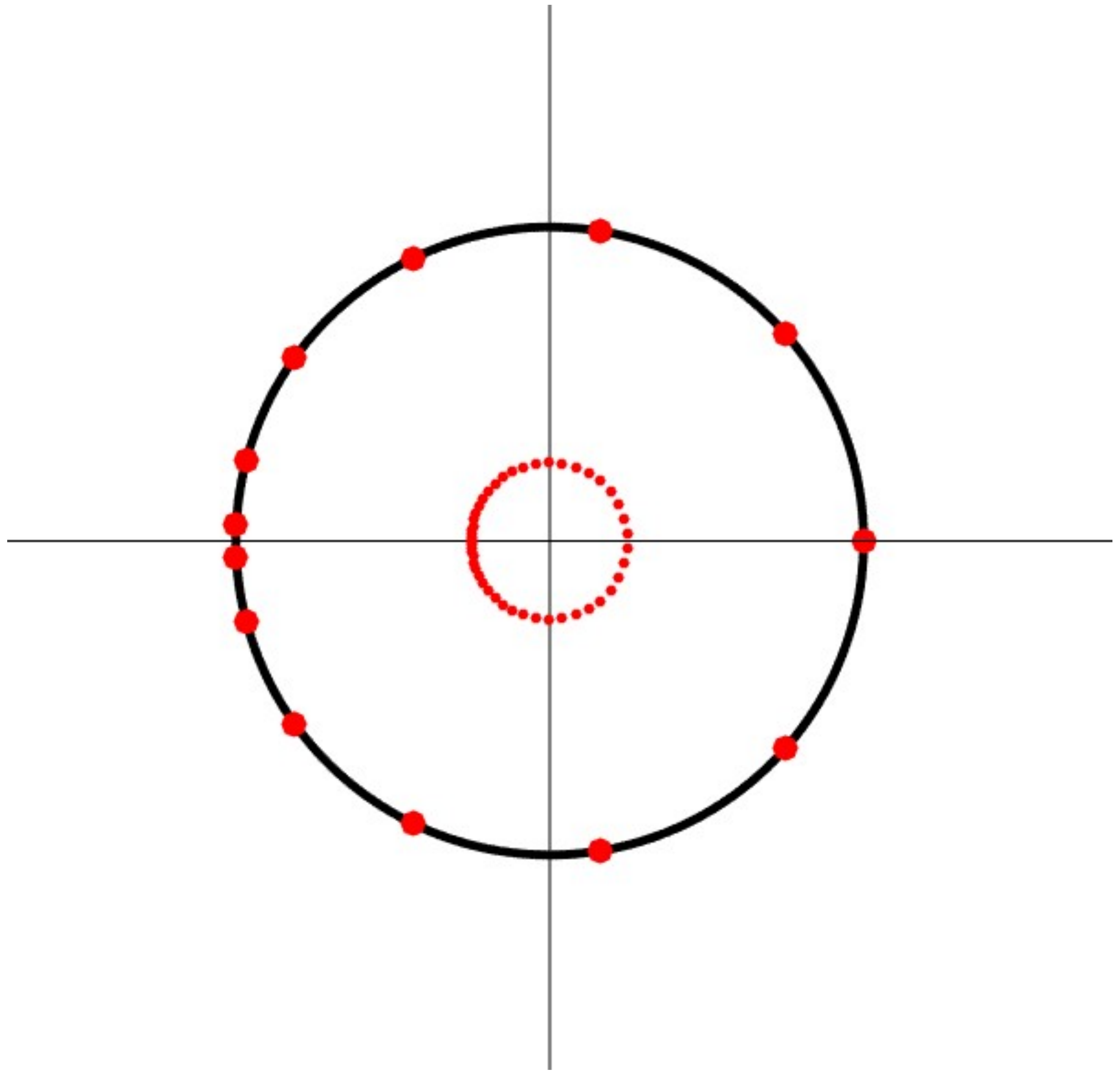
... and this is what I get!





Next task is the obvious one: I expect that if I put the points I generated via our effective quadrature into the quadrature formula for derivatives in zero, I will get the correct results

