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

Francesco Di Renzo (University of Parma and INFN)

EMMI - Aspects of criticality 2

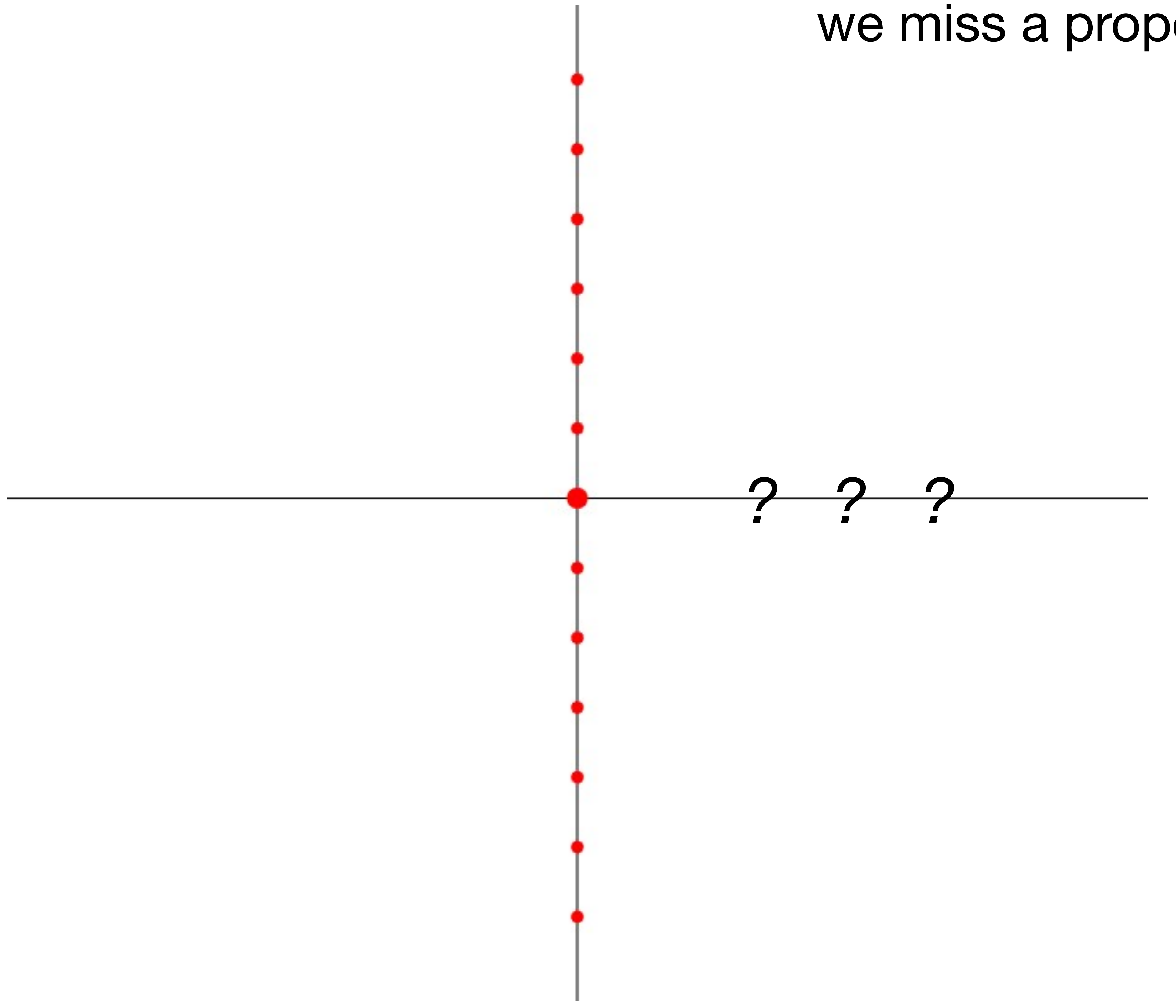
Wroclaw, 03/07/2024

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

(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** …

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

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

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

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

$$\ldots$$

$$P_m(z_k)-f(z_k)Q_n(z_k)=f(z_k)$$

$$P'_m(z_k)-f'(z_k)Q_n(z_k)-f(z_k)Q'_n(z_k)=f'(z_k)$$

$$\ldots$$

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 $\nexists\, z_0 \,:\, P_m(z_0) = \tilde{Q}_n(z_0) = 0$

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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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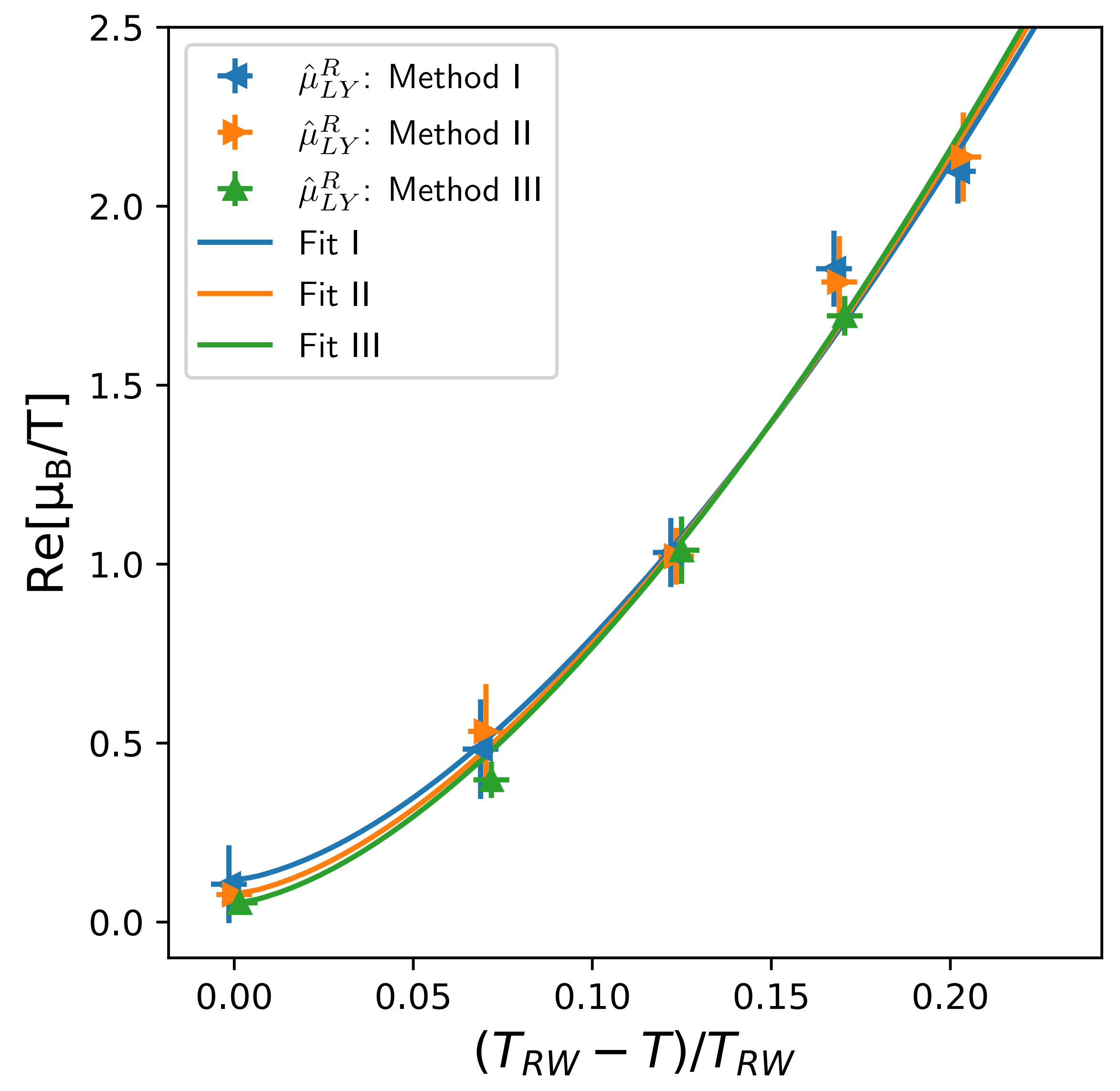

FIG. 9. Scaling fit to the Lee-Yang edge singularities in the vicinity of the Roberge-Weiss transition to the *Ansatz* (22). Shown are three distinct data sets for the real parts of the $\hat{\mu}_B$ (imaginary parts of h) as a function of the reduced temperature $(T_{\rm RW} - T)/T_{\rm RW}$, as obtained from methods I–III.

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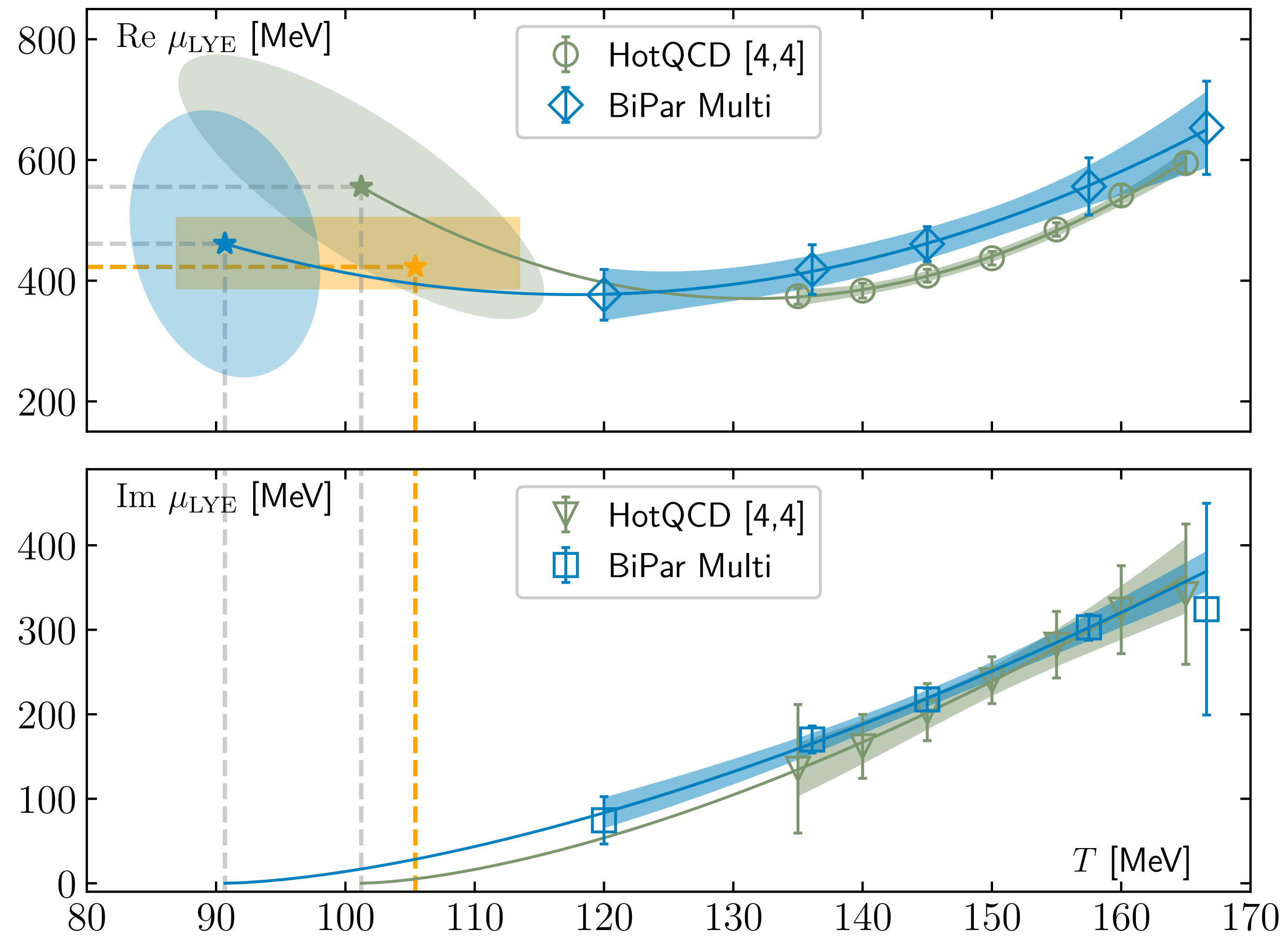

FIG. 4. Scaling fits for the LYE singularities related to the CEP. Green data come from a [4,4] Padé from Ref. [7]. Blue data come from the multi-point Padé. *Top*: Scaling of the real part. *Bottom*: Scaling of the imaginary part. The ellipses shown in the top panel represent the 68% confidence region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

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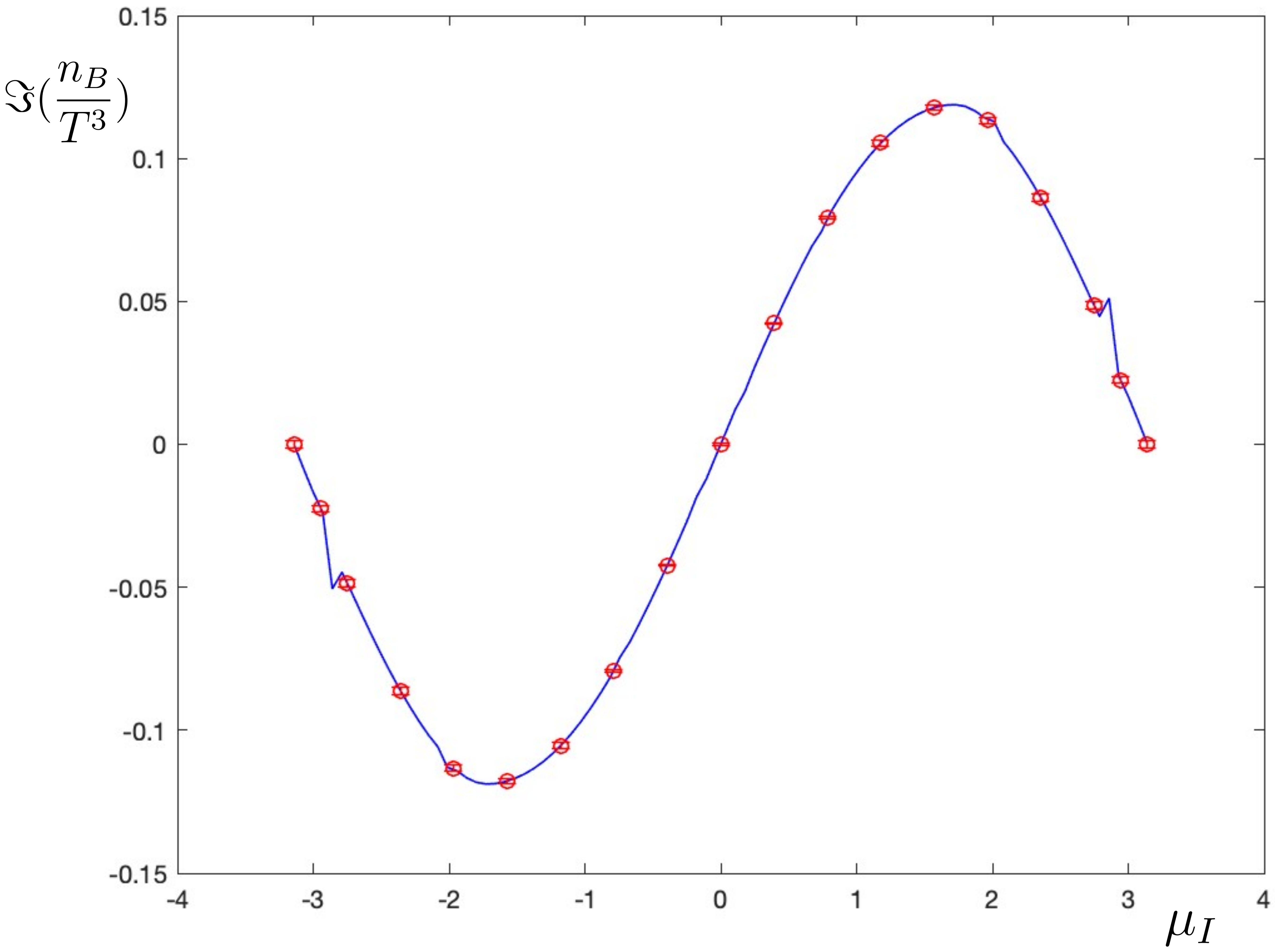
$T = 157.5\ (\sim 155)$ MeV



... 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 (*negligible*...)

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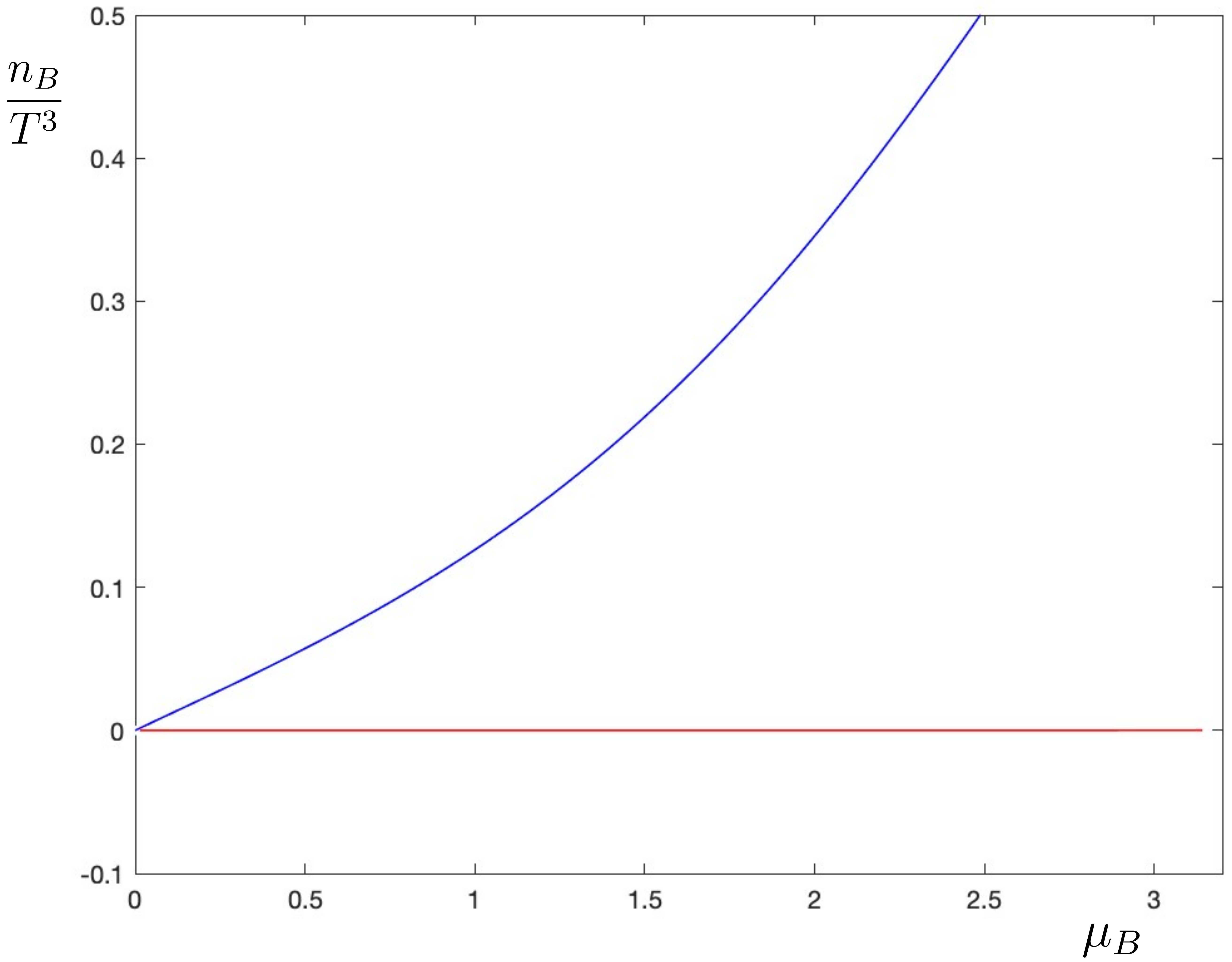

... which is pretty simple (we will be concerned with the number density):

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 ... we know how to compute them, but here we are concerned with *trends*,,, FIXED CUTOFF!

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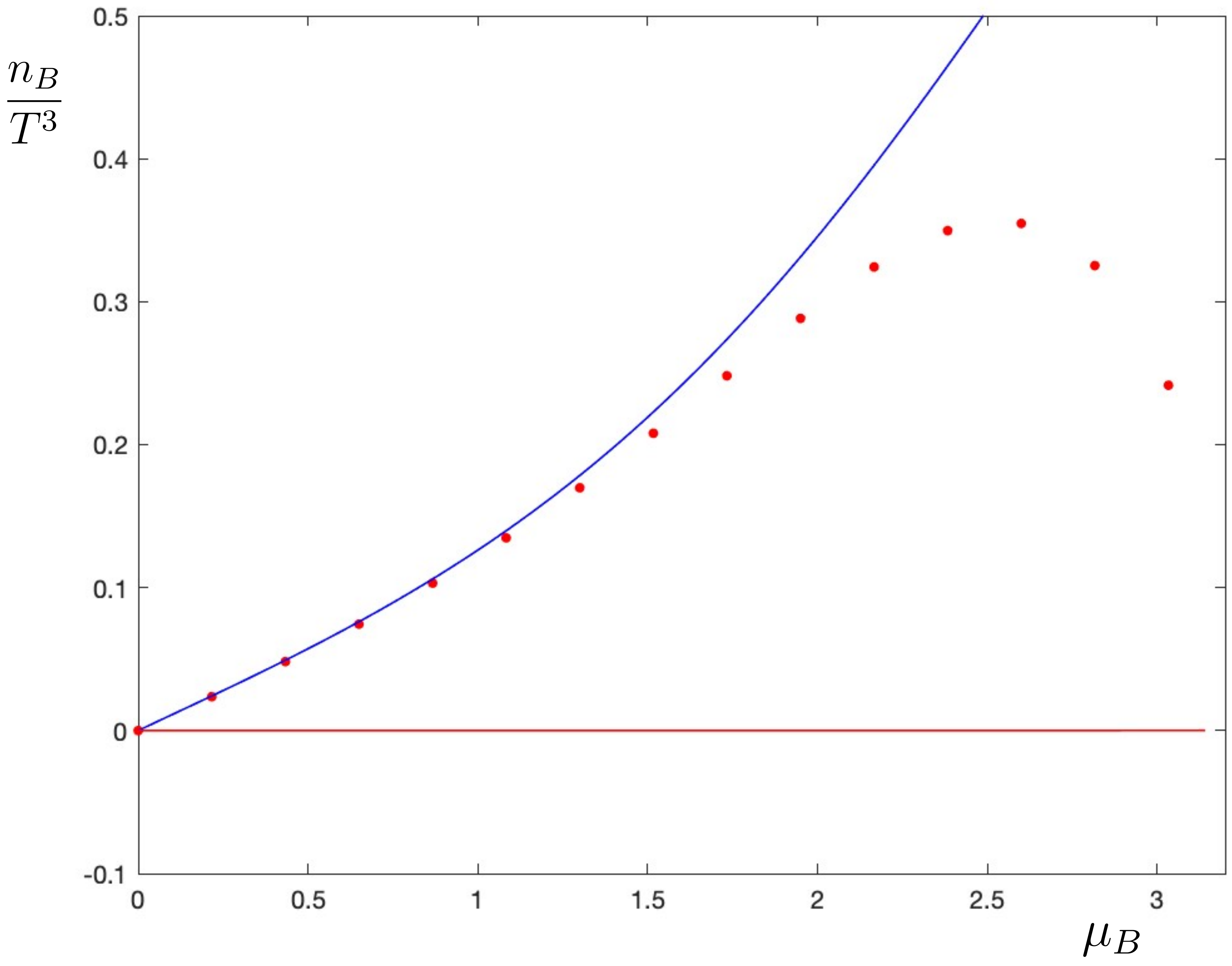

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... and you simply compute it for REAL VALUES of μ_B

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 ... we know how to compute them, but here we are concerned with *trends*,,, FIXED CUTOFF!

Finite density QCD as an inverse problem

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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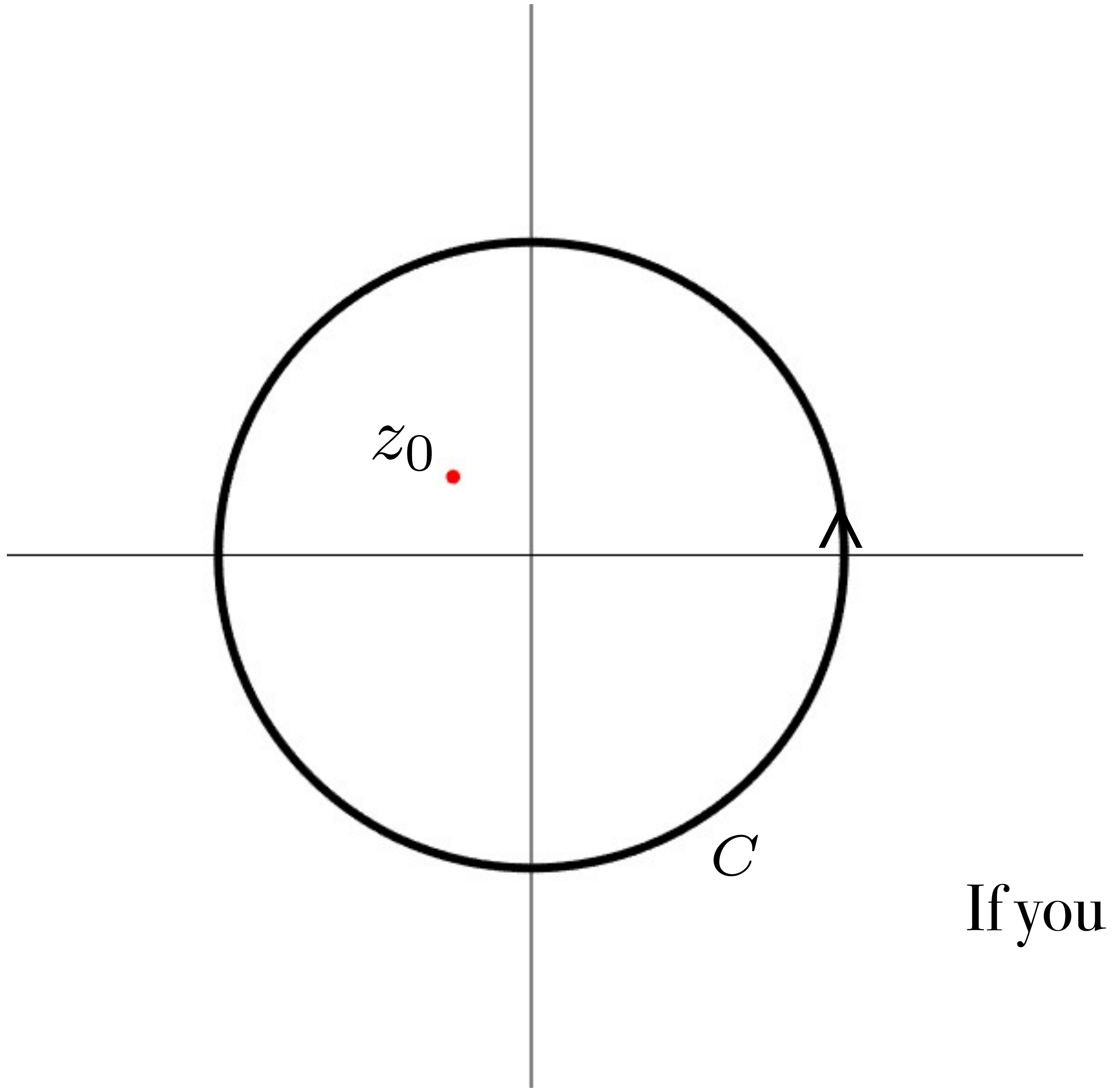

CAUCHY FORMULA

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

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

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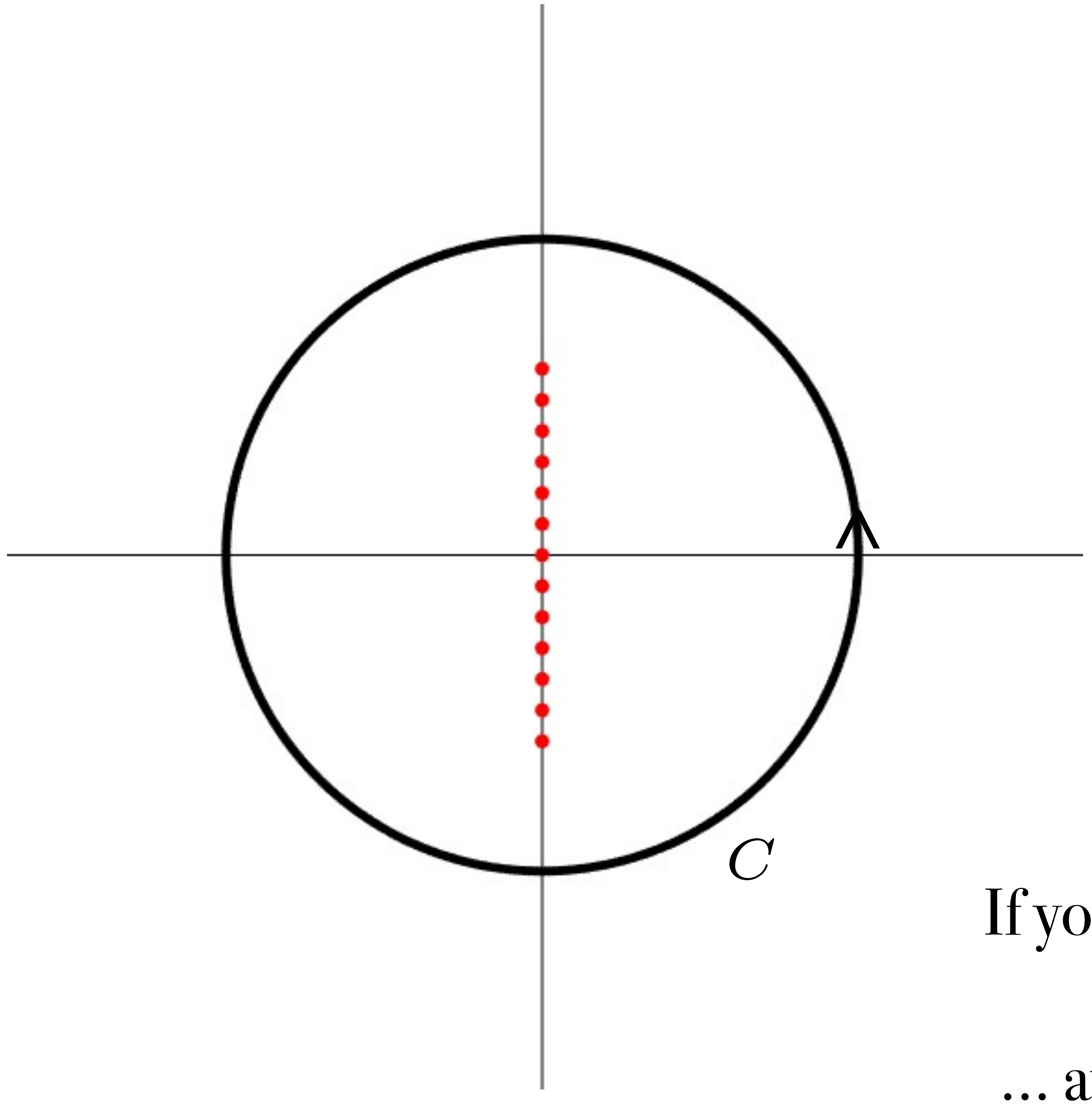

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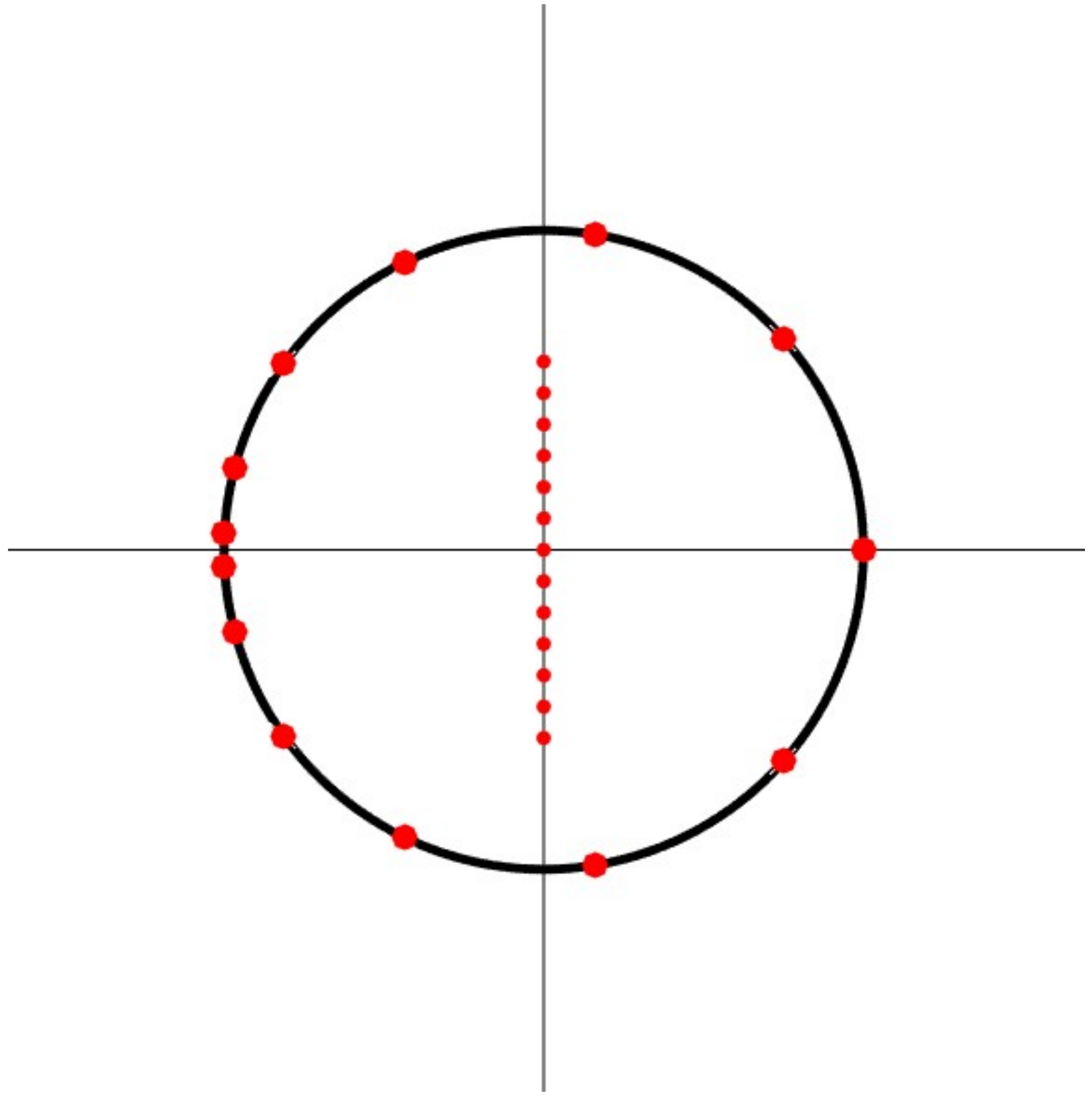
… at any point, including the (only) ones we can compute (on the imaginary axis) in our case…

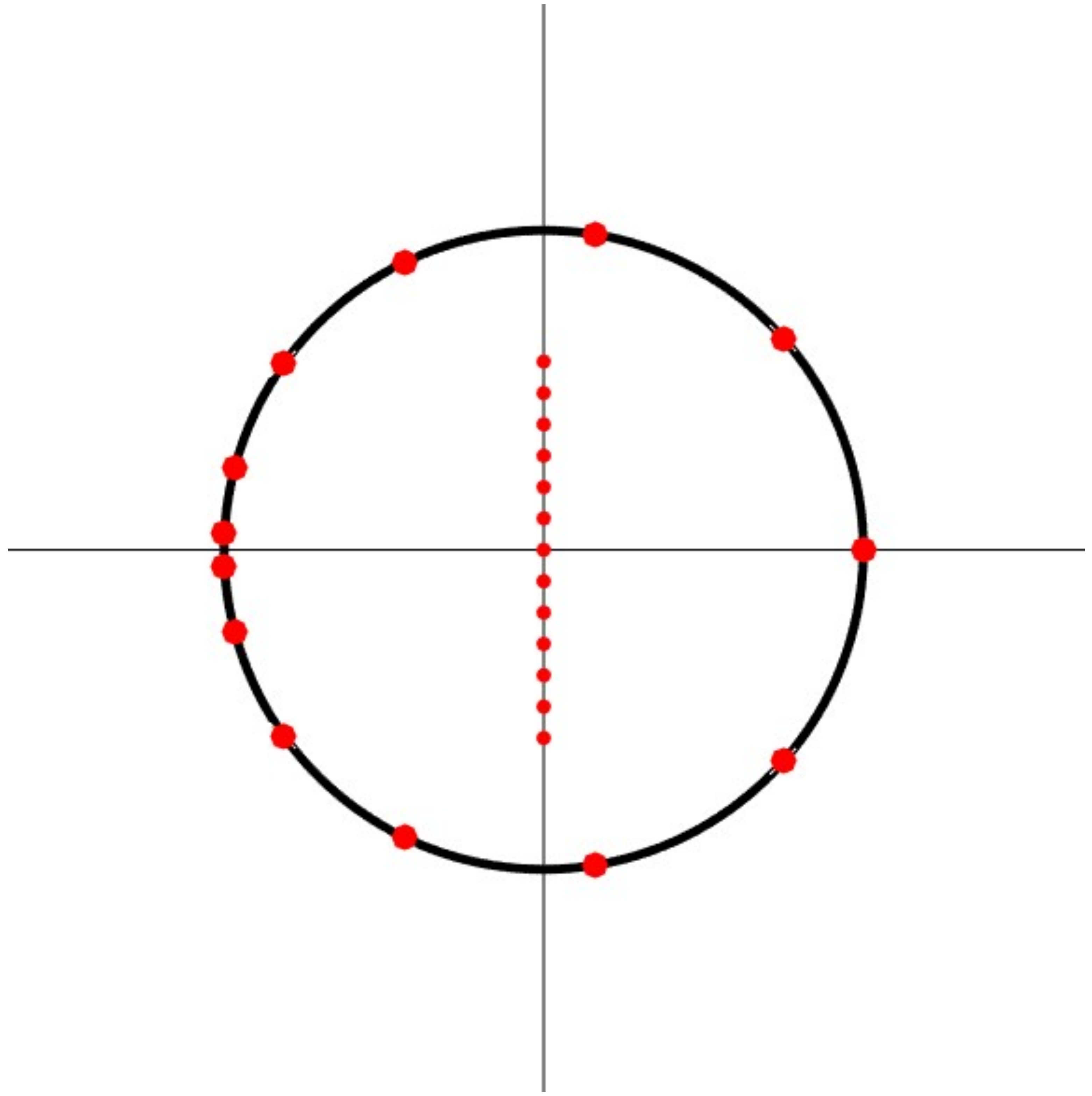


With your favourite QUADRATURE method ... you can go numeric!