It must work …



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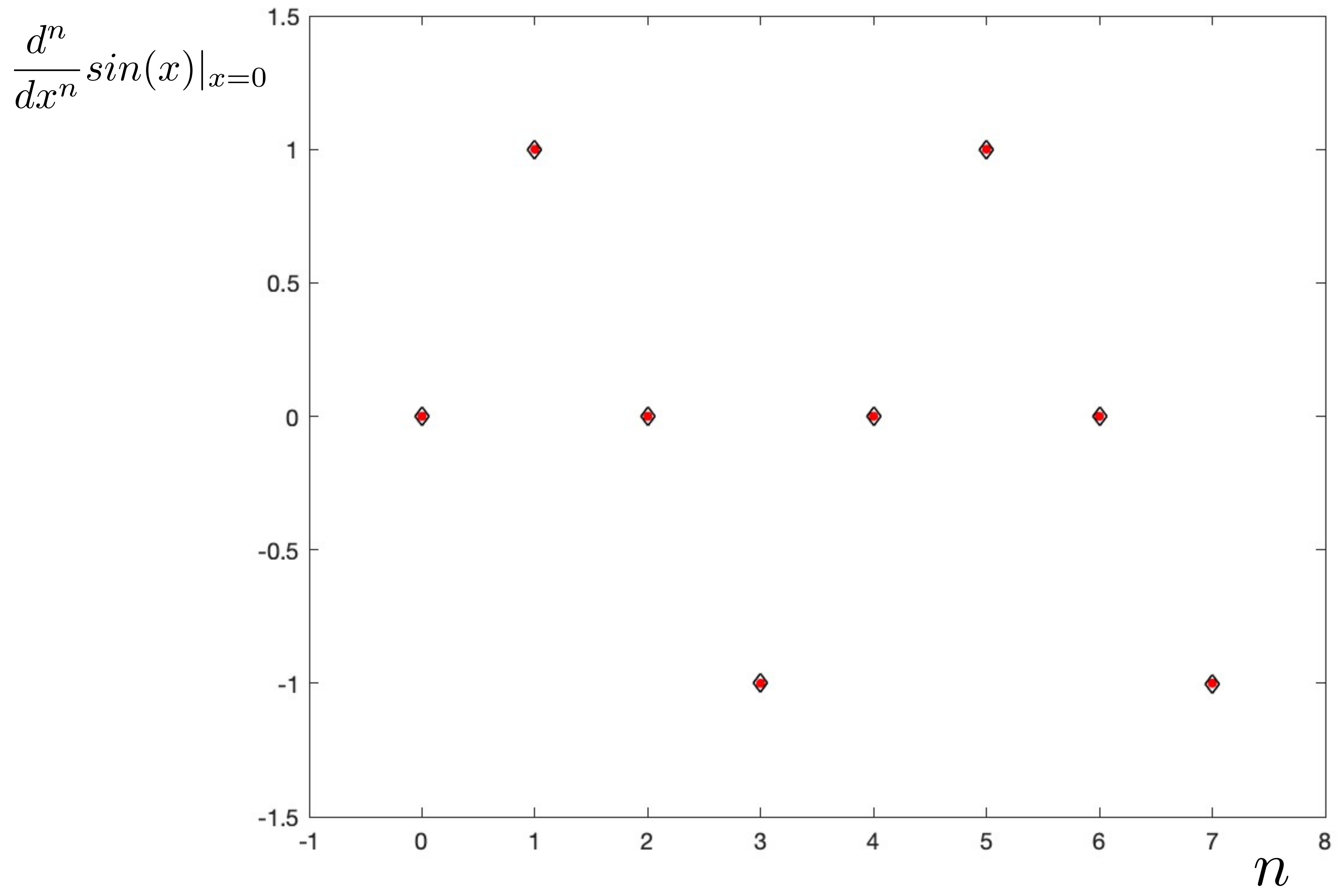