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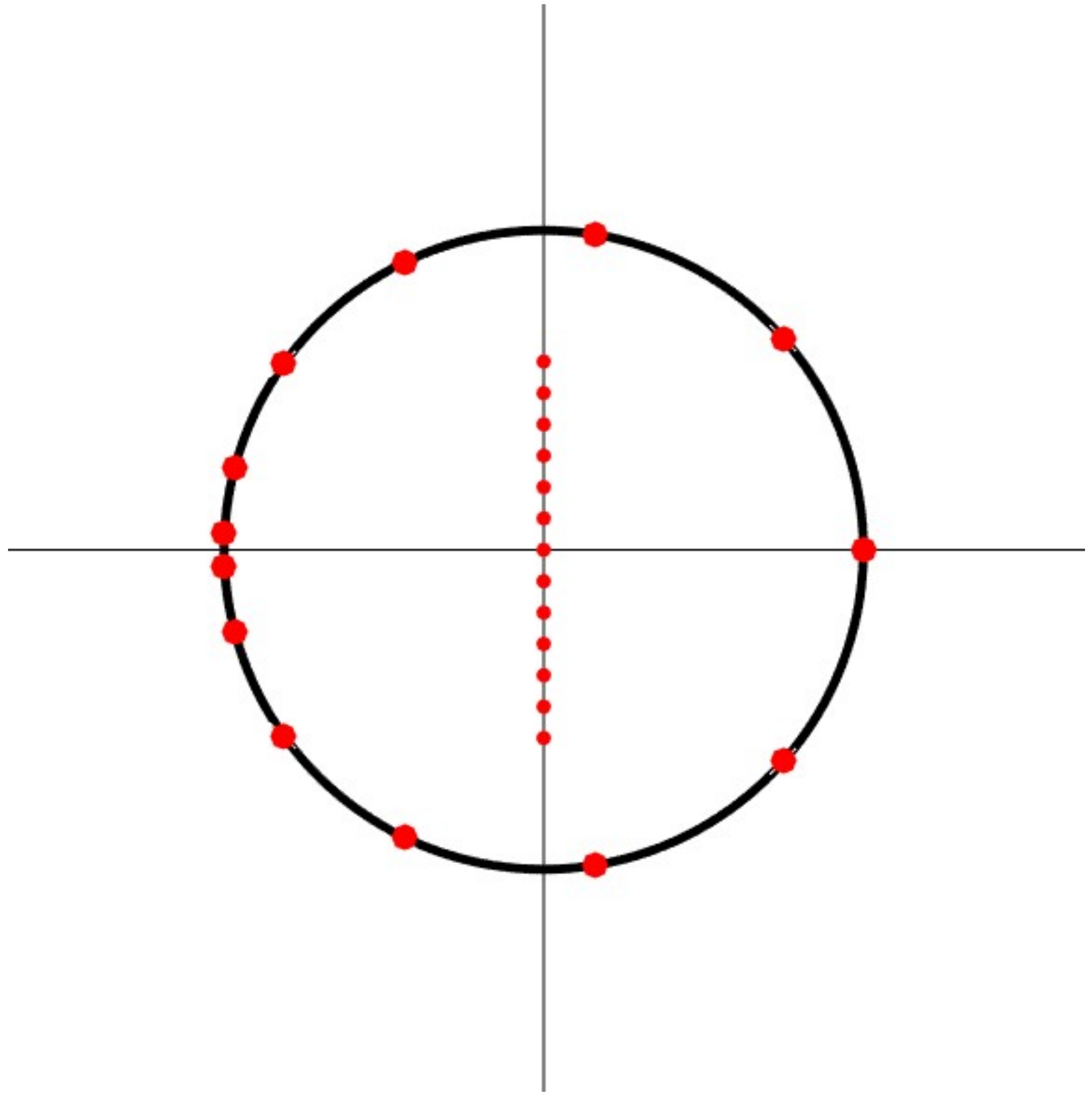
... and then you are ready for your (BRAVE) INVERSE PROBLEM!



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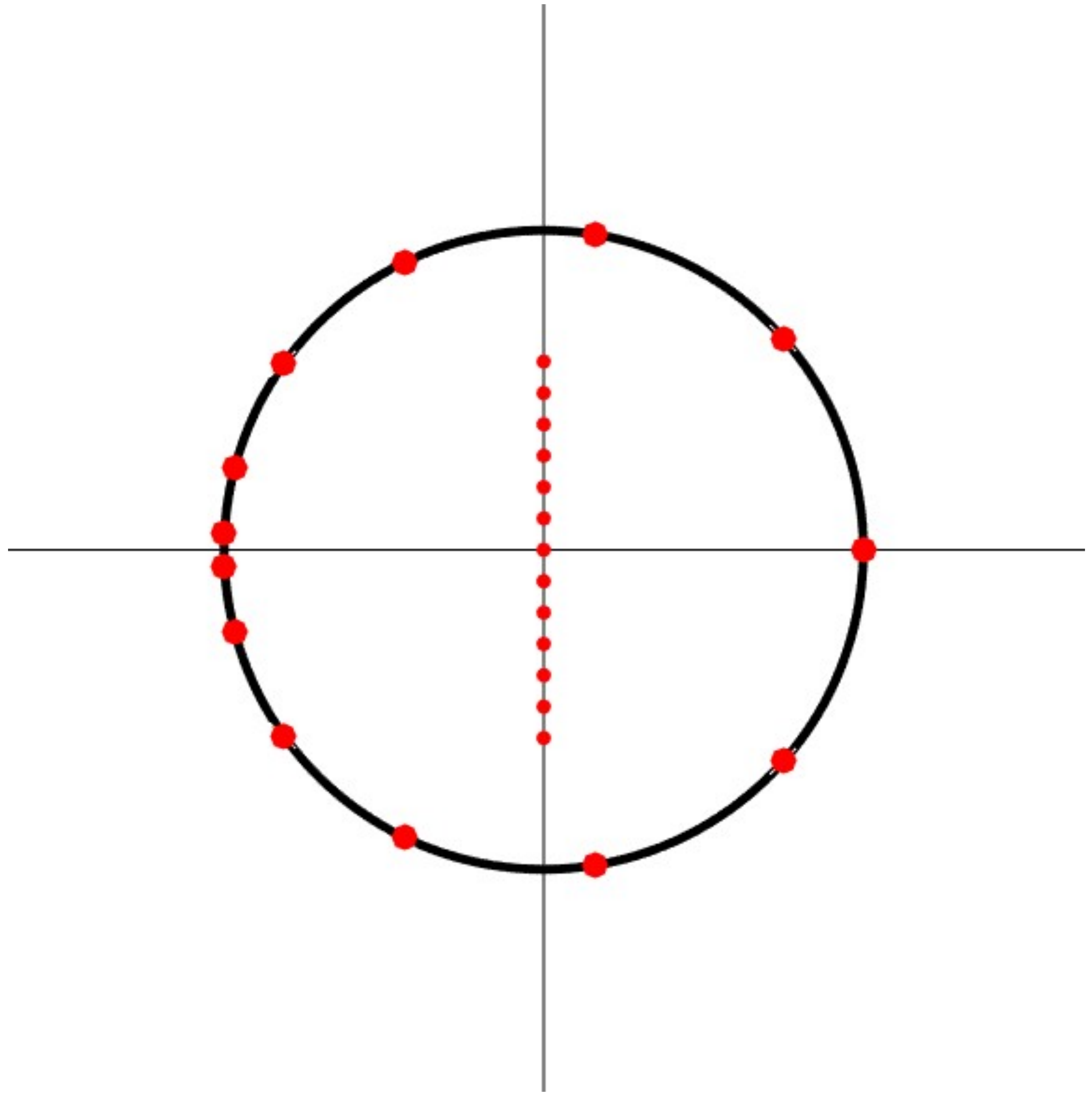
$$A_{ik} = \frac{1}{2\pi} \, w_k \, \frac{R\, e^{i\theta_k}}{R\, e^{i\theta_k} - z_i}$$

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

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



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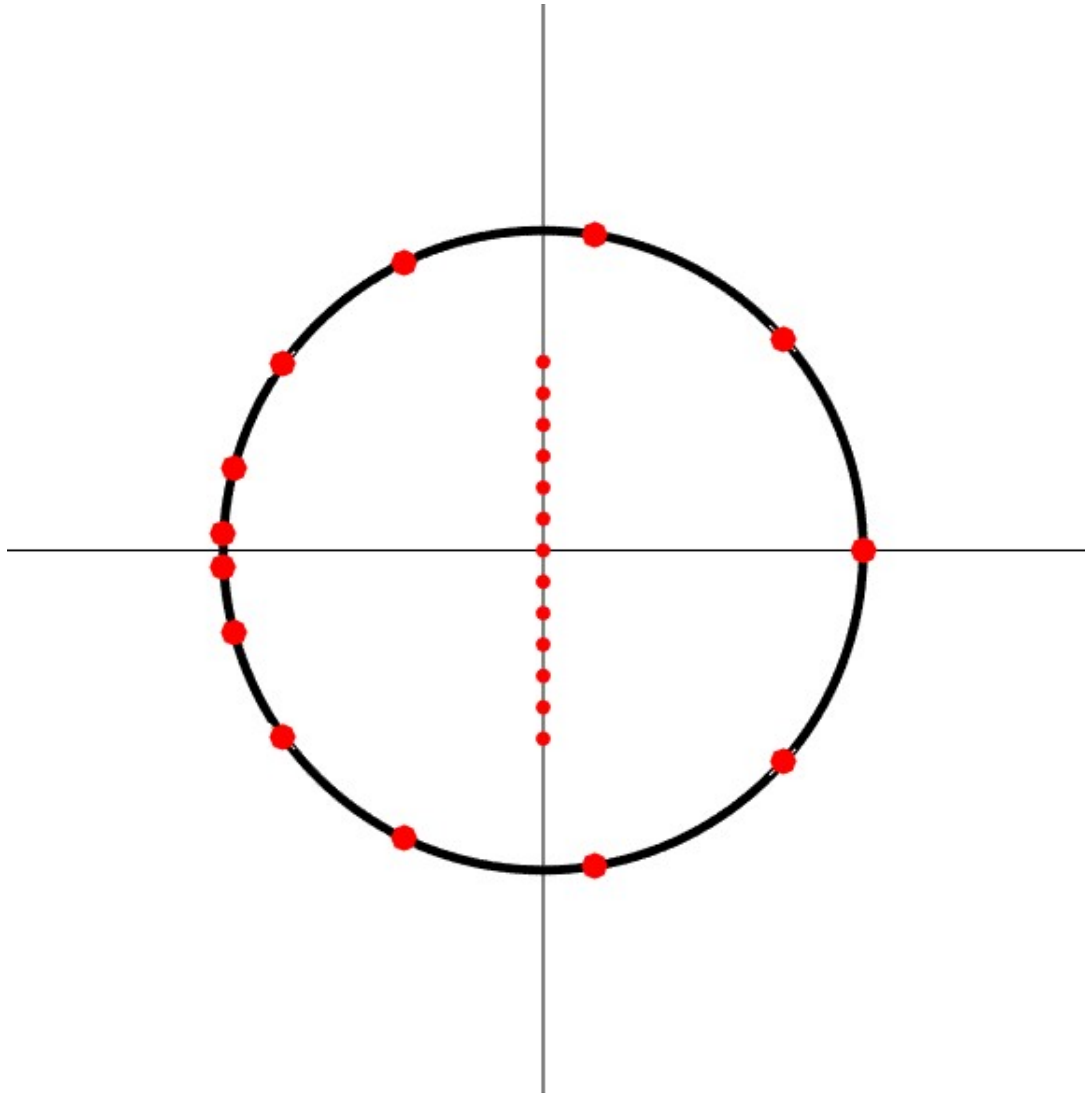
A very SIMPLE idea! ... a NAIVE one ... INVERSE PROBLEM!!!



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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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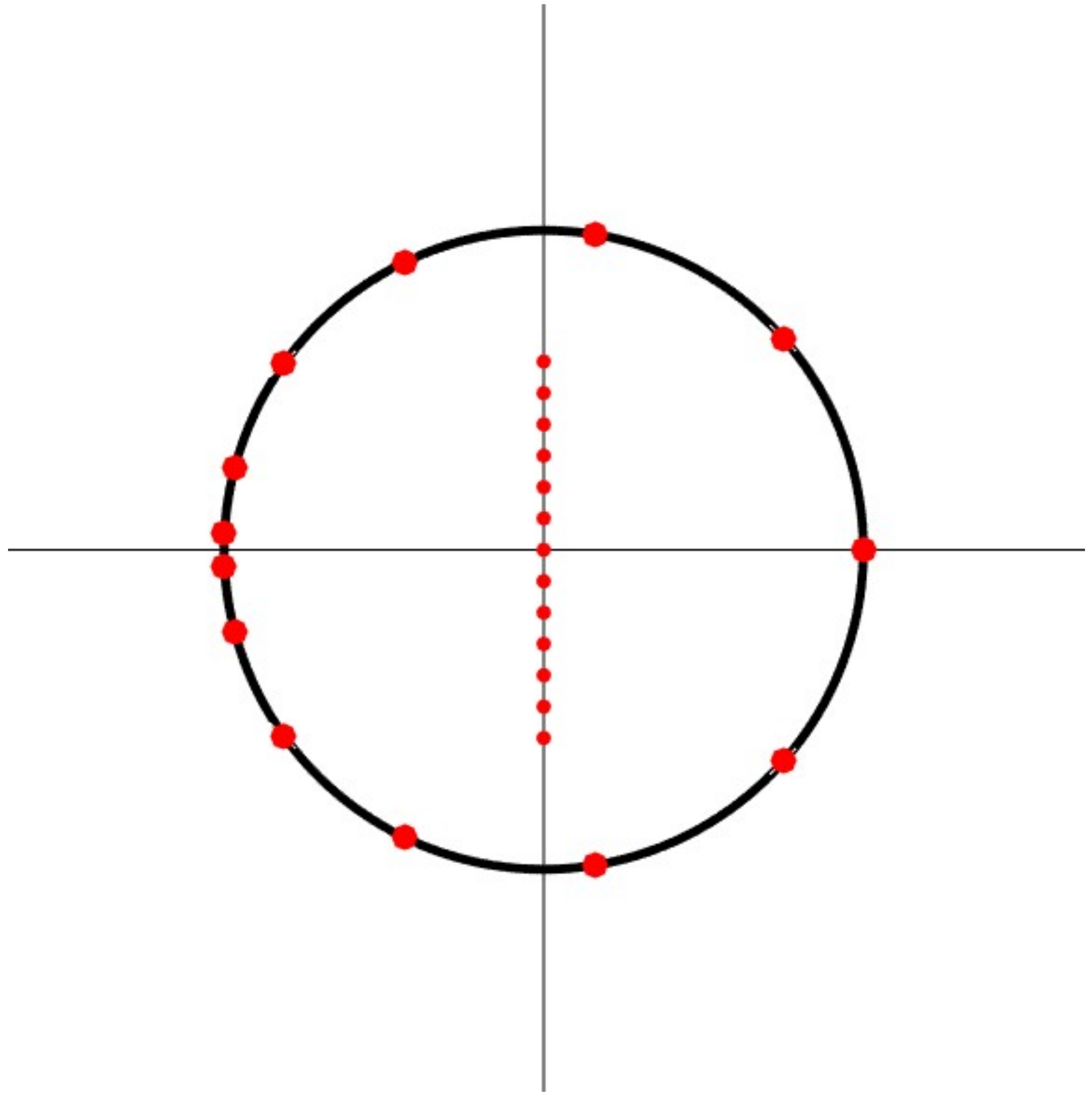

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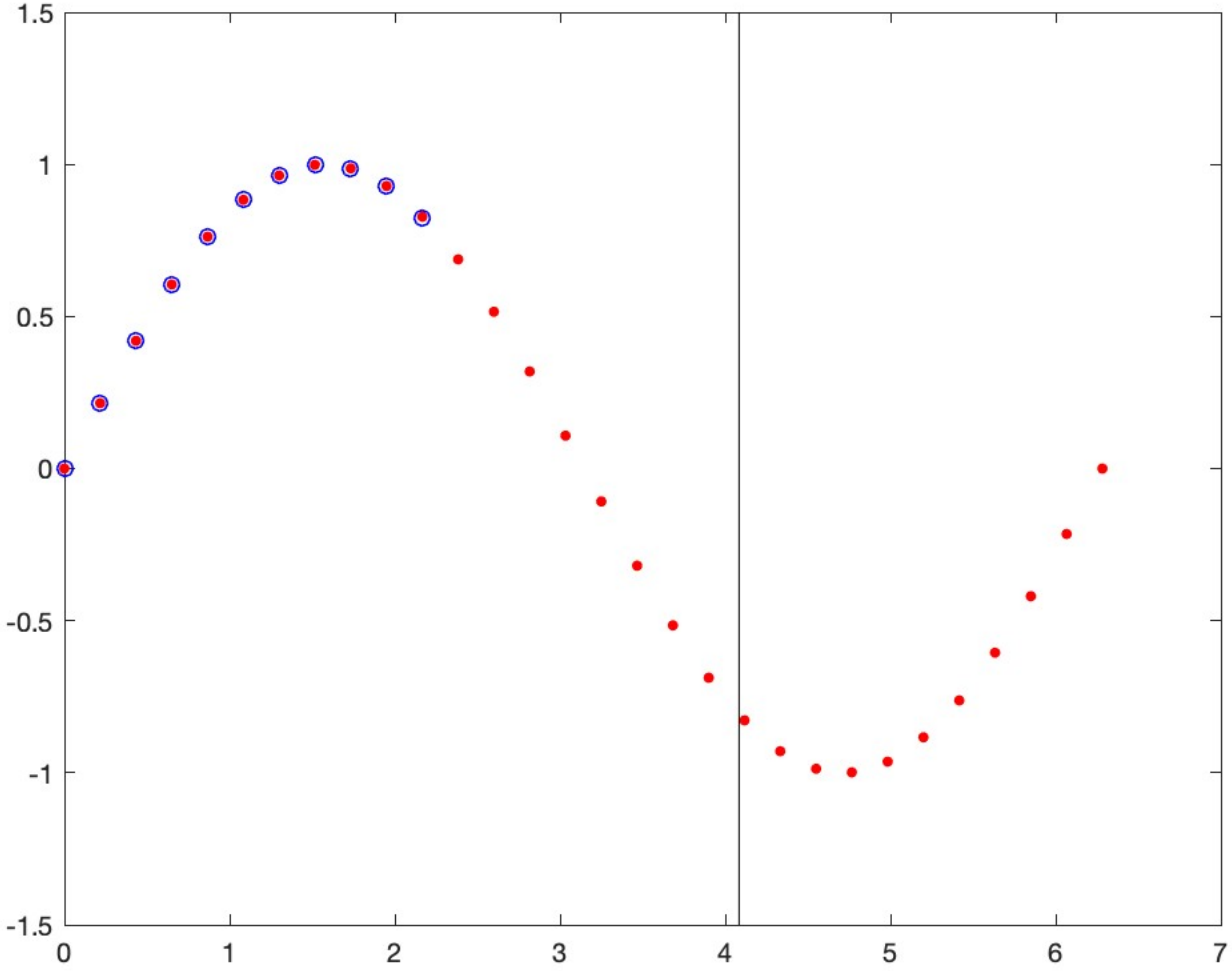
Radius (*ca 4*) and number of points (*13*) chosen having in mind what we have to live with in finite density QCD!

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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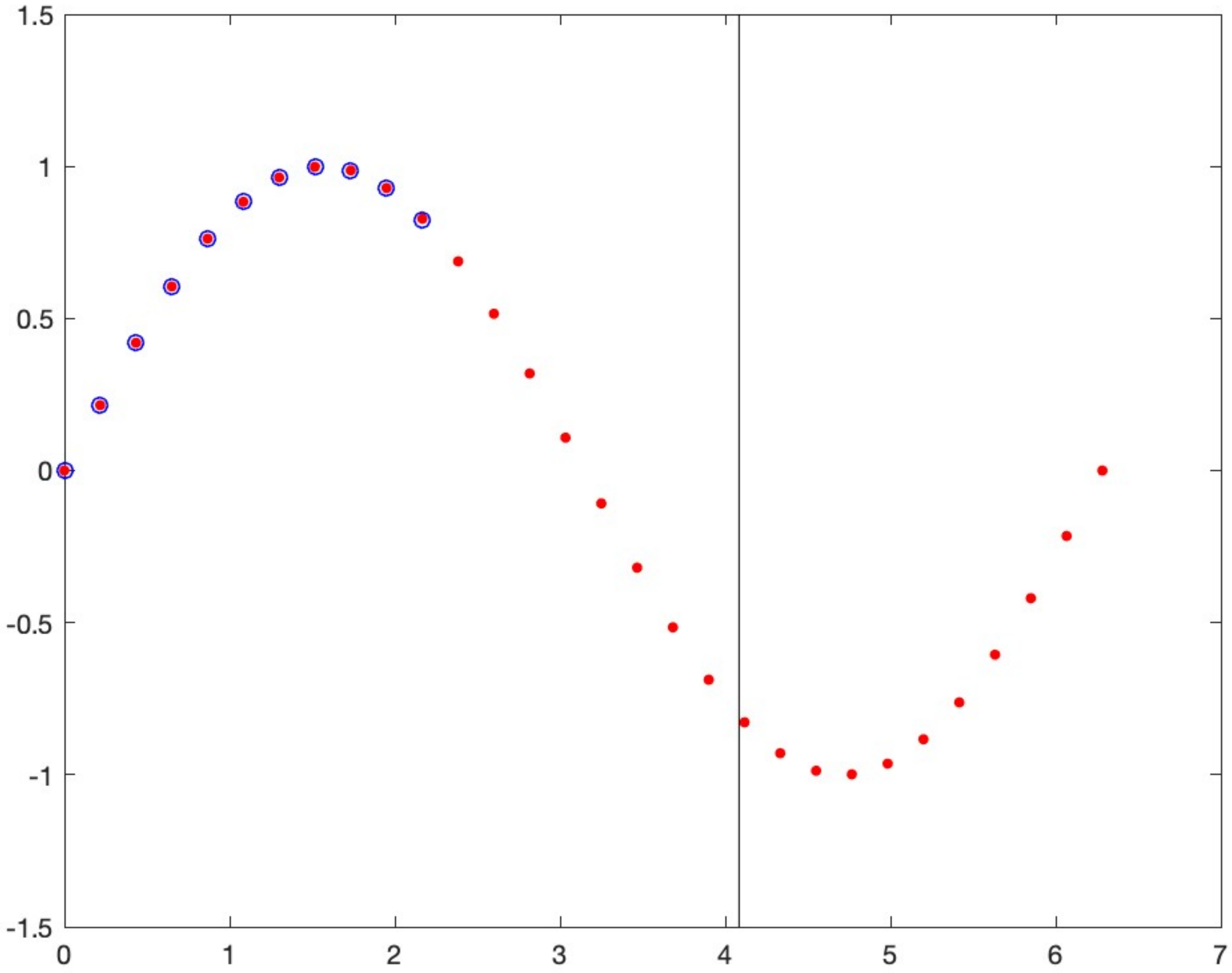

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(a) bad condition number of the linear system
(b) the quadrature formula being NOT exact

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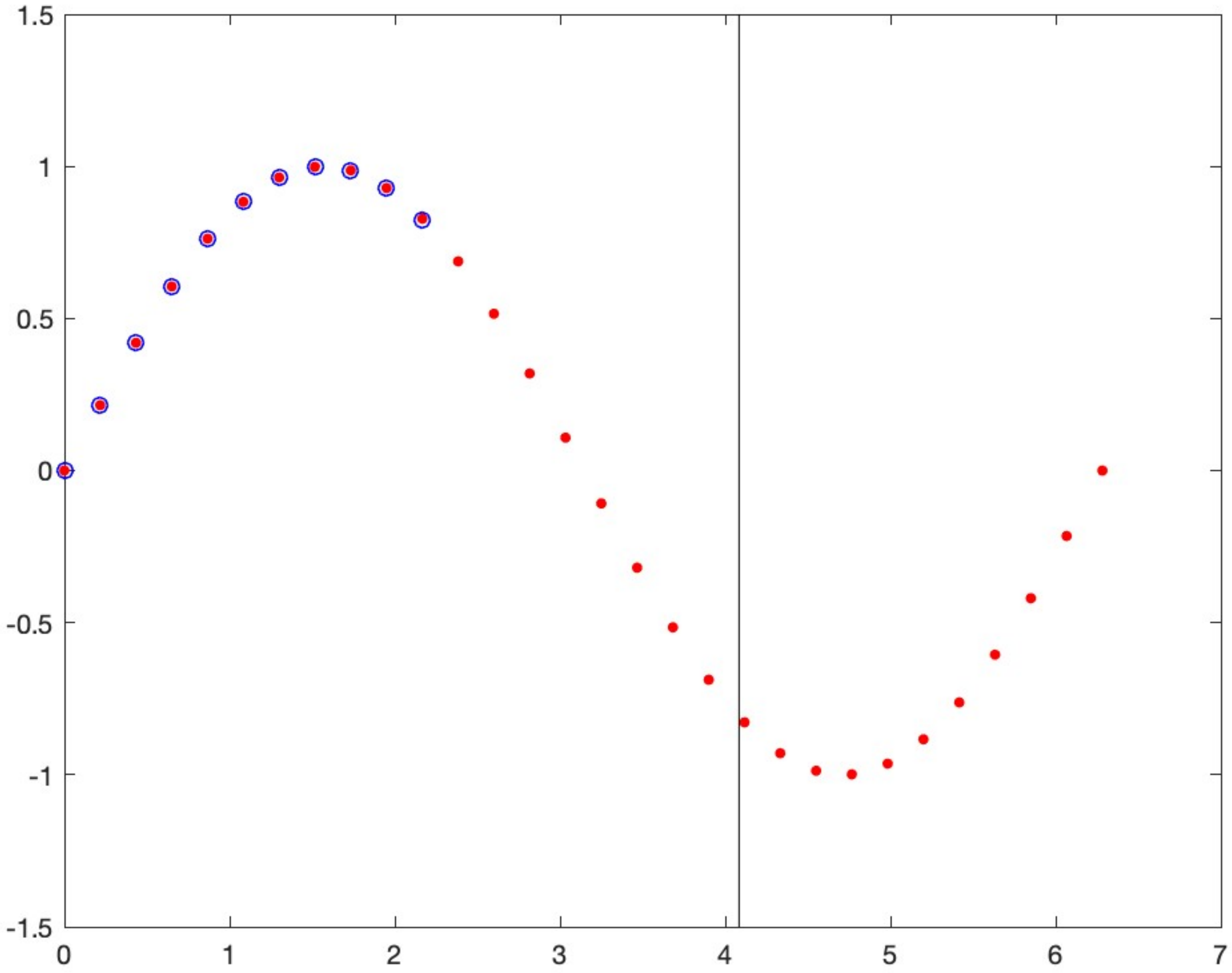

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… and as a matter of fact the *solution* you get
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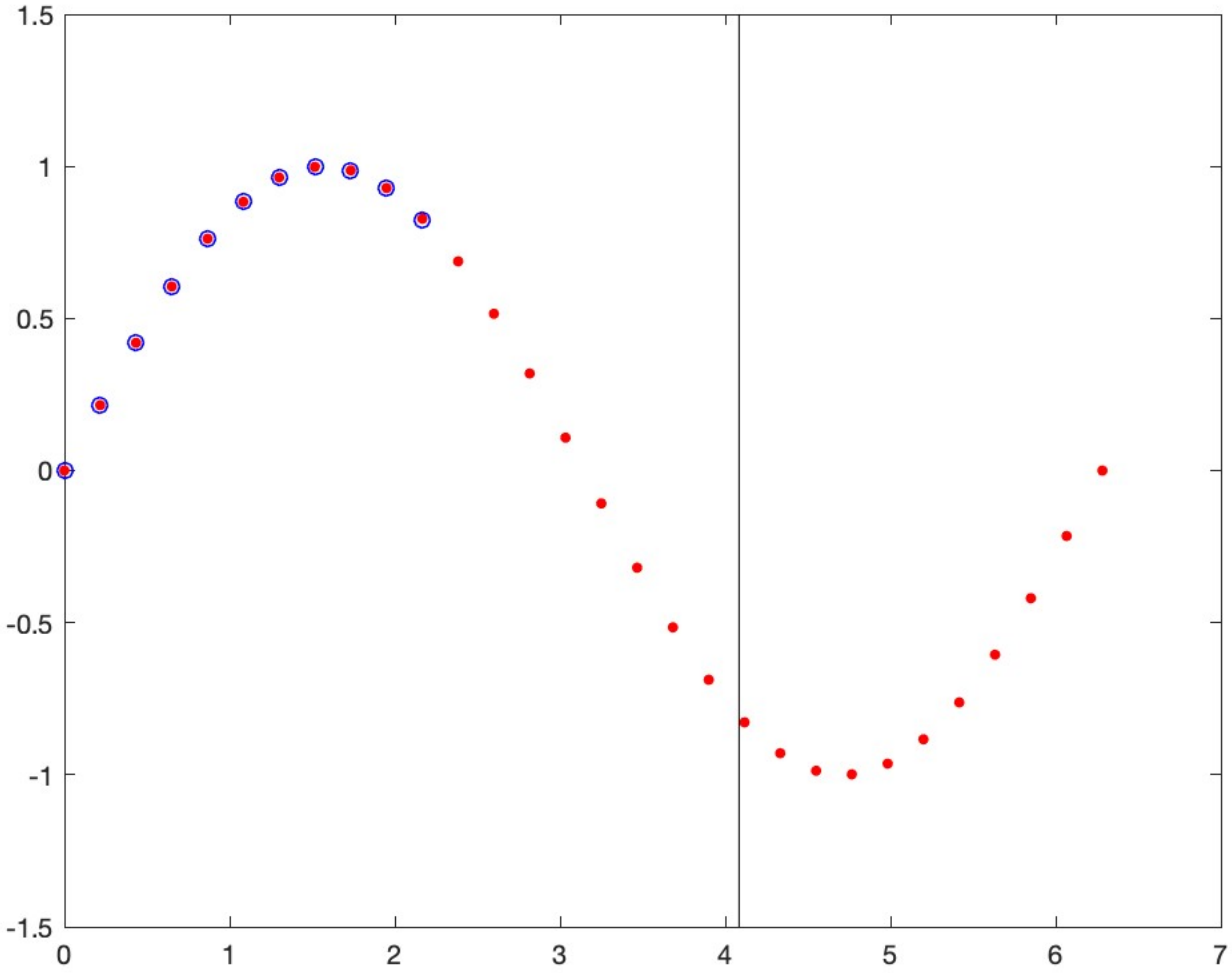

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… and as a matter of fact the *solution* you get has *nothing to do with the sin function evaluated at the expected (quadrature) points*

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

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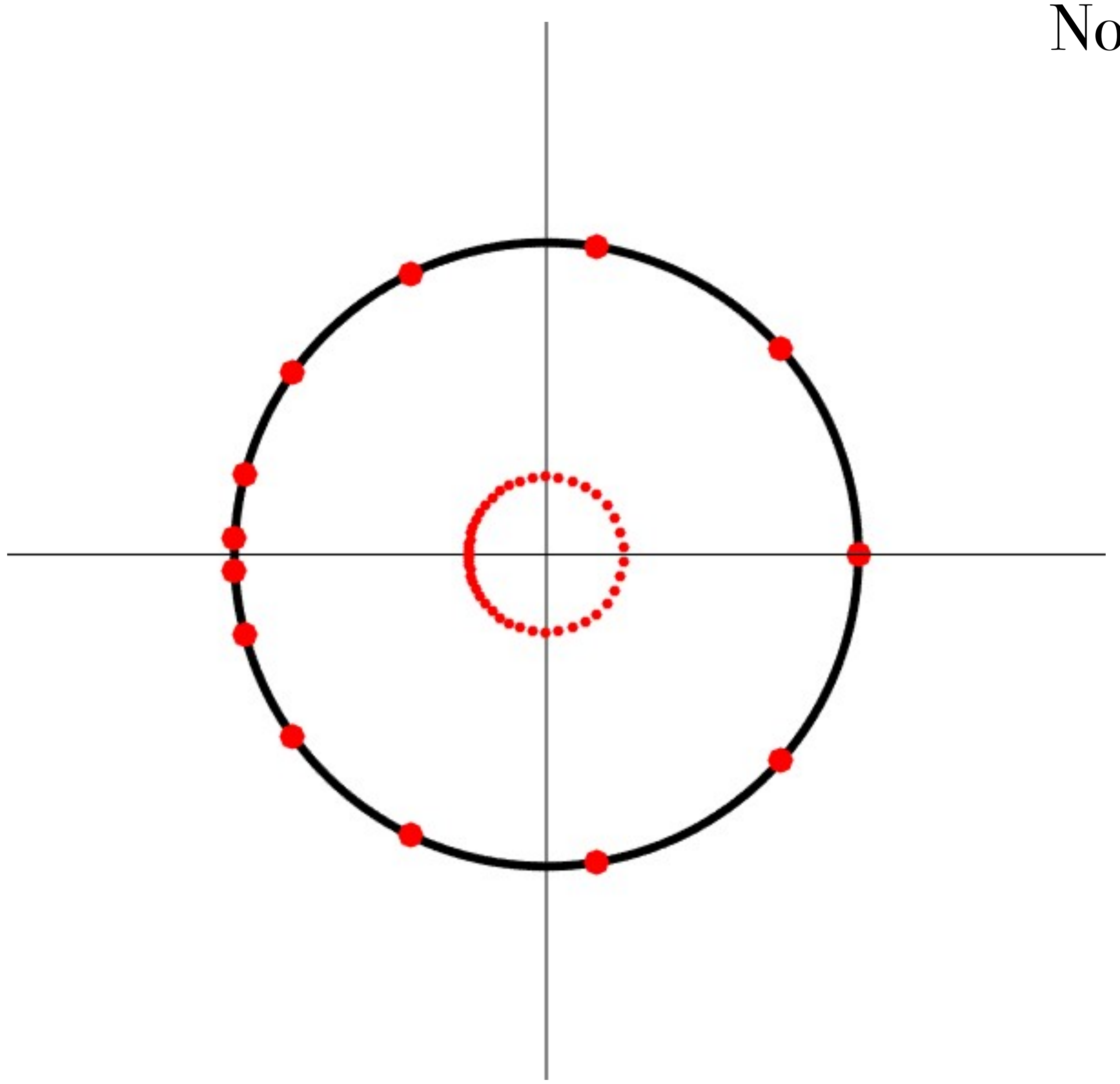
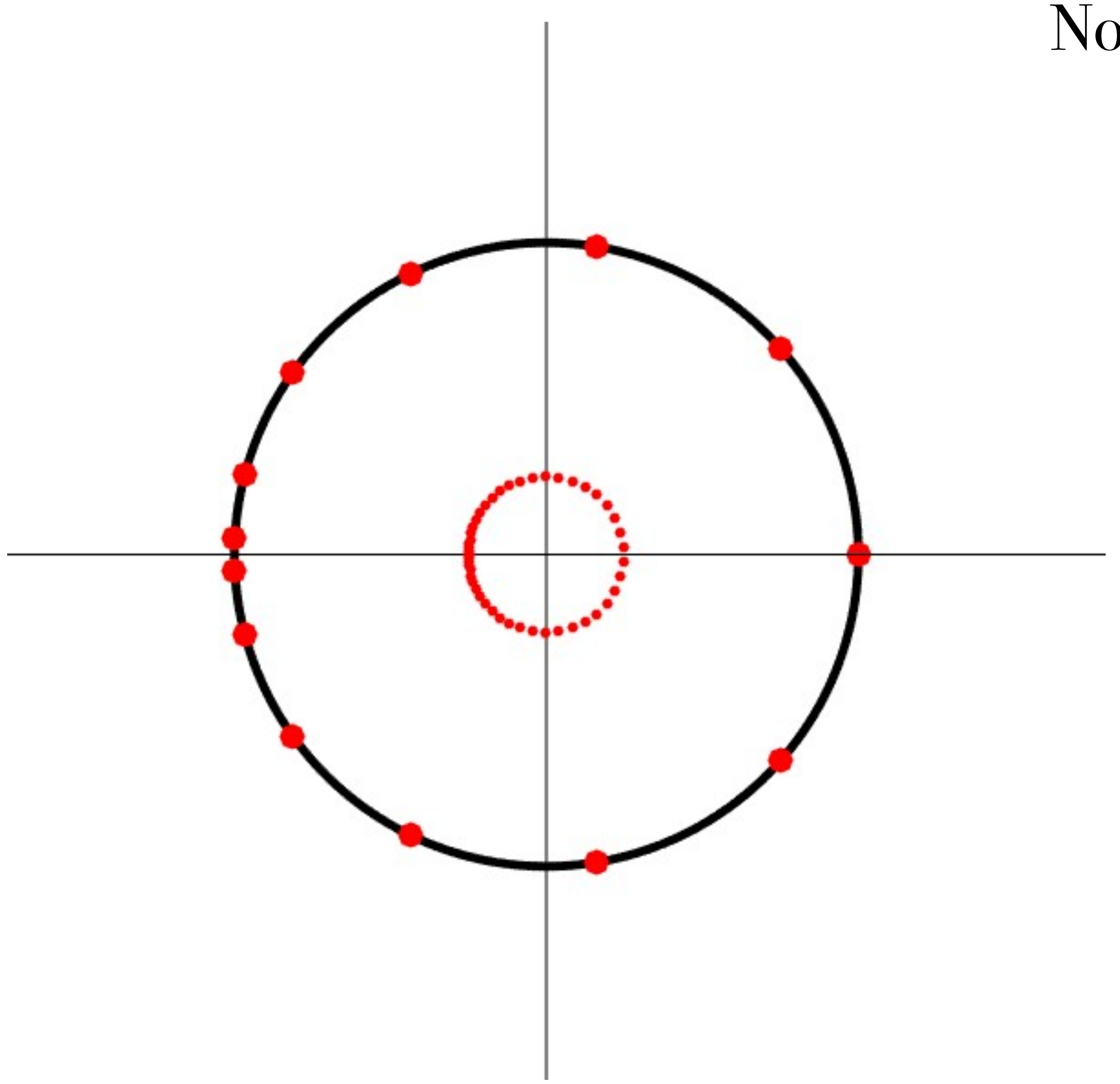