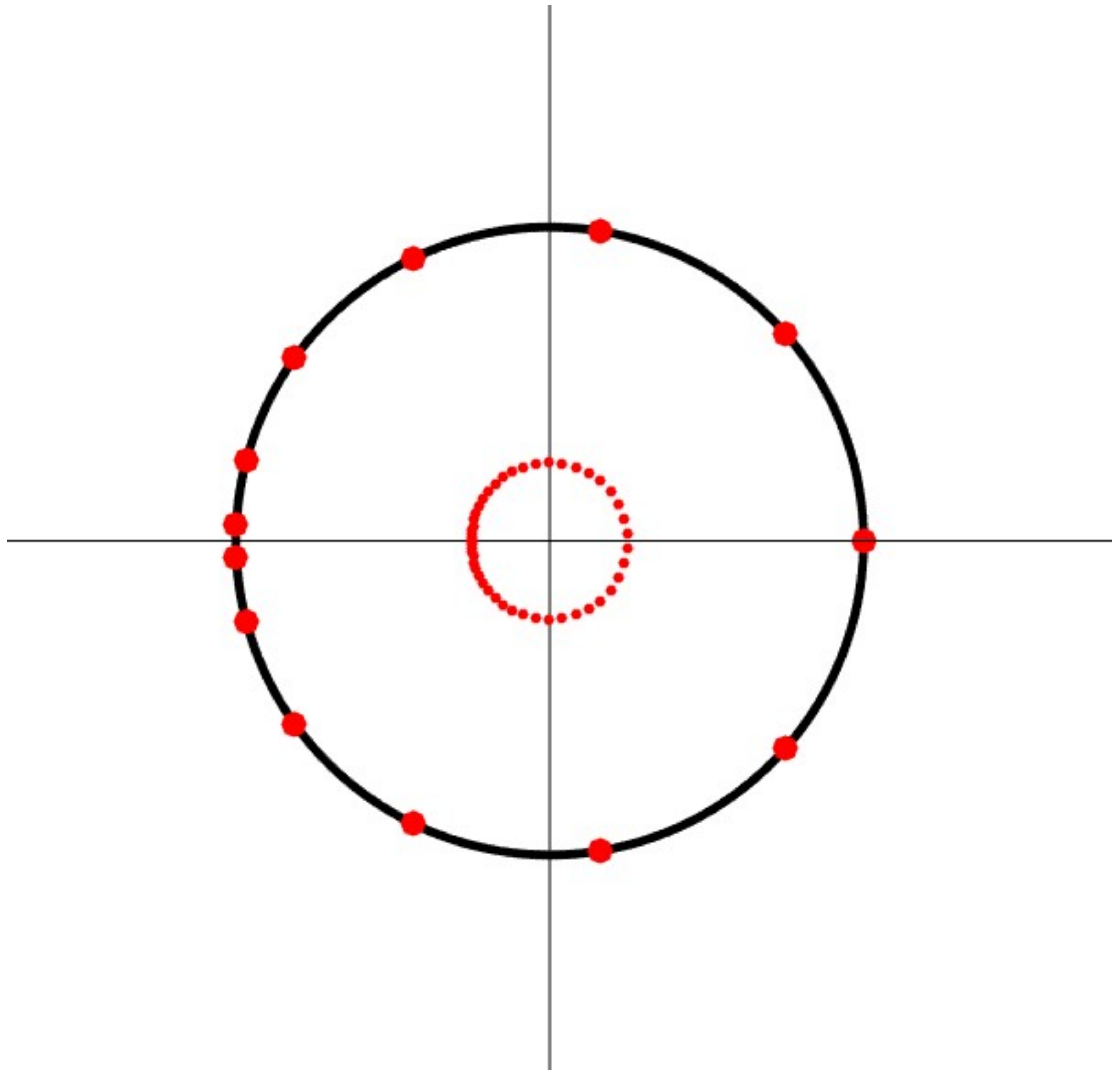

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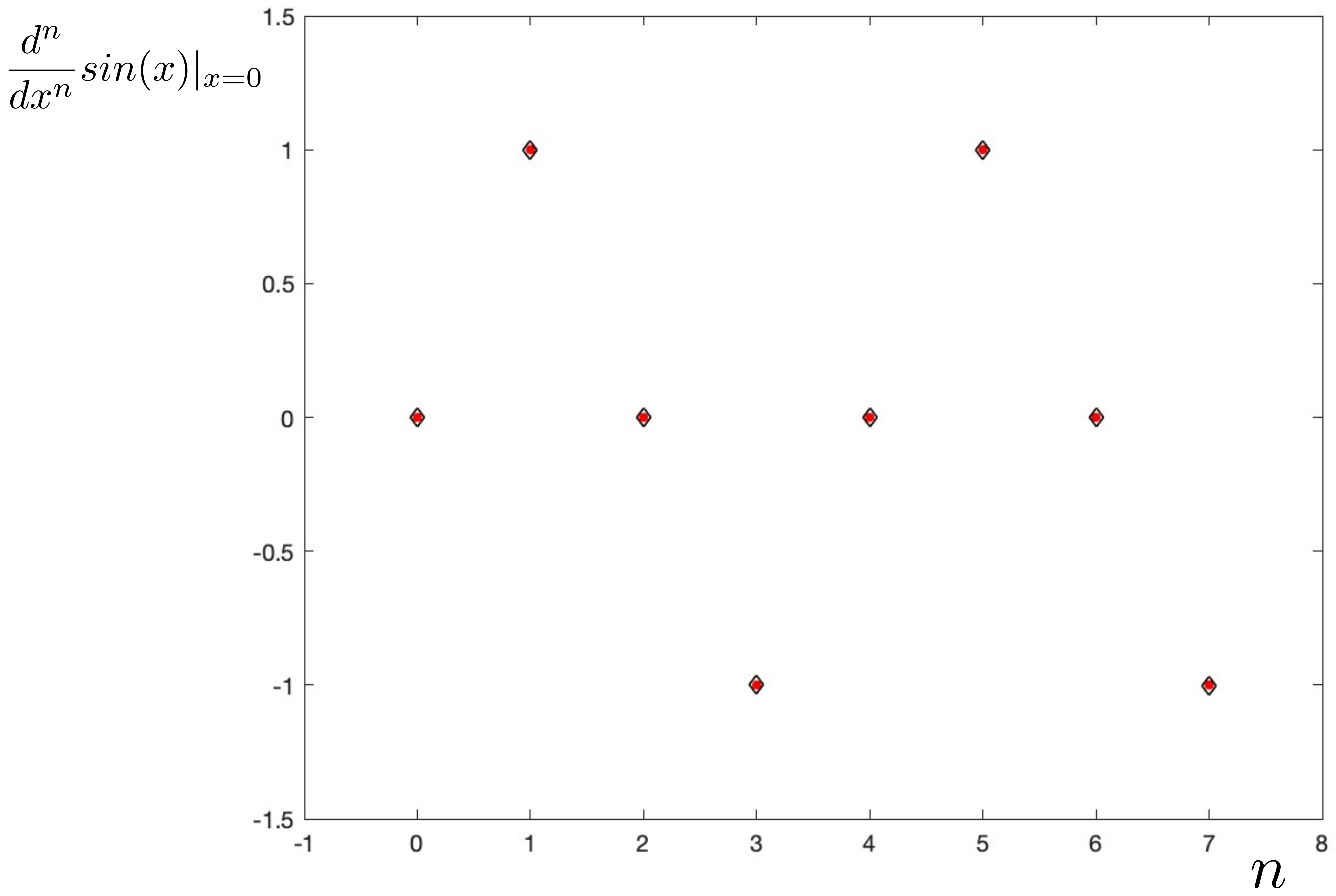

…but here comes the point! This is exactly the same result I get if I directly use our original effective quadrature! … so, everything is consistent!

… OK! … but then … WHAT ABOUT QCD?

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...we can compare **TAYLOR COEFFICIENTS AT ZERO**
with what we get from their “DIRECT” ESTIMATION!
(*see previous talk by M. Aliberti*)

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```
ans =

    0.1100
    0.0898
    0.0179
```

$\chi_2\ ,\ \chi_4\ ,\ \chi_6$

```
ans =

  -0.0000 + 0.0000i
   0.1100 - 0.0000i
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… changing the amount of information…

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ans =

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$\chi_2\,,\,\chi_4\,,\,\chi_6\,,\,\chi_8$