Now, forget about the inverse problem, and remember Cauchy formula for derivatives

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



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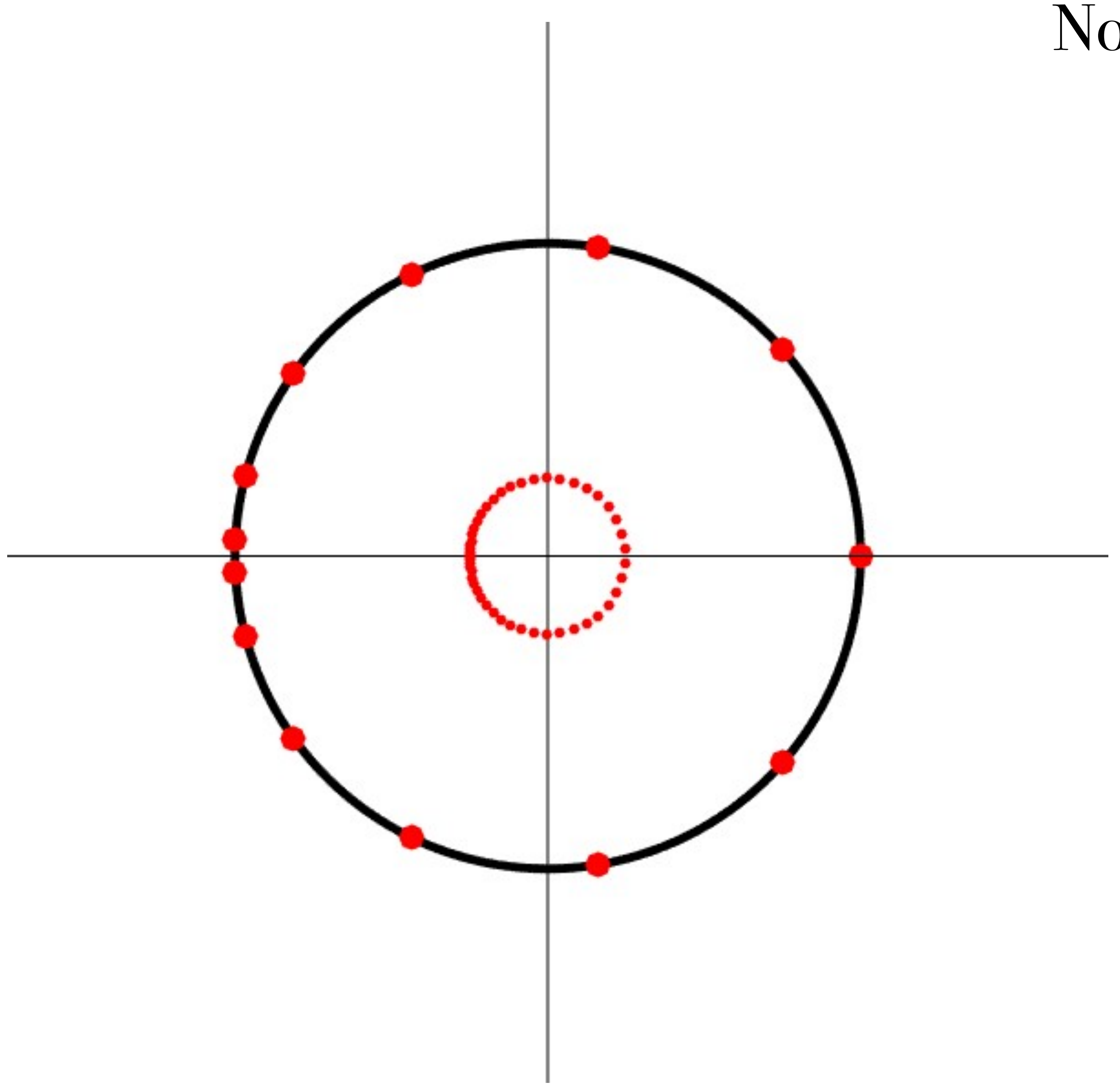
I took quite some quadrature points (50) on a much shorter contour, closer to the origin. We will now compute derivatives of our function in $z_0 = 0$



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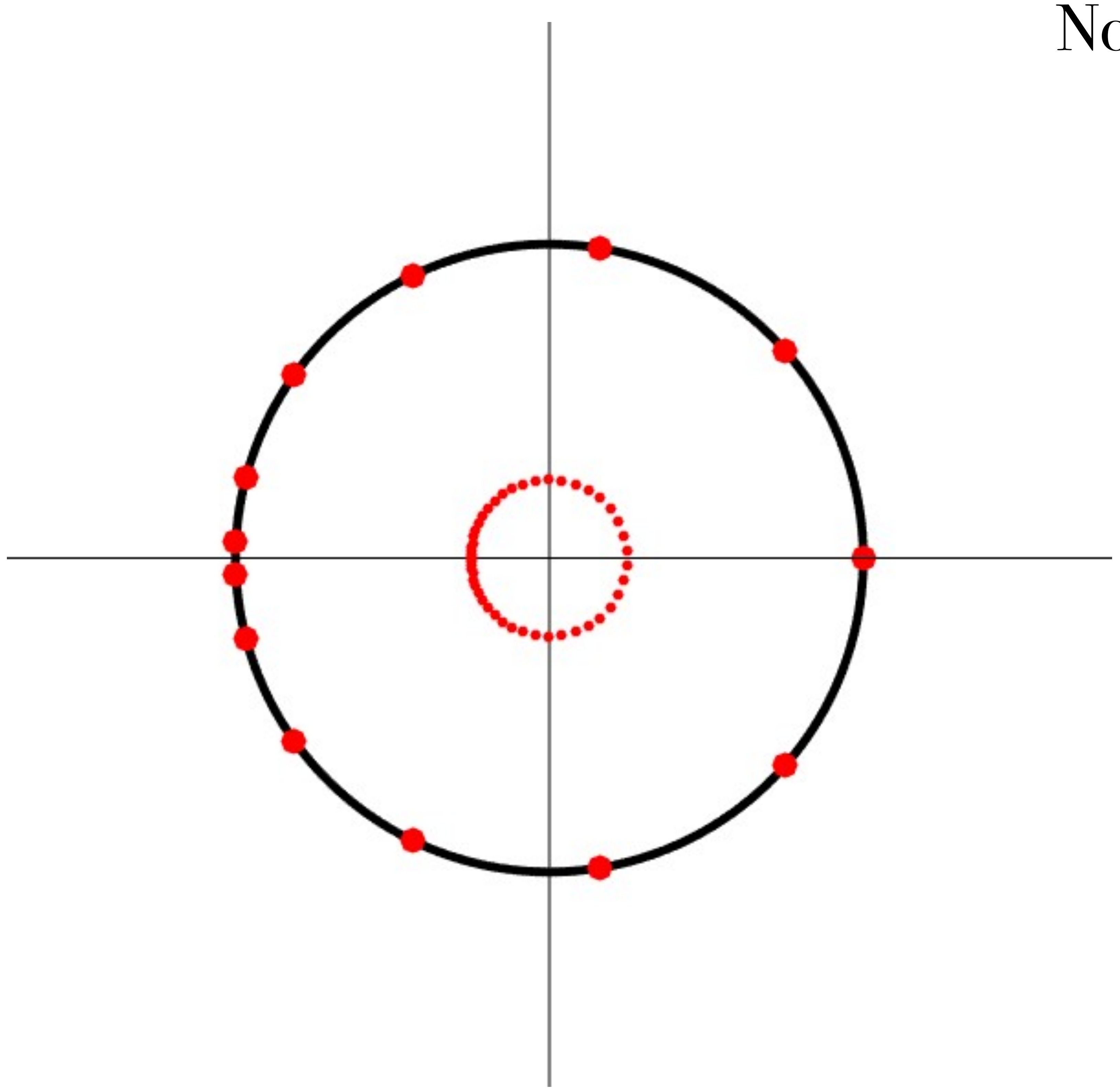

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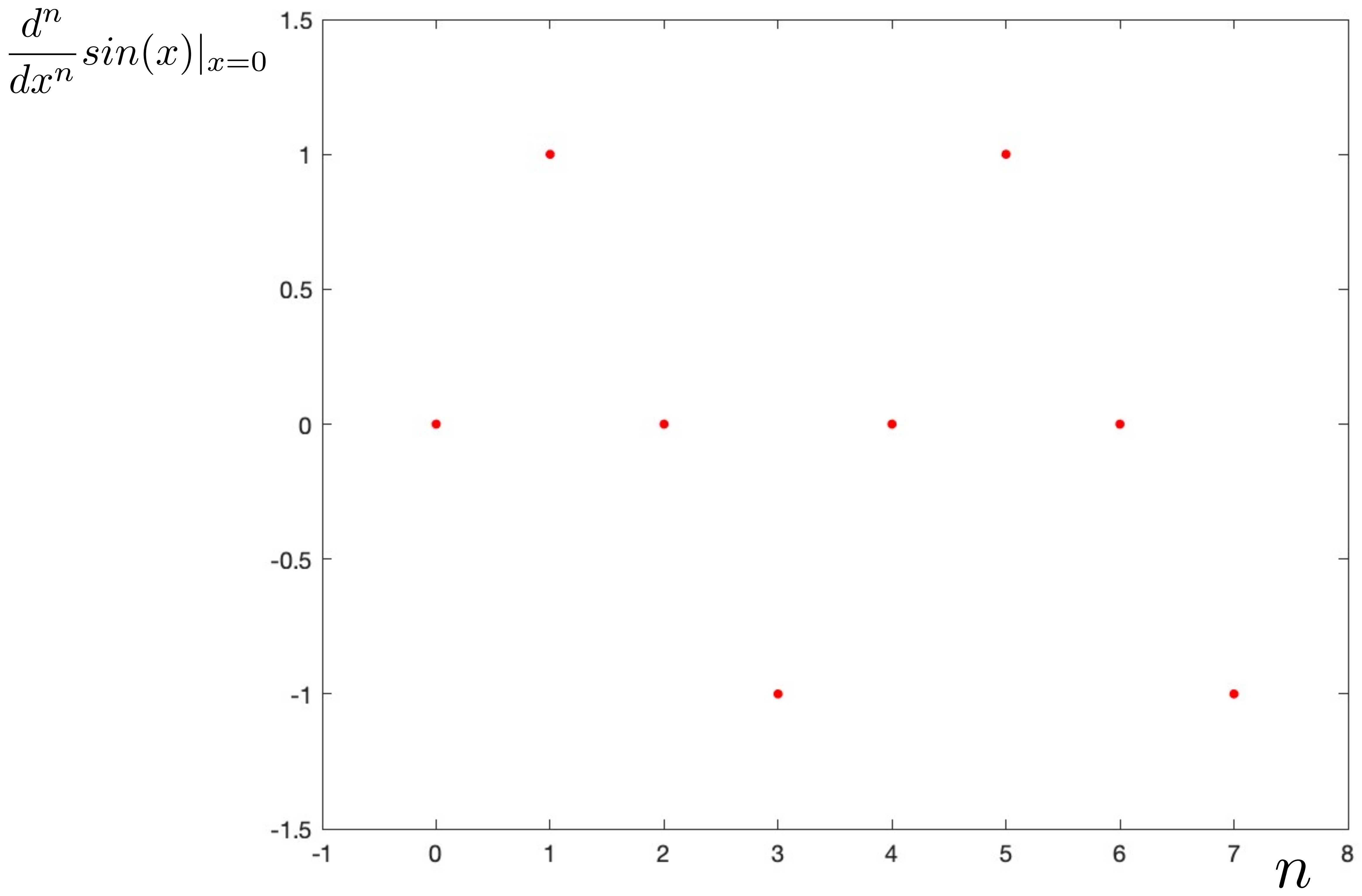

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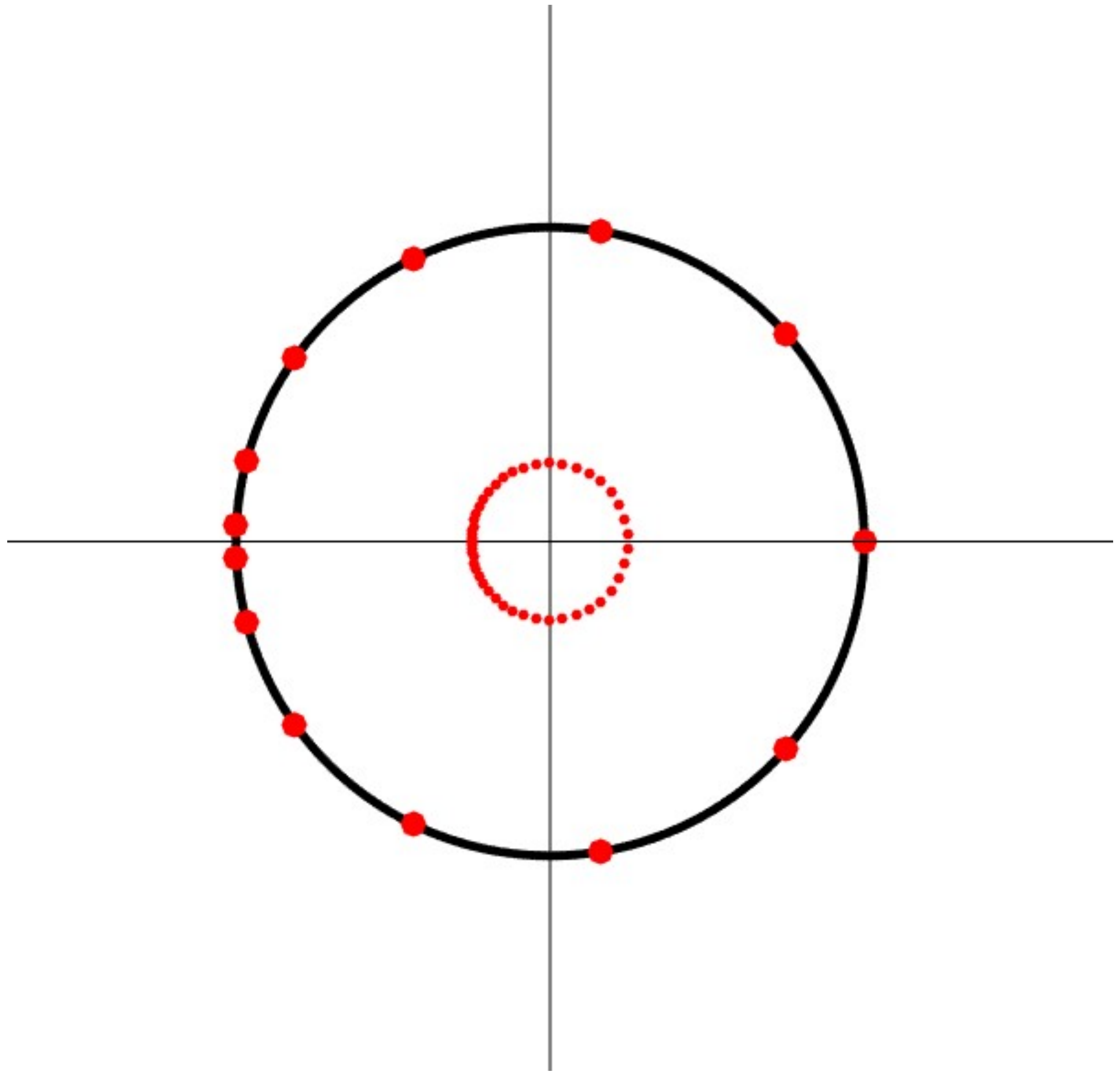

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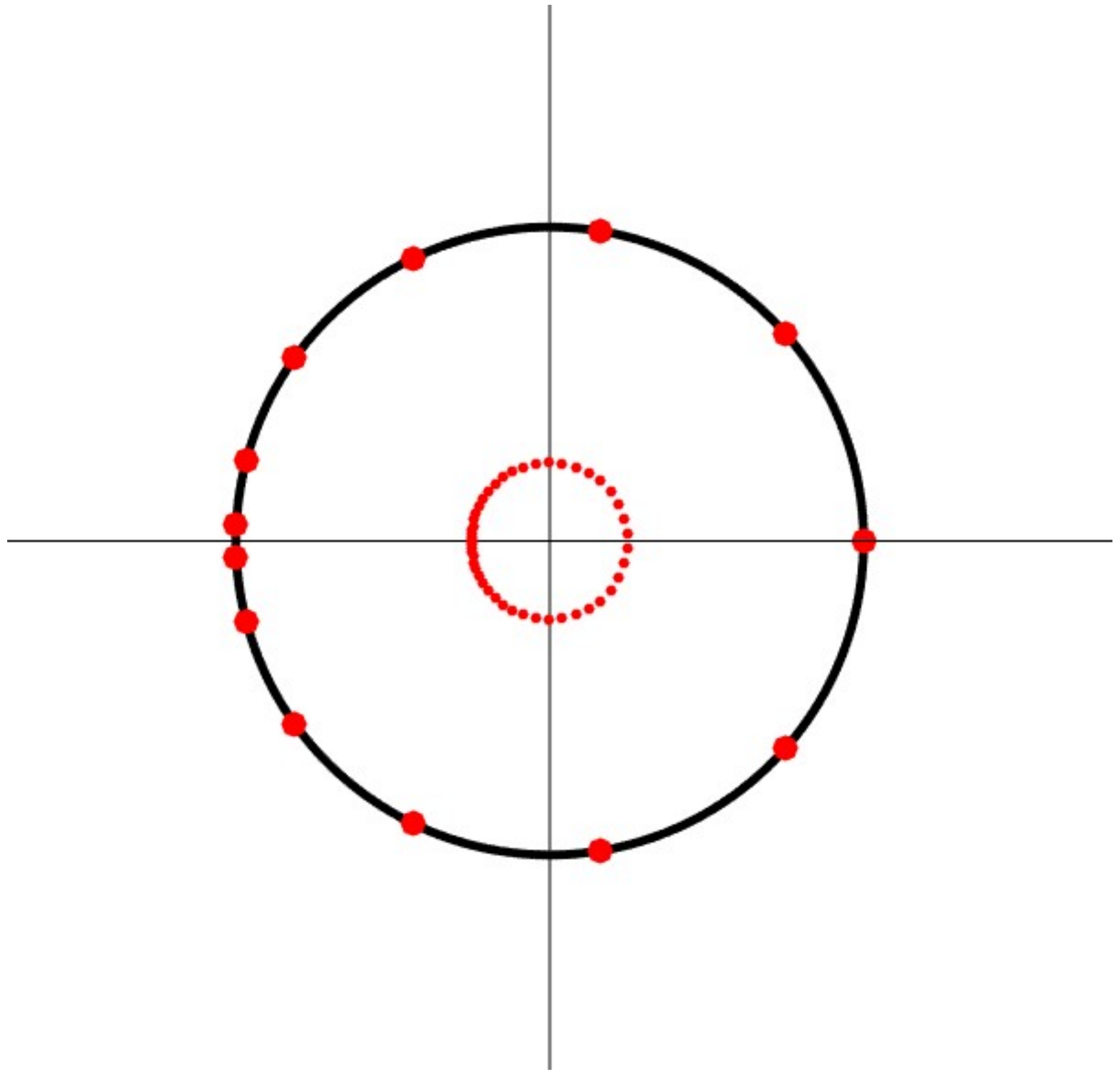
Does it work?



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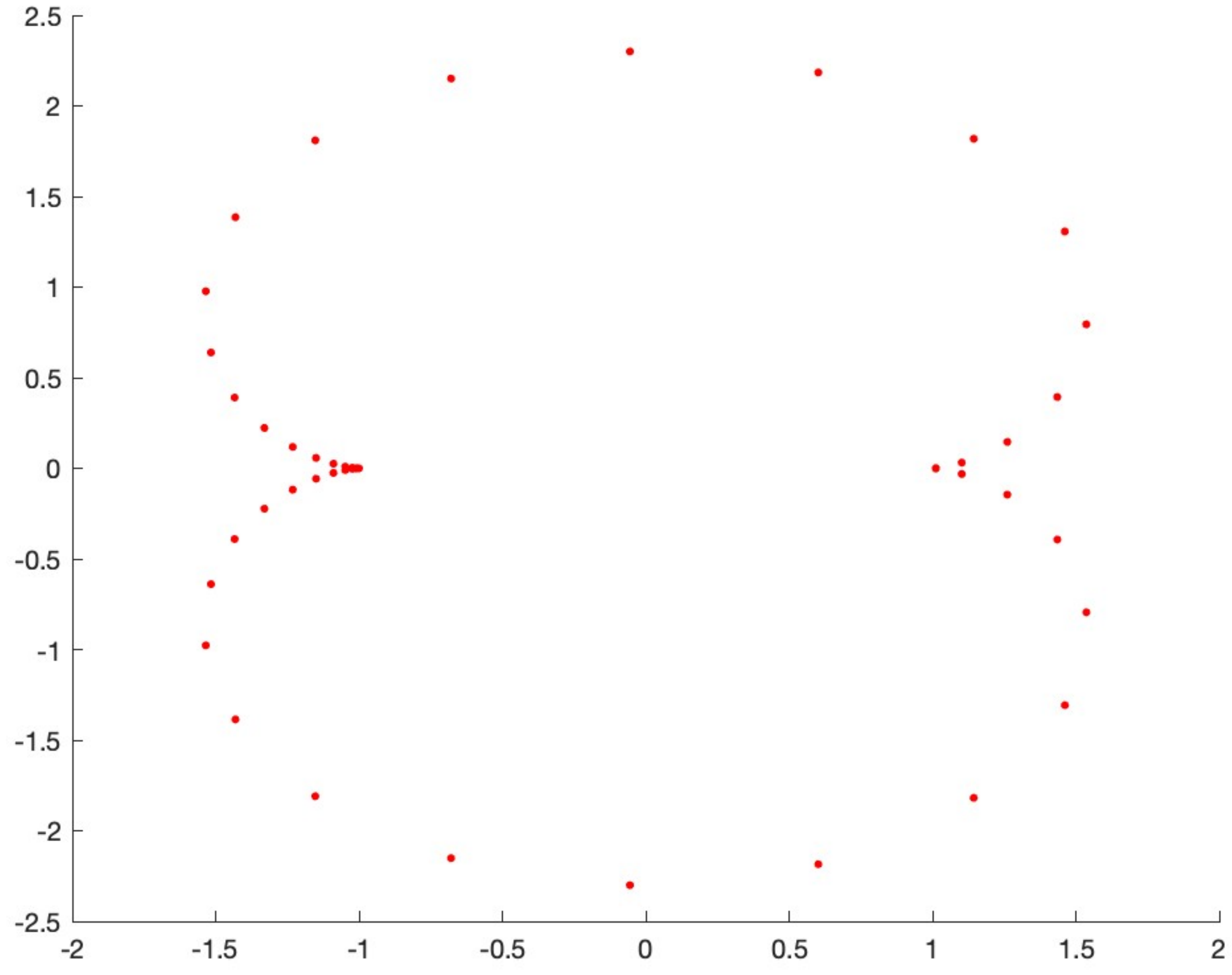
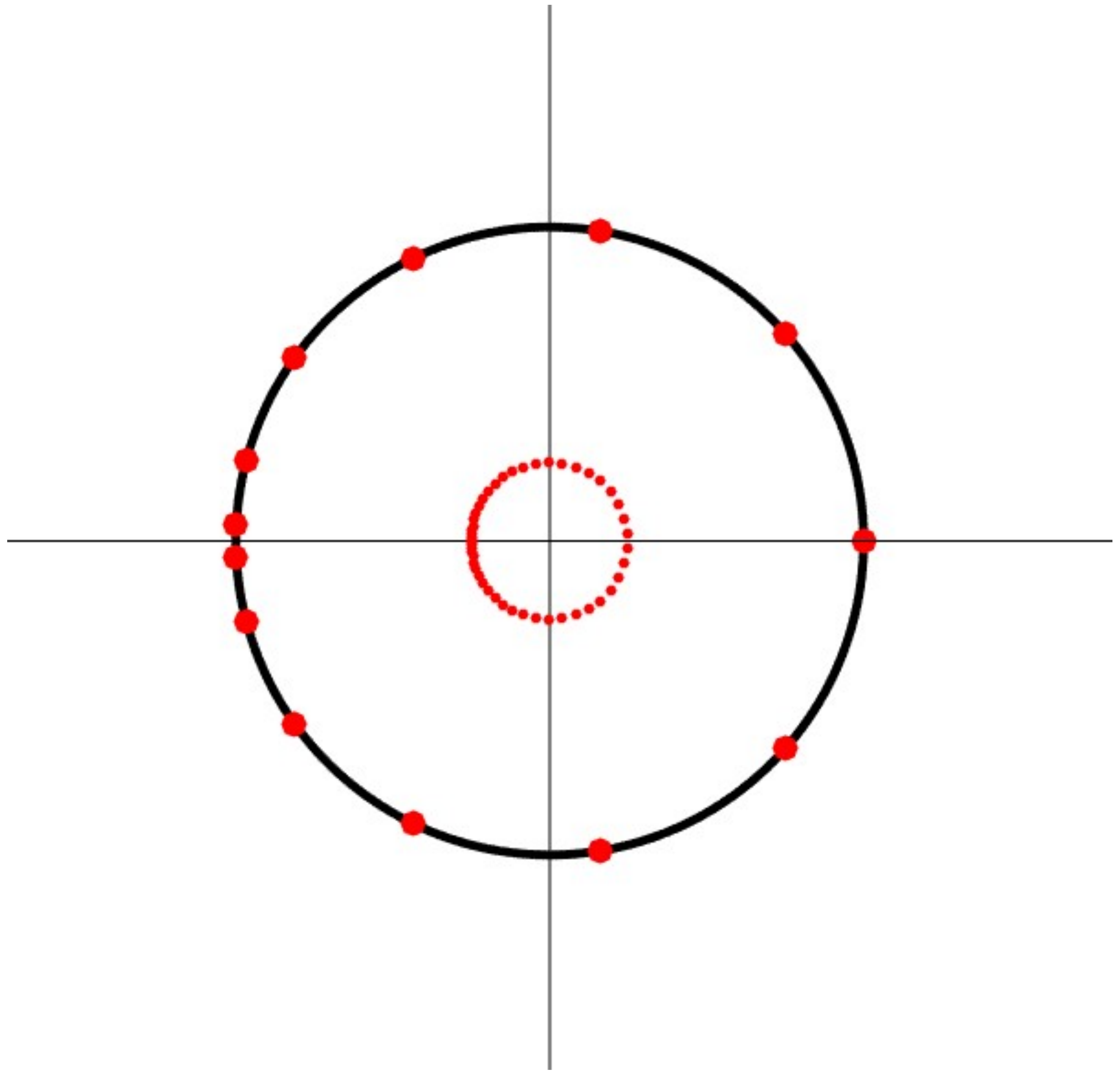
Let me plot (on the complex plane) the values I have to get





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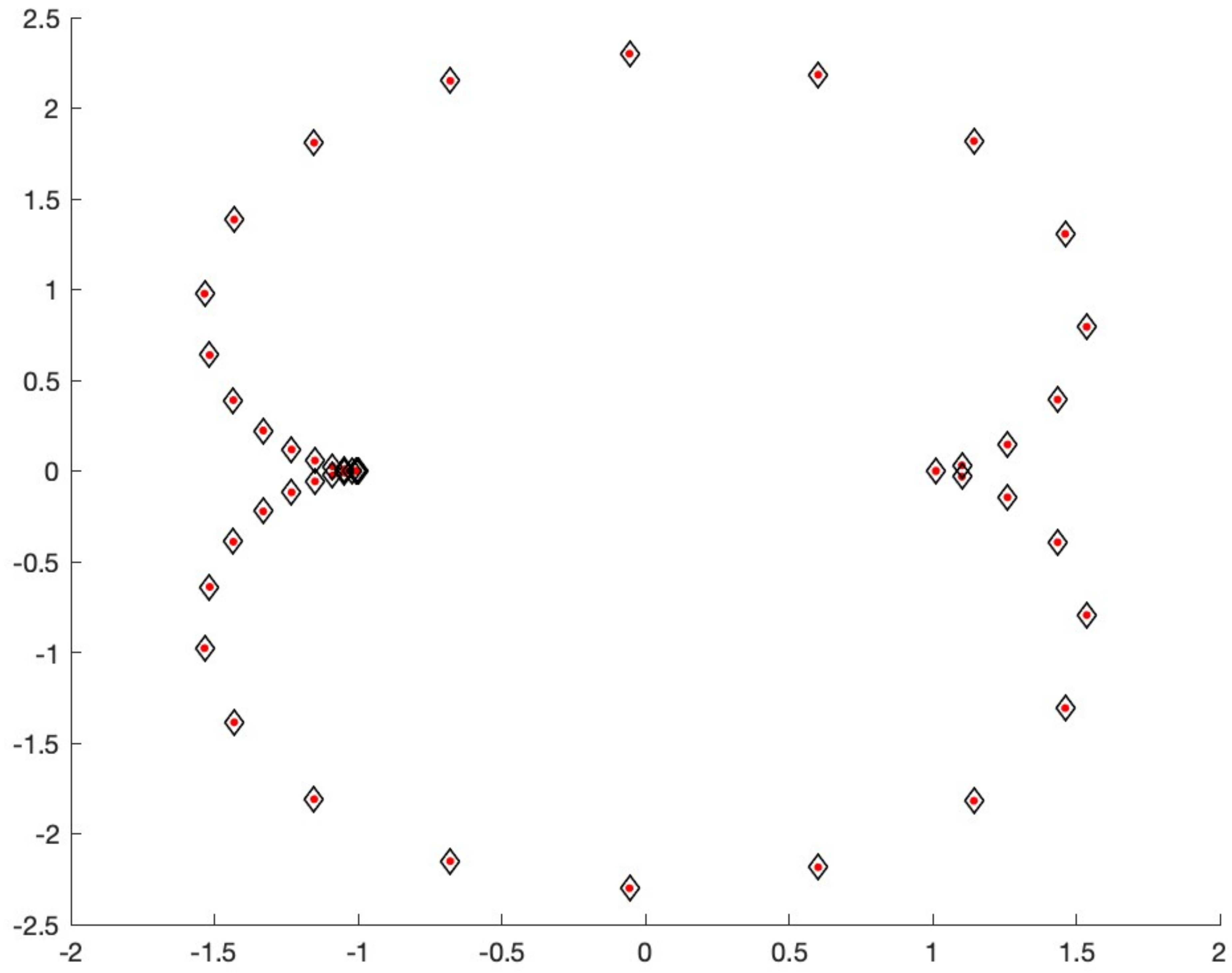
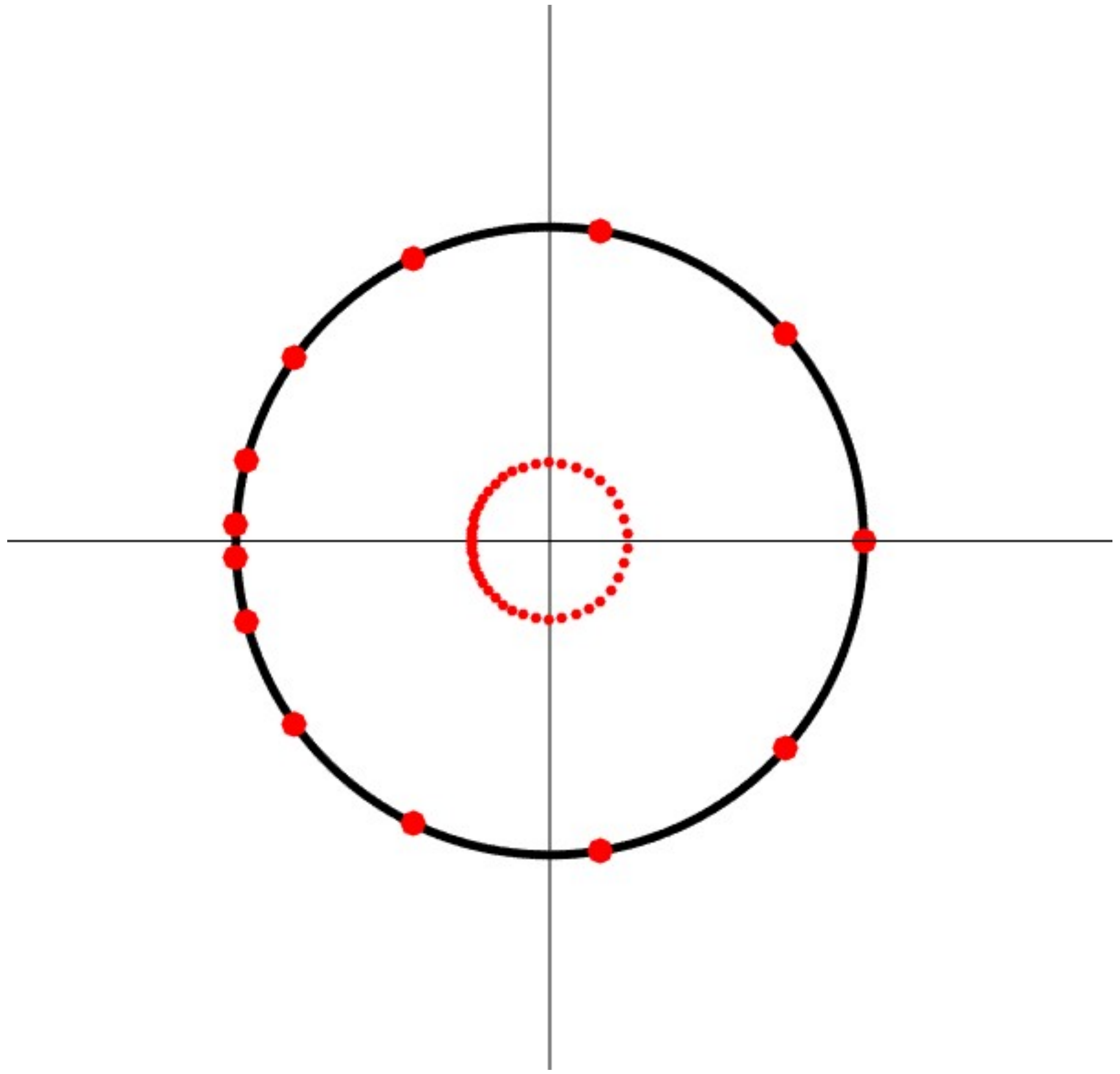
... and this is what I get!





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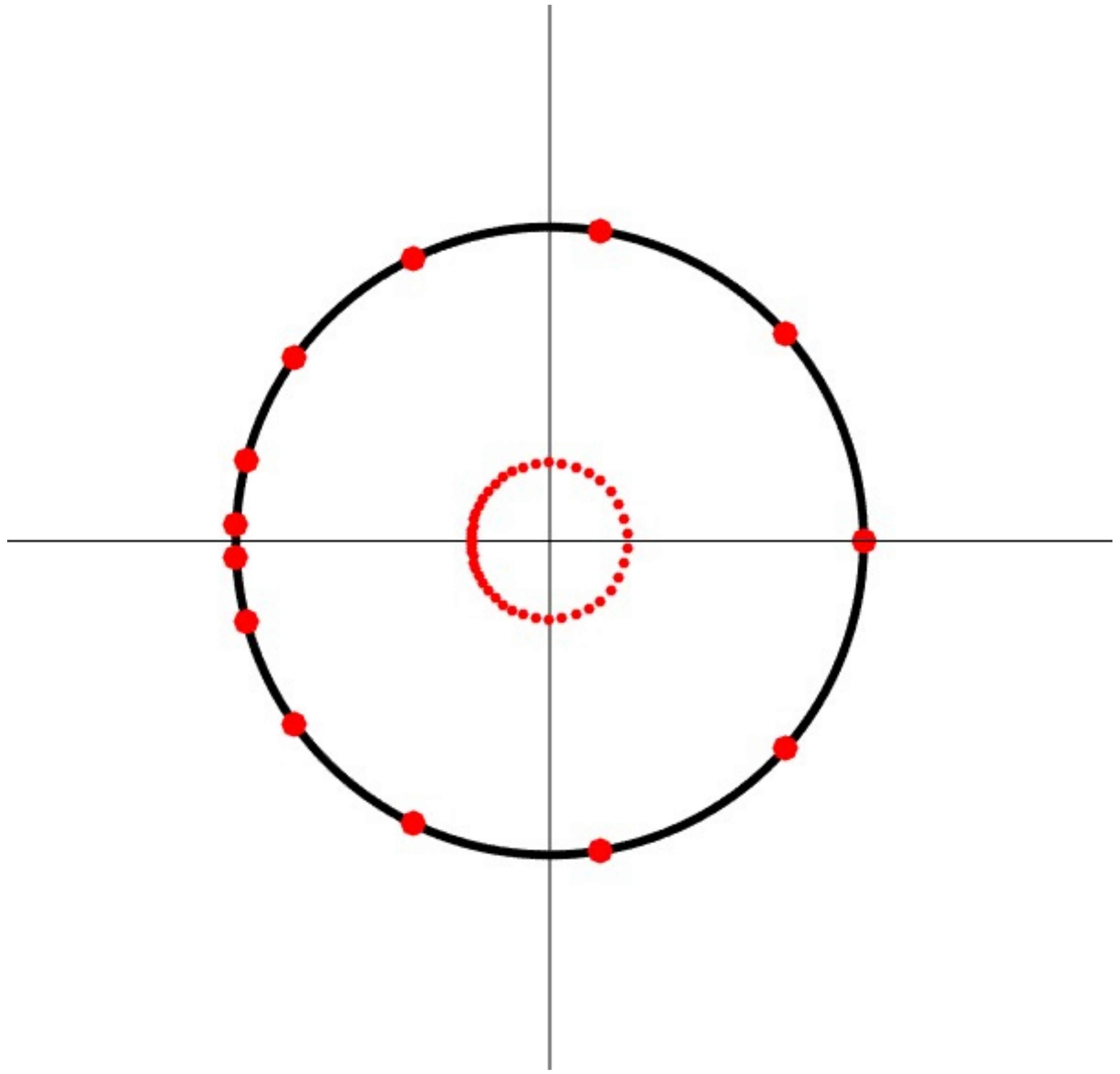