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  -0.0000 + 0.0000i
  -1.0574 + 0.0000i
```

They are exactly the SAME!

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… so WE DID NOT LEARN ANYTHING NEW with this funny inverse problem … NOT TRUE!

SOMETHING ELSE you can do with the inverse problem machinery:
we can play the same game for inverse Laplace transform …

$$f(s) = \int_0^\infty e^{-ts}\, F(t)\, dt \qquad\qquad f(s) = \int_0^\infty e^{-t}\, e^{-t(s-1)}\, F(t)\, dt$$

$$f(s) = \int_0^\infty e^{-t}\, e^{-t(s-1)}\, F(t)\, dt \ \sim \sum_j w_j\, e^{-t_j(s-1)}\, F(t_j)$$

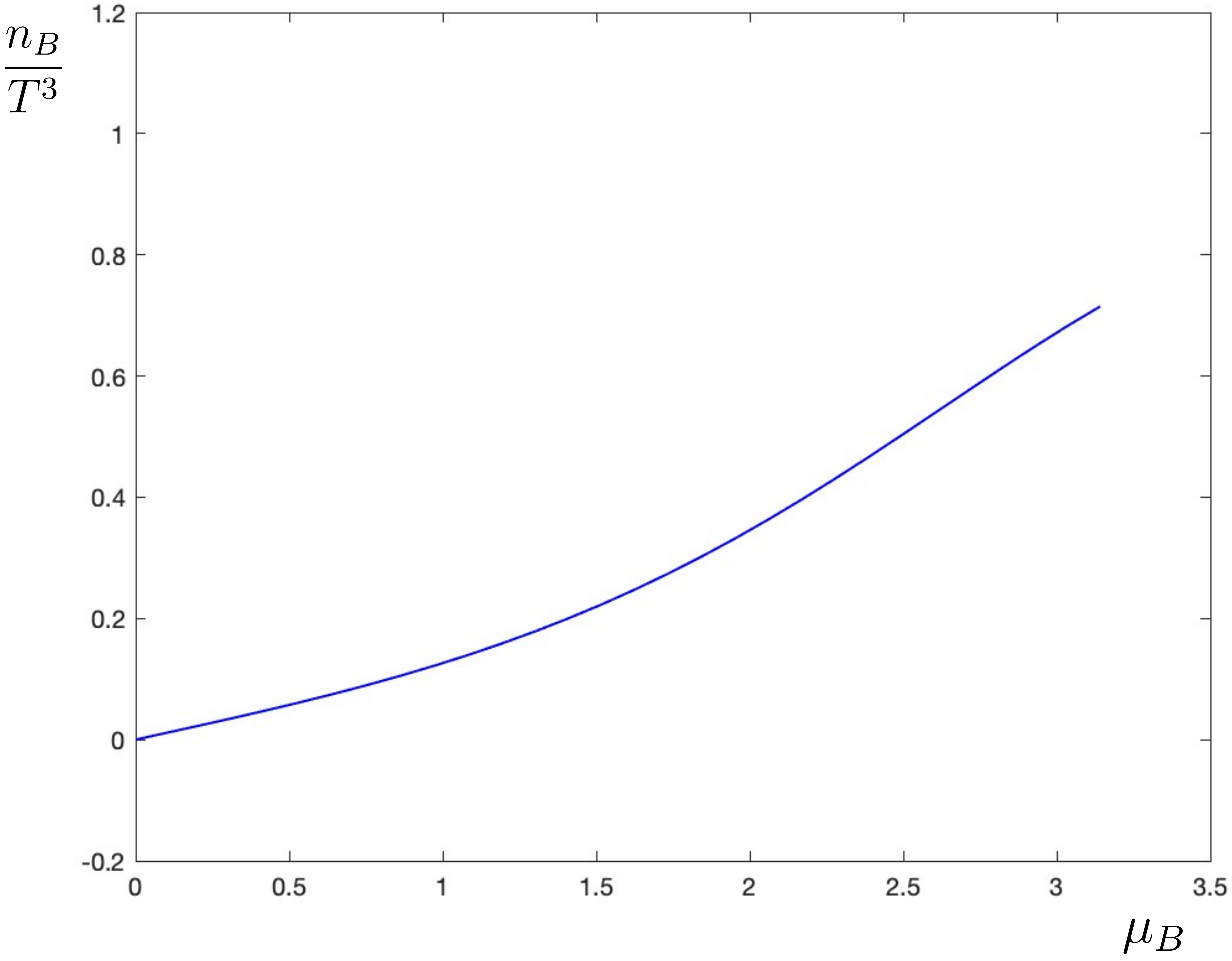
This time, Laguerre quadratures …

For a few test functions, we could play effectively with some tricks and reconstruct the inverse Laplace transform …

In the end … Any **conclusion** about
analytic continuation in finite density QCD?

We wanted to **compare methods**
and possibly **cross check** results

$T = 157.5 \ (\sim 155) \ \text{MeV}$



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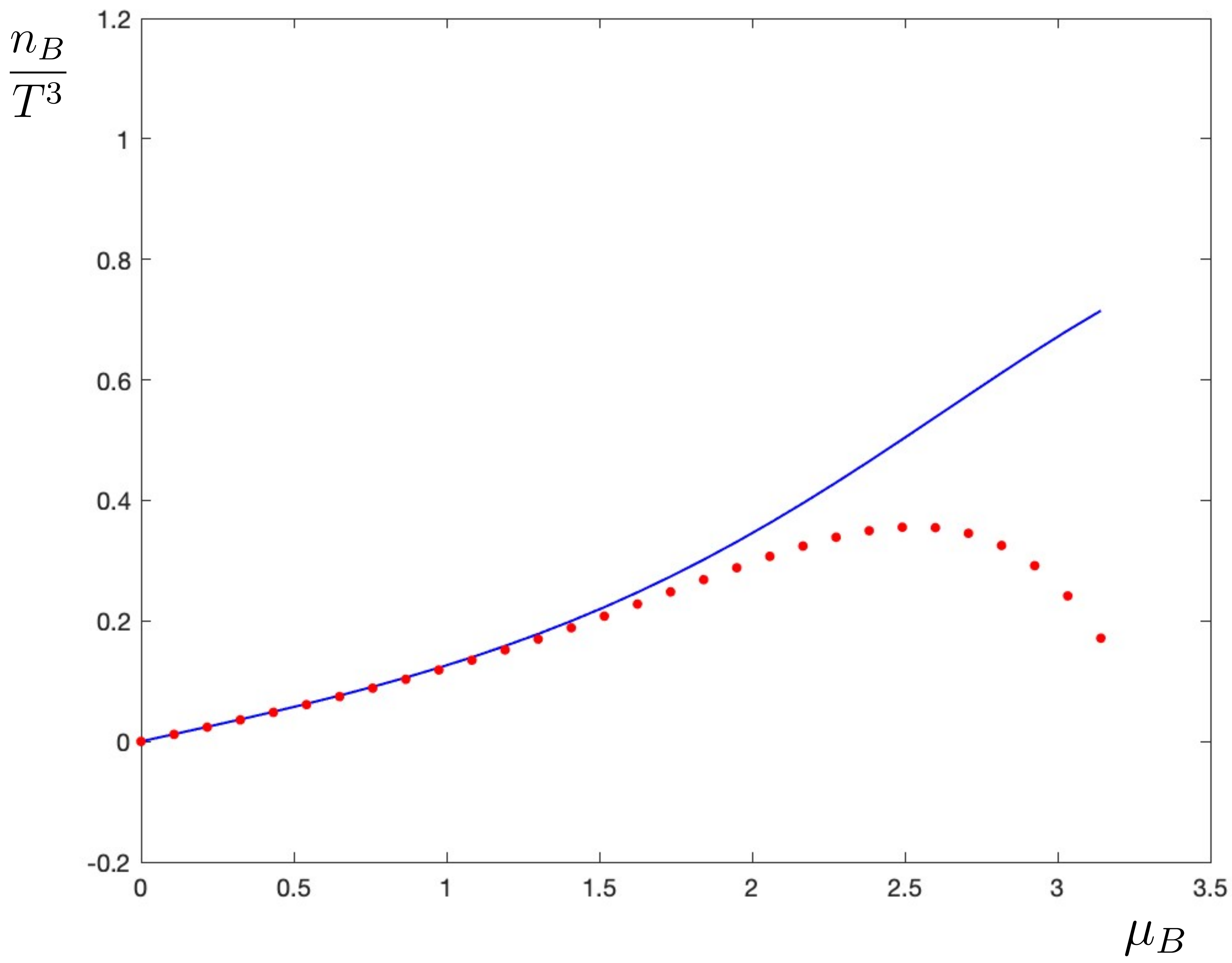
We saw we can go via Padé analytic continuation.

CAVEAT: FIXED CUTOFF! $N_\tau = 6$

$T = 157.5\ (\sim 155)$ MeV