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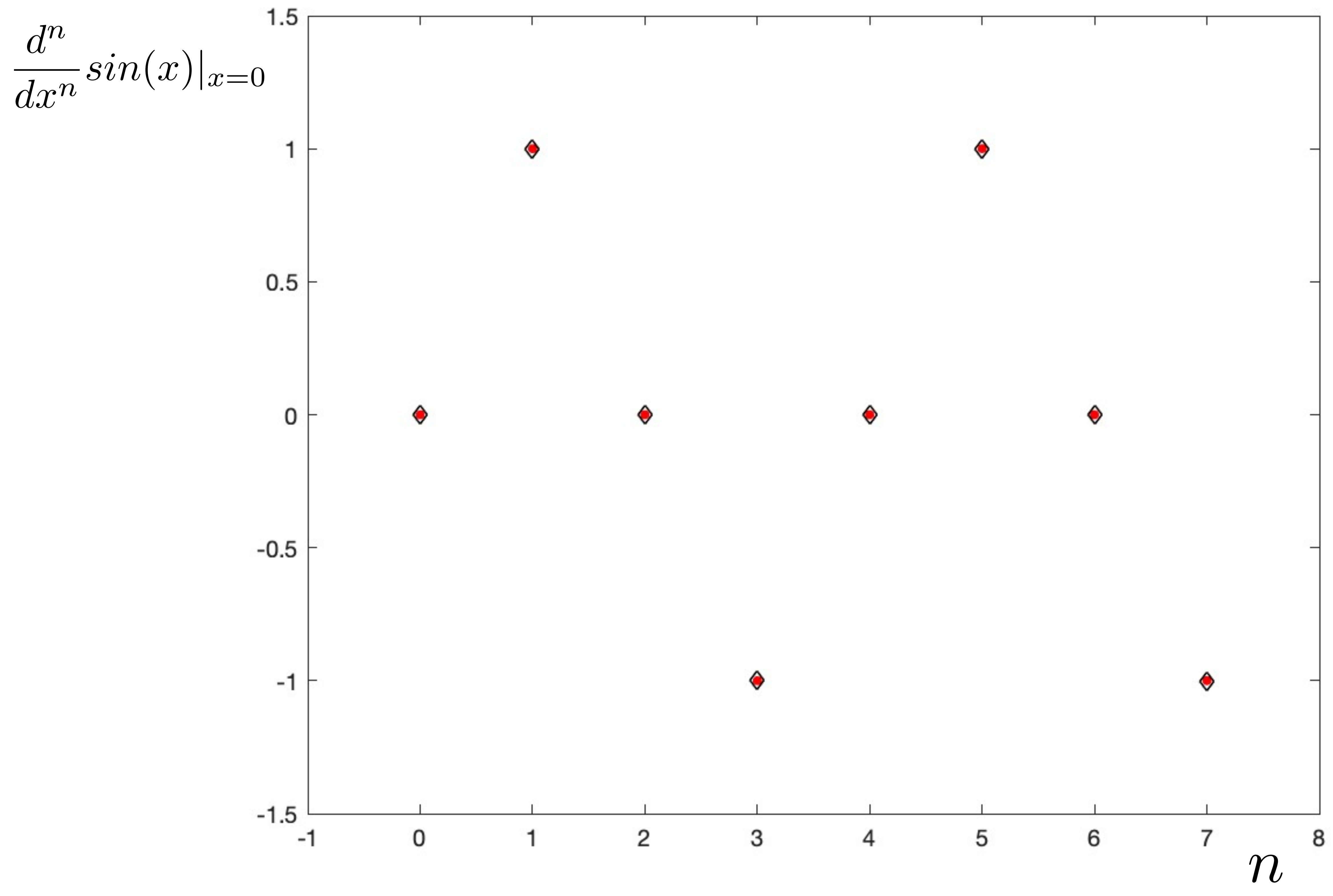

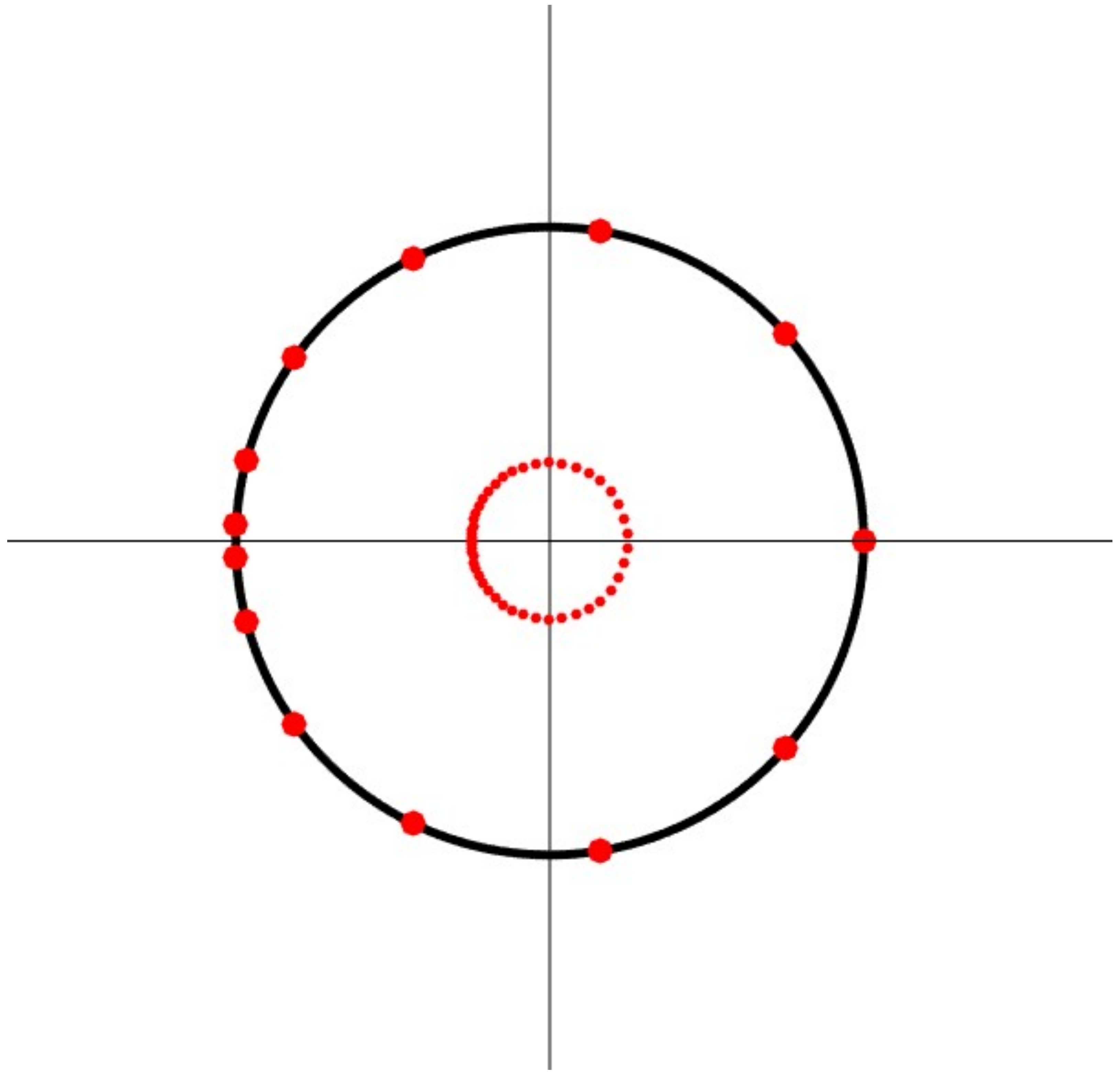

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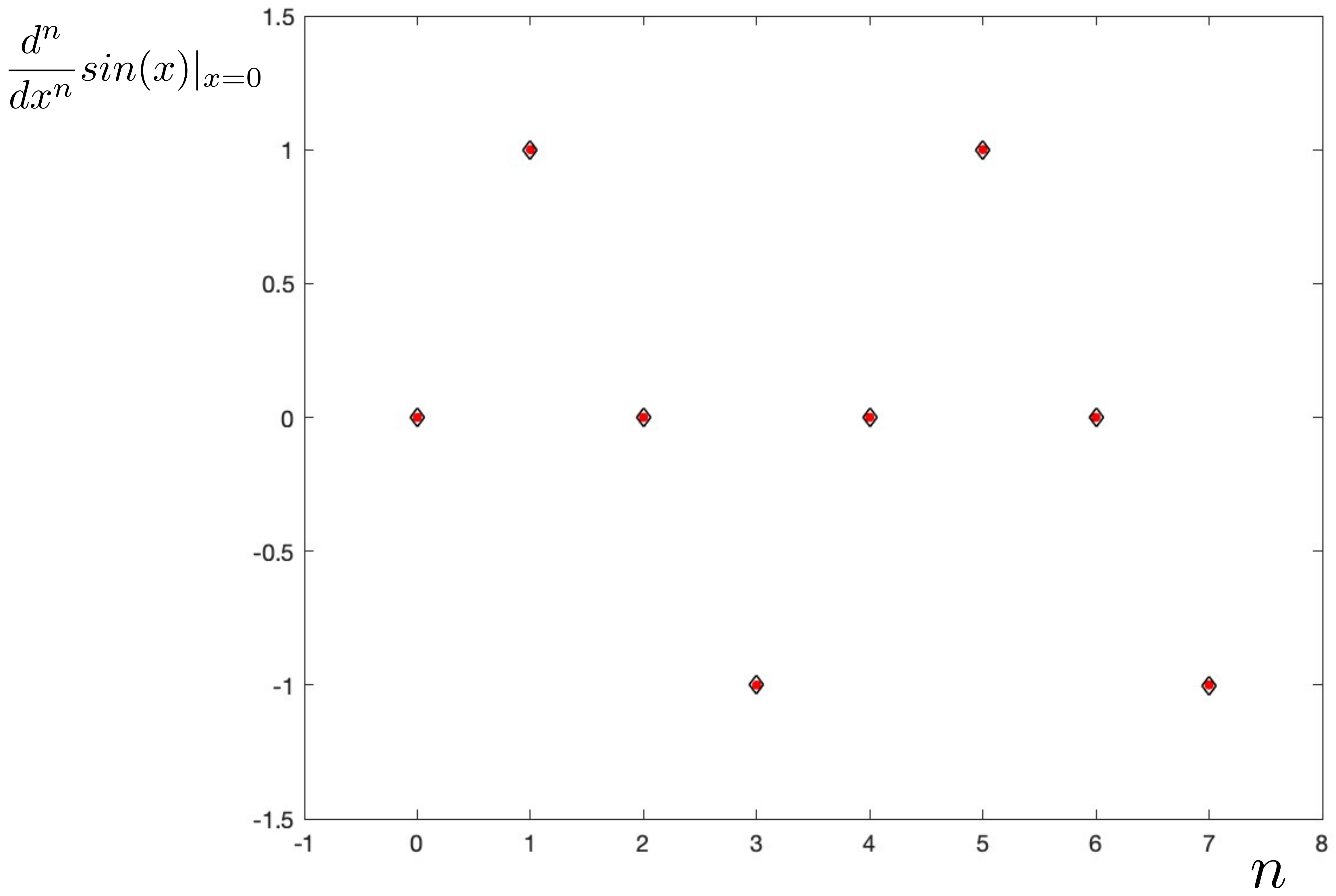
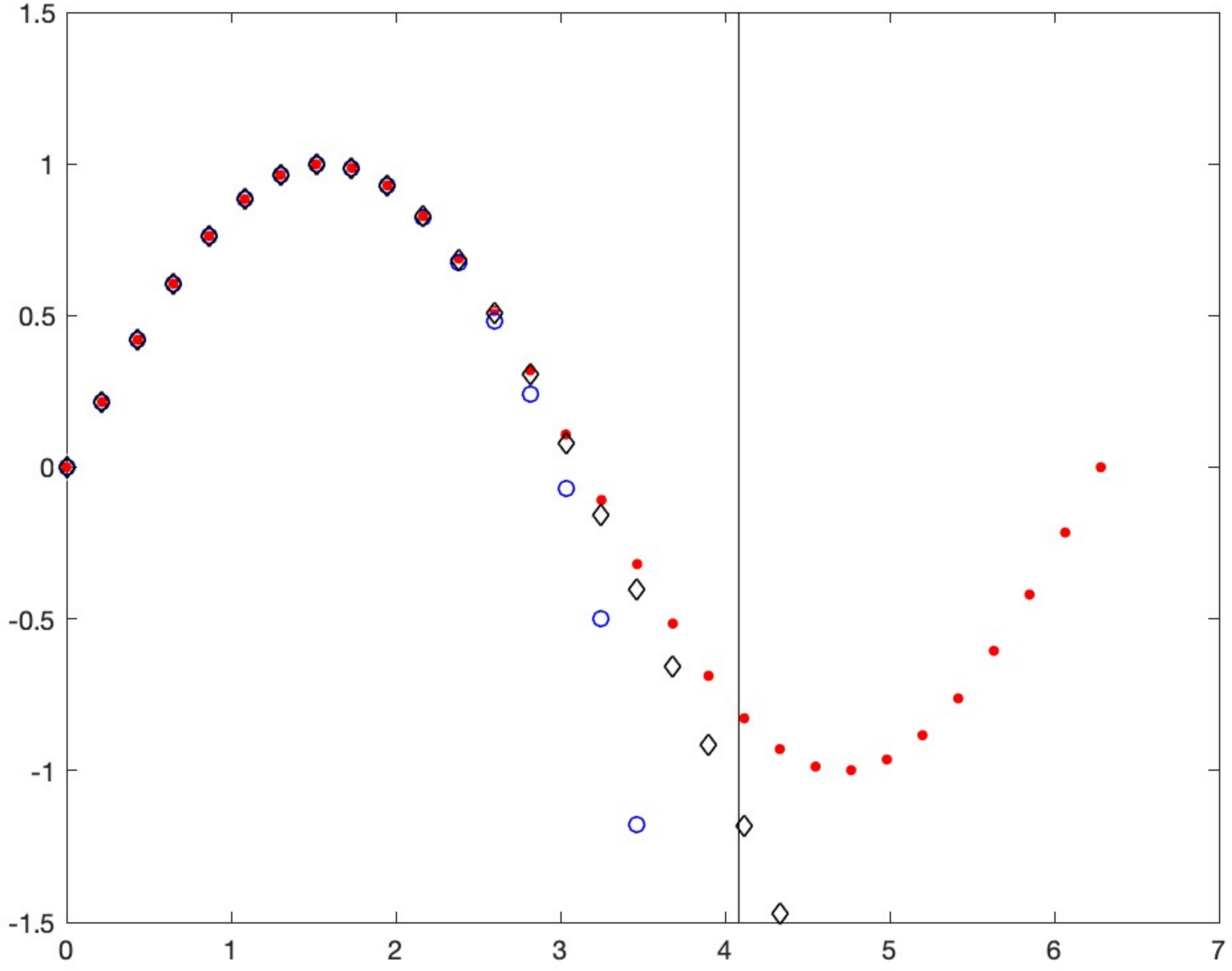


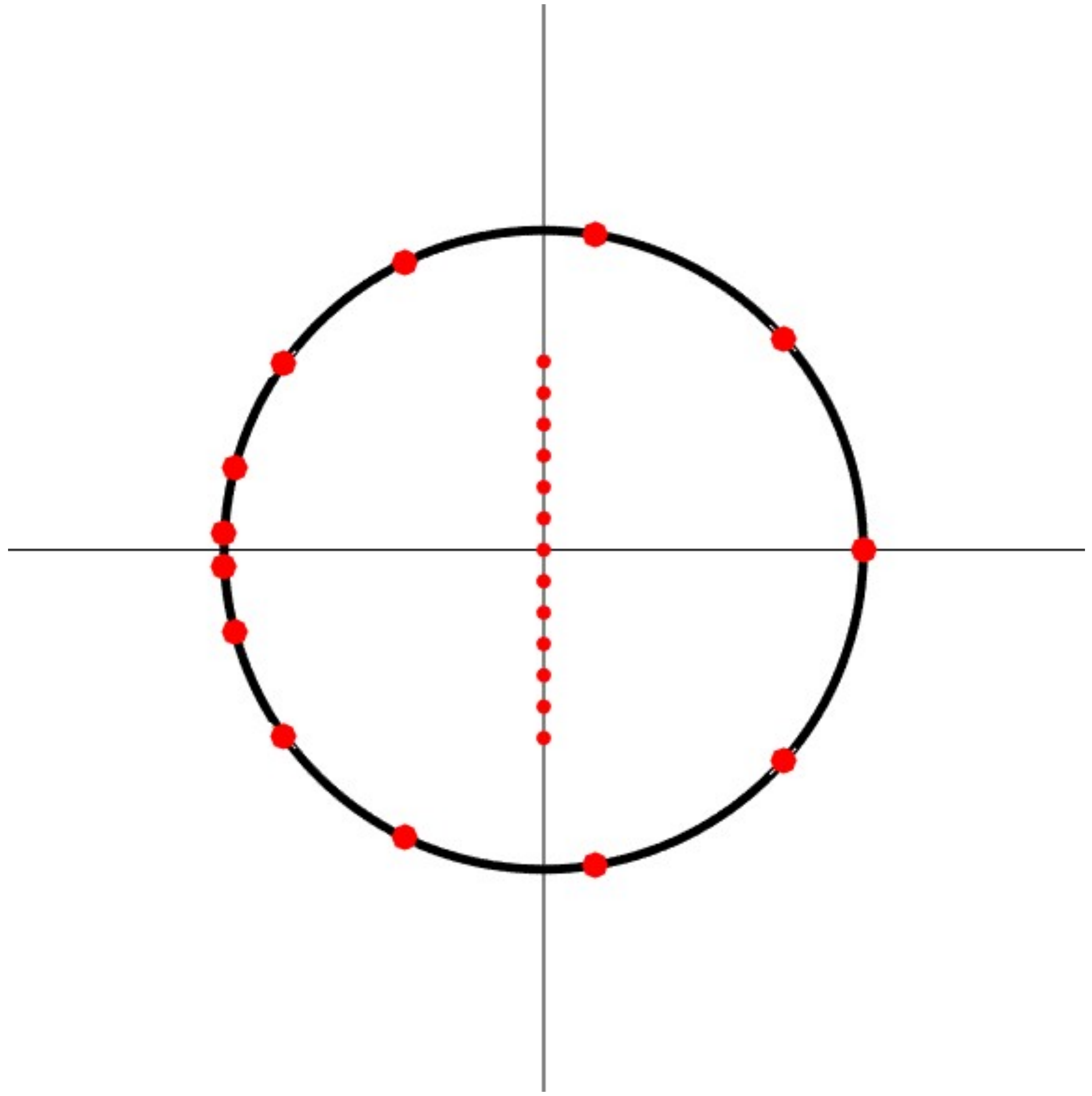
...but here comes the point! This is exactly the same result I get if I directly use our original effective quadrature! ... so, everything is consistent!

Finally, this is our computation of the *sin* function via our inverse problem (i.e., we started on the imaginary axis and we got values on the real axis)

A final comment: the values we get via Taylor expansion in zero (diamonds) are more accurate than the direct computation for increasing values of x (*not surprisingly…*)



Let's summarise ...