In the end … Any **conclusion** about analytic continuation in finite density QCD?

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We could compare with HotQCD results.

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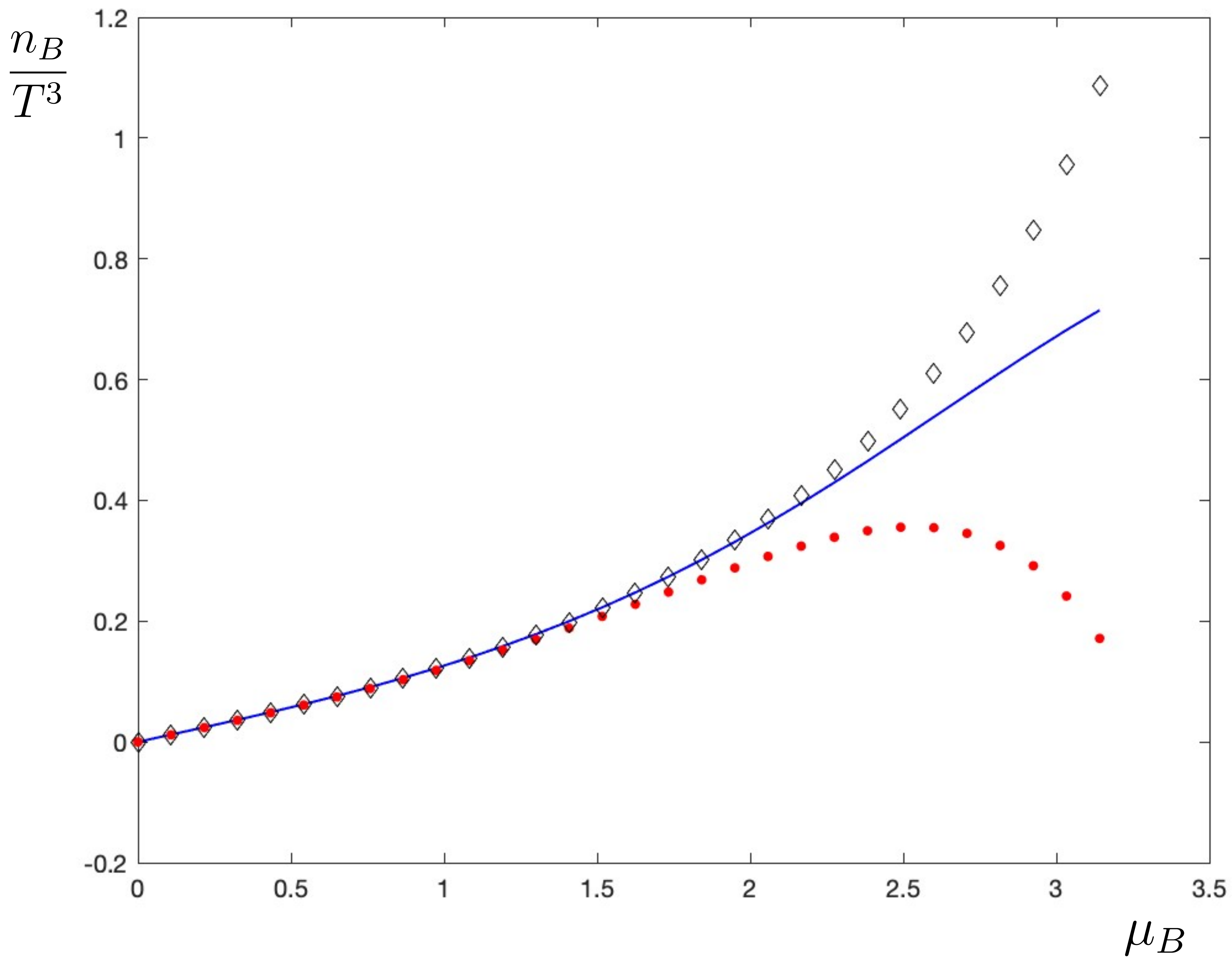

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We saw we can go via Cauchy formula (inverse problem).

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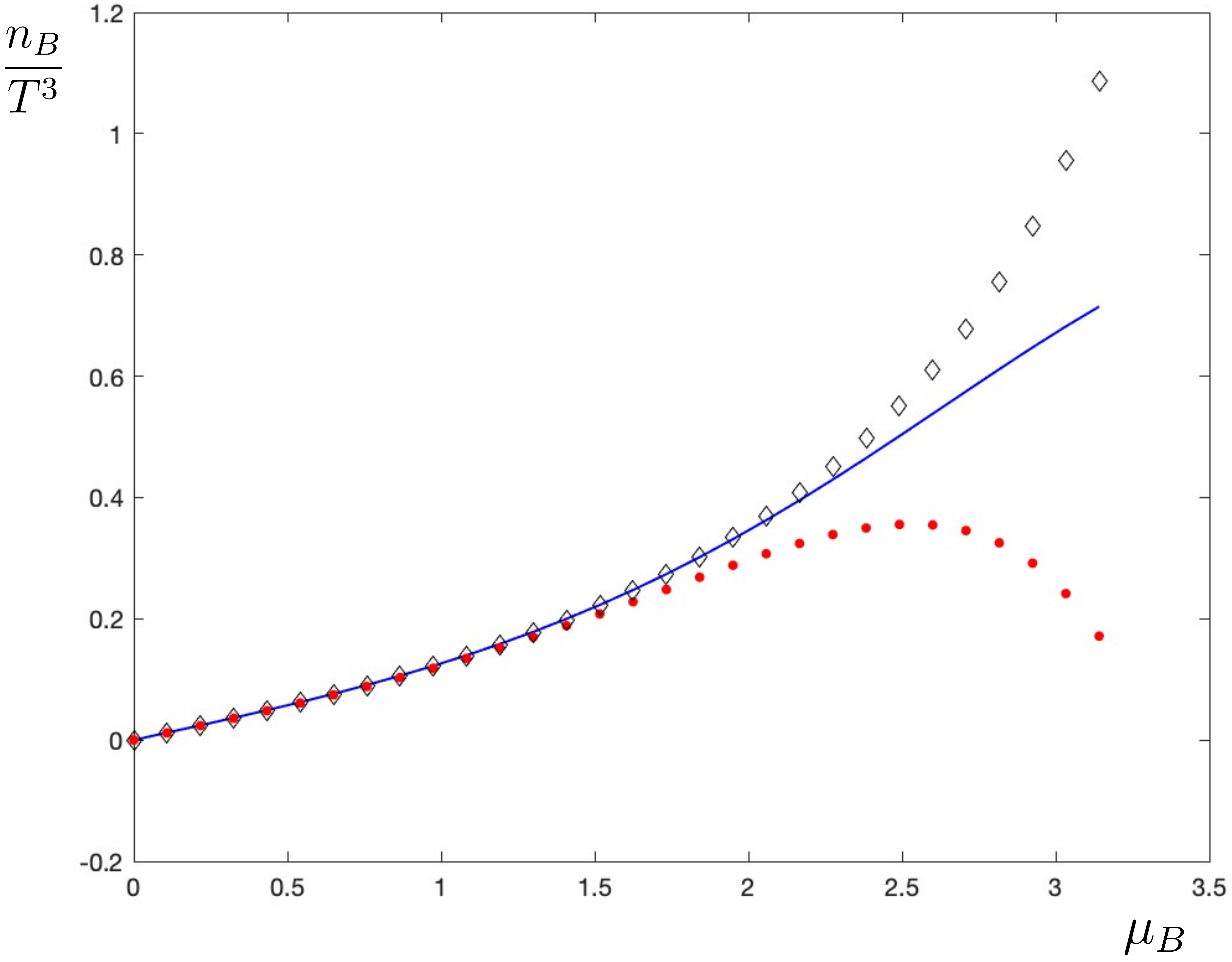

In the end … Any **conclusion** about analytic continuation in finite density QCD?

We saw we can go via Cauchy formula (inverse problem).

And remember: other applications possible …

$$f(s) = \int_0^\infty e^{-t}\, e^{-t(s-1)}\, F(t)\, dt \;\; = \int_0^\infty e^{-t}\, e^{-t(s-1)}\, F(t)\, dt \sim \sum_j w_j\, e^{-t_j(s-1)}\, F(t_j)$$

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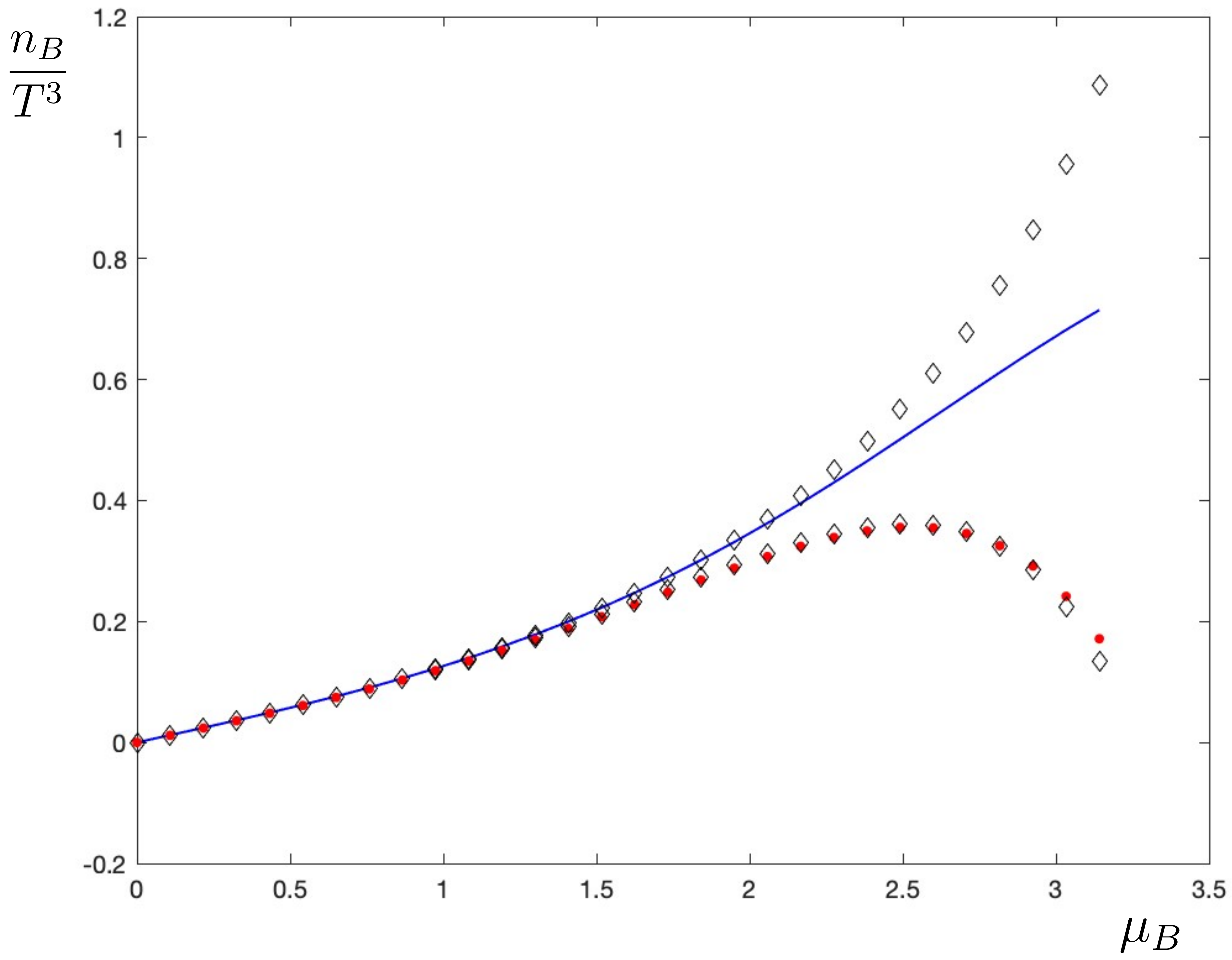

In the end ... Any **conclusion** about analytic continuation in finite density QCD?

In general, beyond a given value of the chemical potential, quite a sensitivity to the input (imaginary) region!

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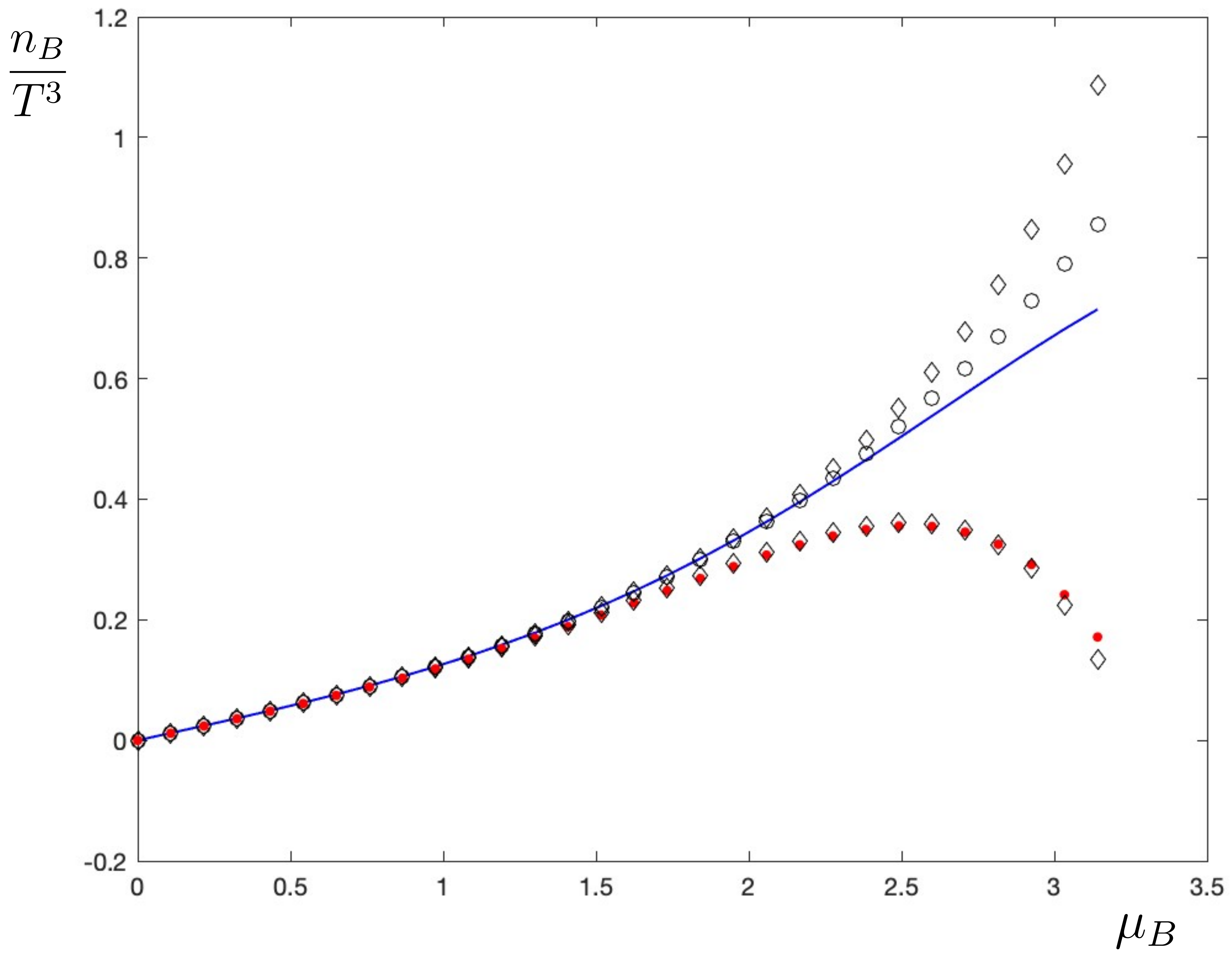

In the end … Any **conclusion** about analytic continuation in finite density QCD?

We saw the inverse problem (Cauchy formula) provides the same results as summation of the Taylor series (Taylor coefficients got with the same amount of information)

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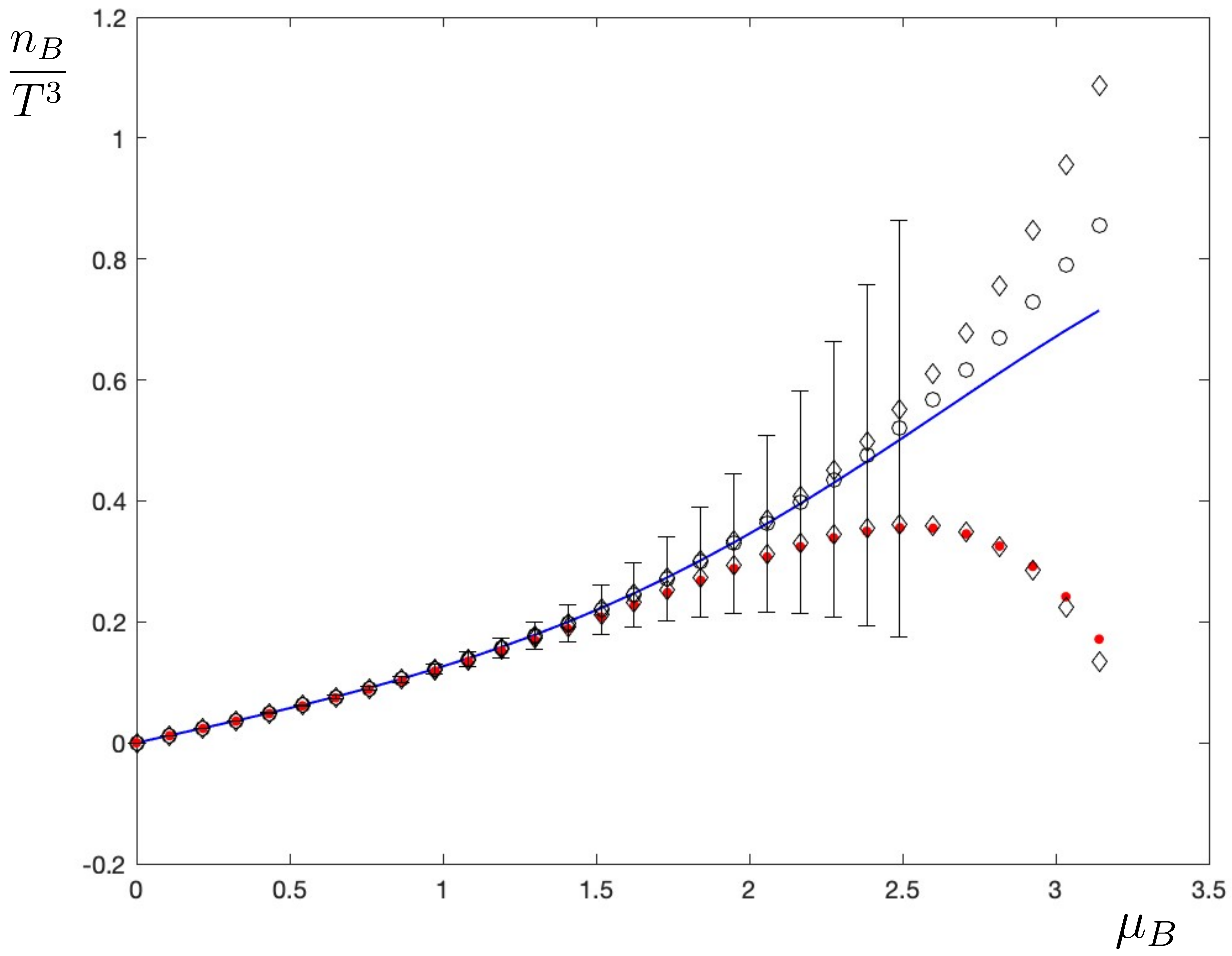

All in all: still a lot of work to understand systematics of different analytic continuation methods working on the same data.

There is a region in which every method provides the same answer.

CAVEAT: FIXED CUTOFF! $N_\tau = 6$