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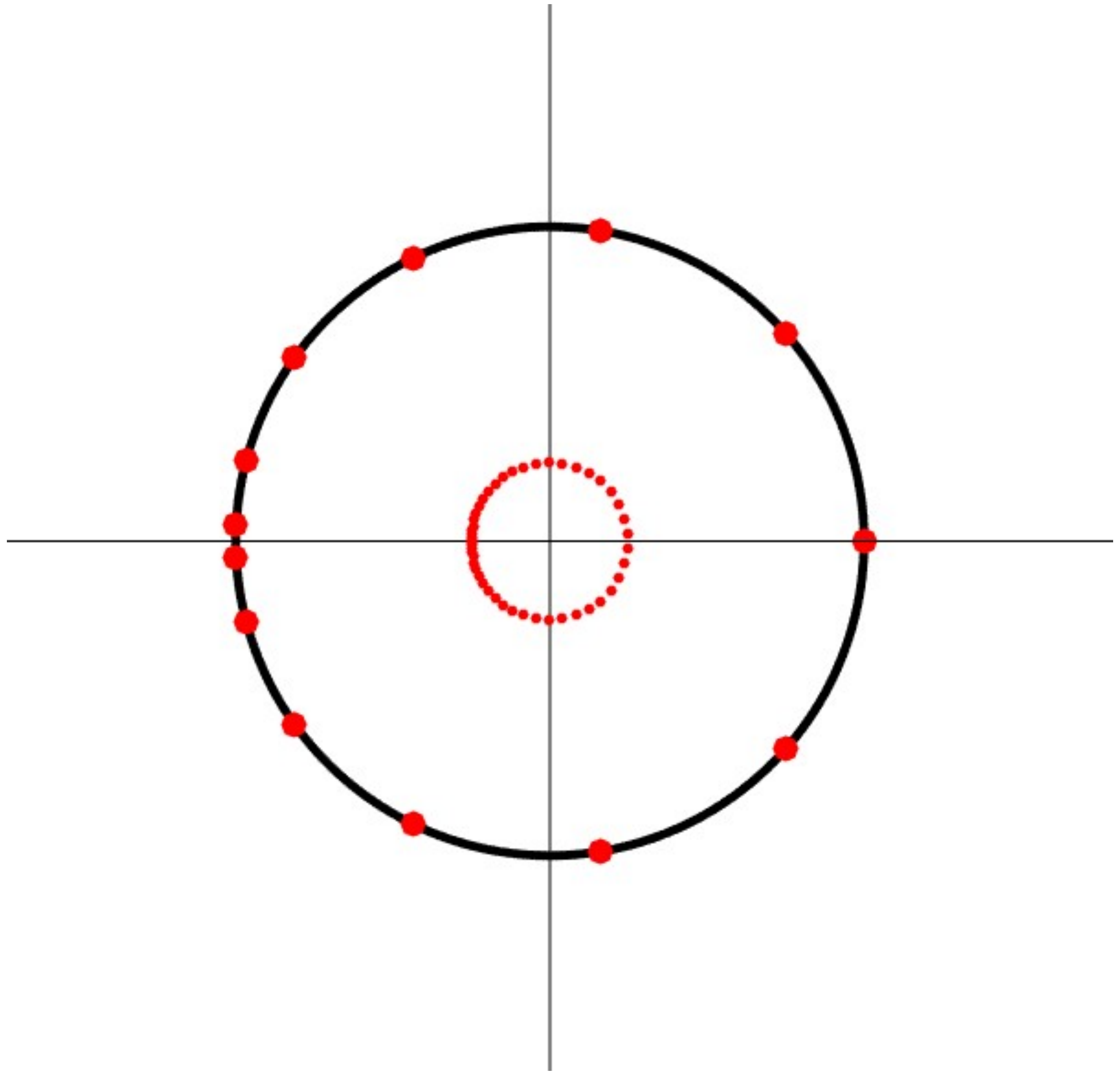

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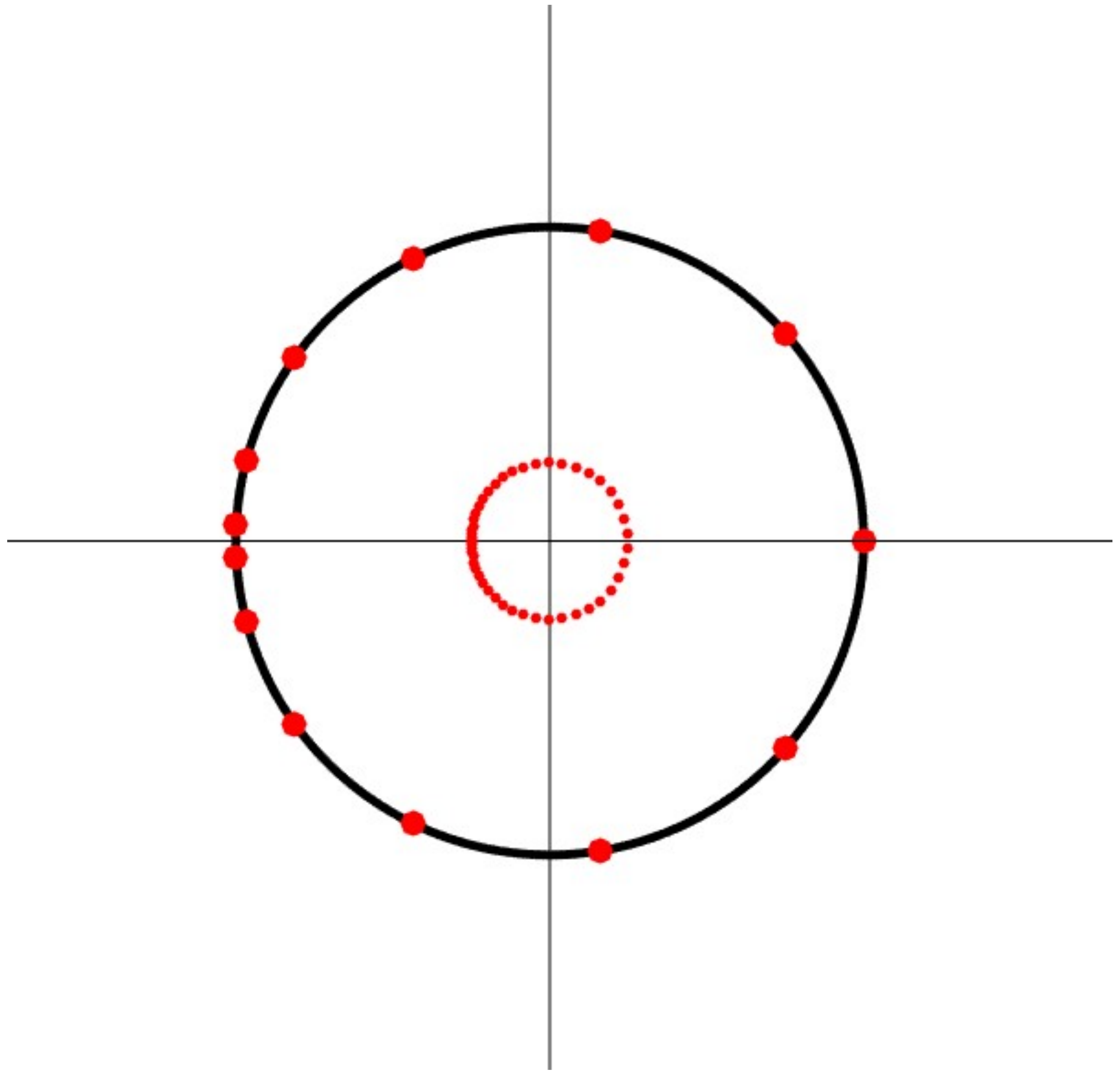

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Intermezzo: we can play the same game for inverse Laplace transform ...

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

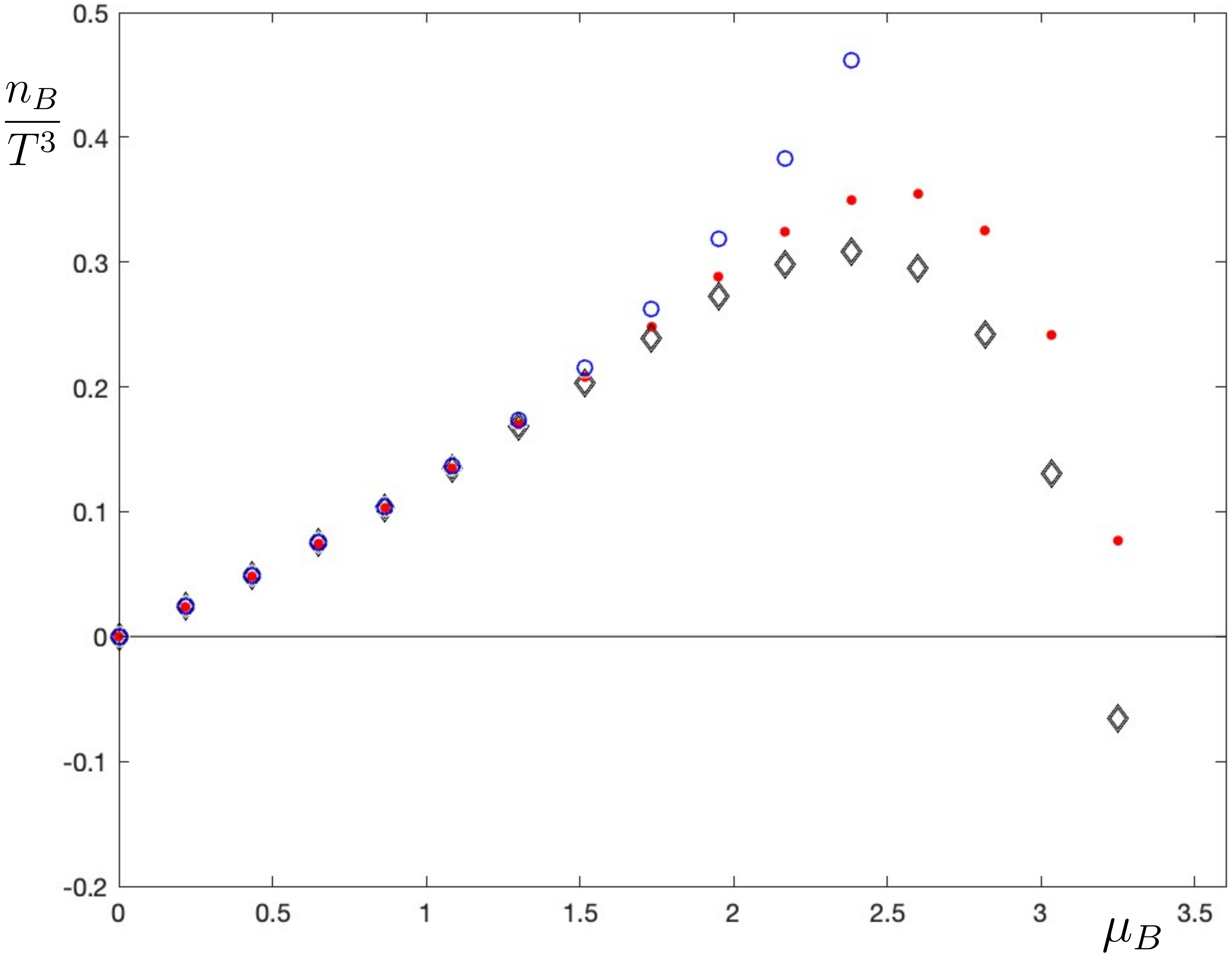
$$f(s) = \int_0^\infty e^{-t}\, e^{-t(s-1)}\, F(t)\, dt \;\sim\; \sum_j w_j\, e^{-t_j(s-1)}\, F(t_j)$$

This time, Laguerre quadratures ...

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

What about finite density QCD as an inverse problem?

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



What about finite density QCD as an inverse problem?

CAVEAT: no error shown … once again, here we are mainly concerned with *trends*,,, (possible scenarios) FIXED CUTOFF!

Conclusions and prospects

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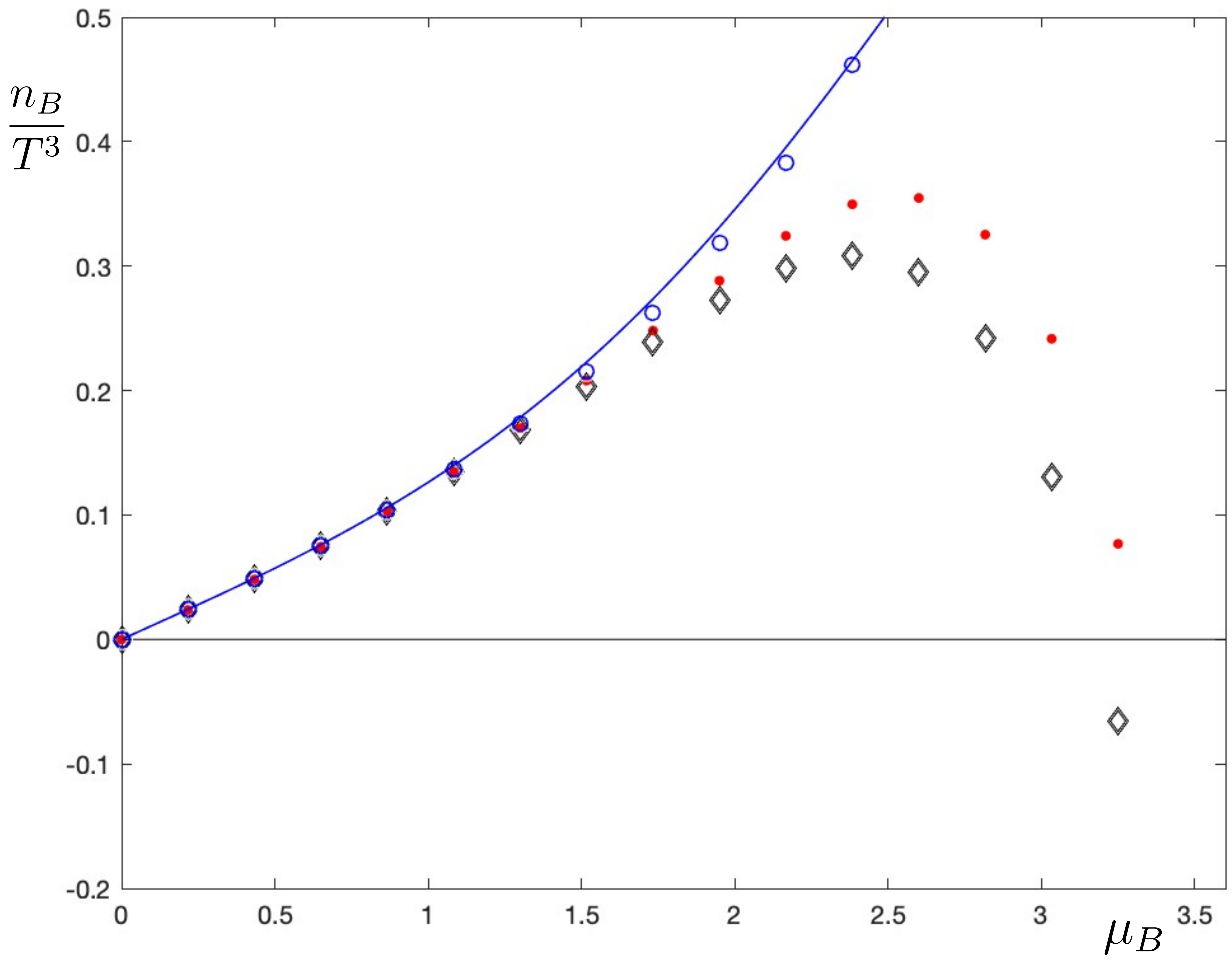

What about finite density QCD as an inverse problem?

We can compare to our Padé analytic continuation.

We have a lot of work in front of us (in particular playing around with consistency checks like the ones we had before).

One interesting thing: indeed we have to test (to some extent *rule out?*) different scenarios

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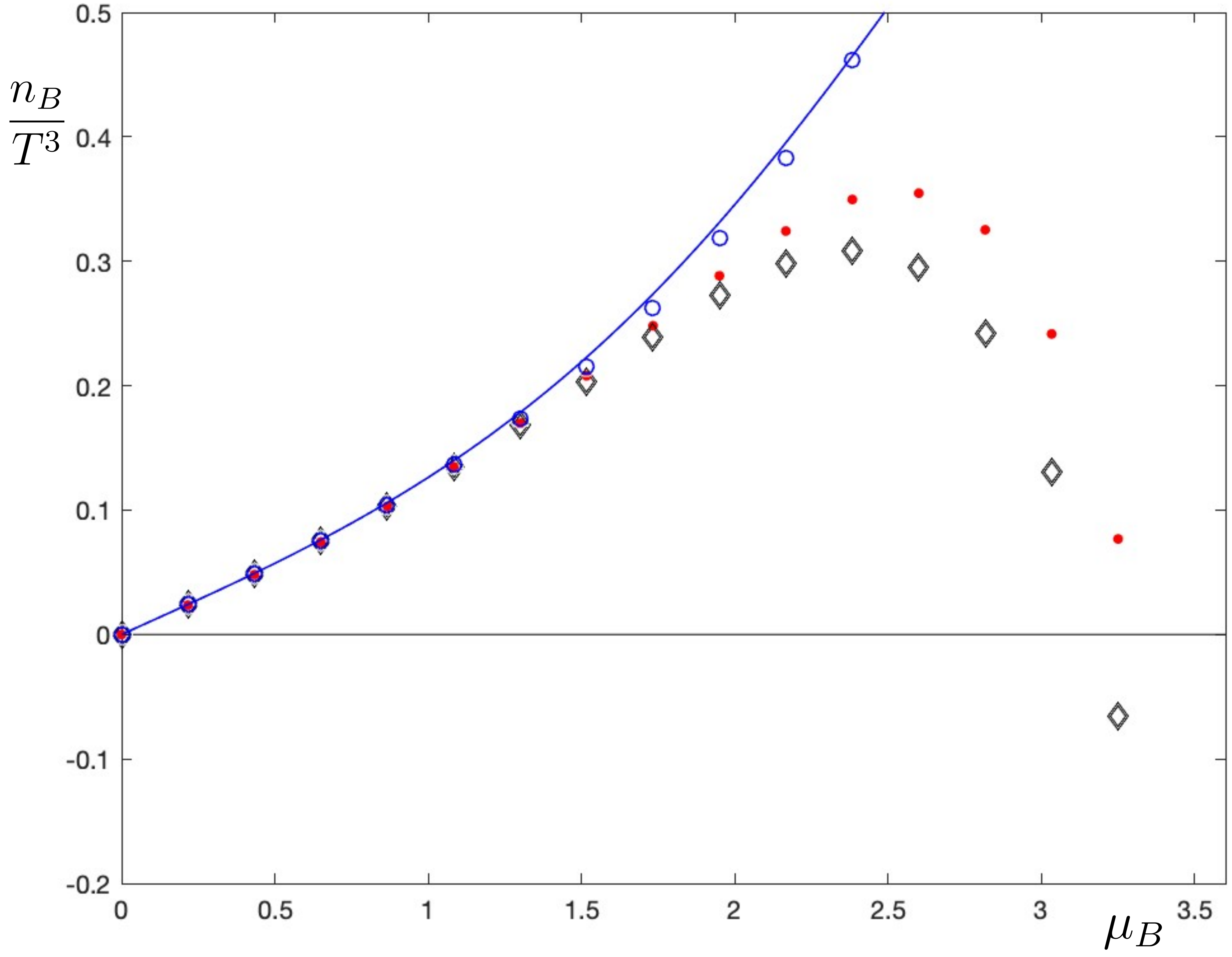

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And remember: other applications possible ...

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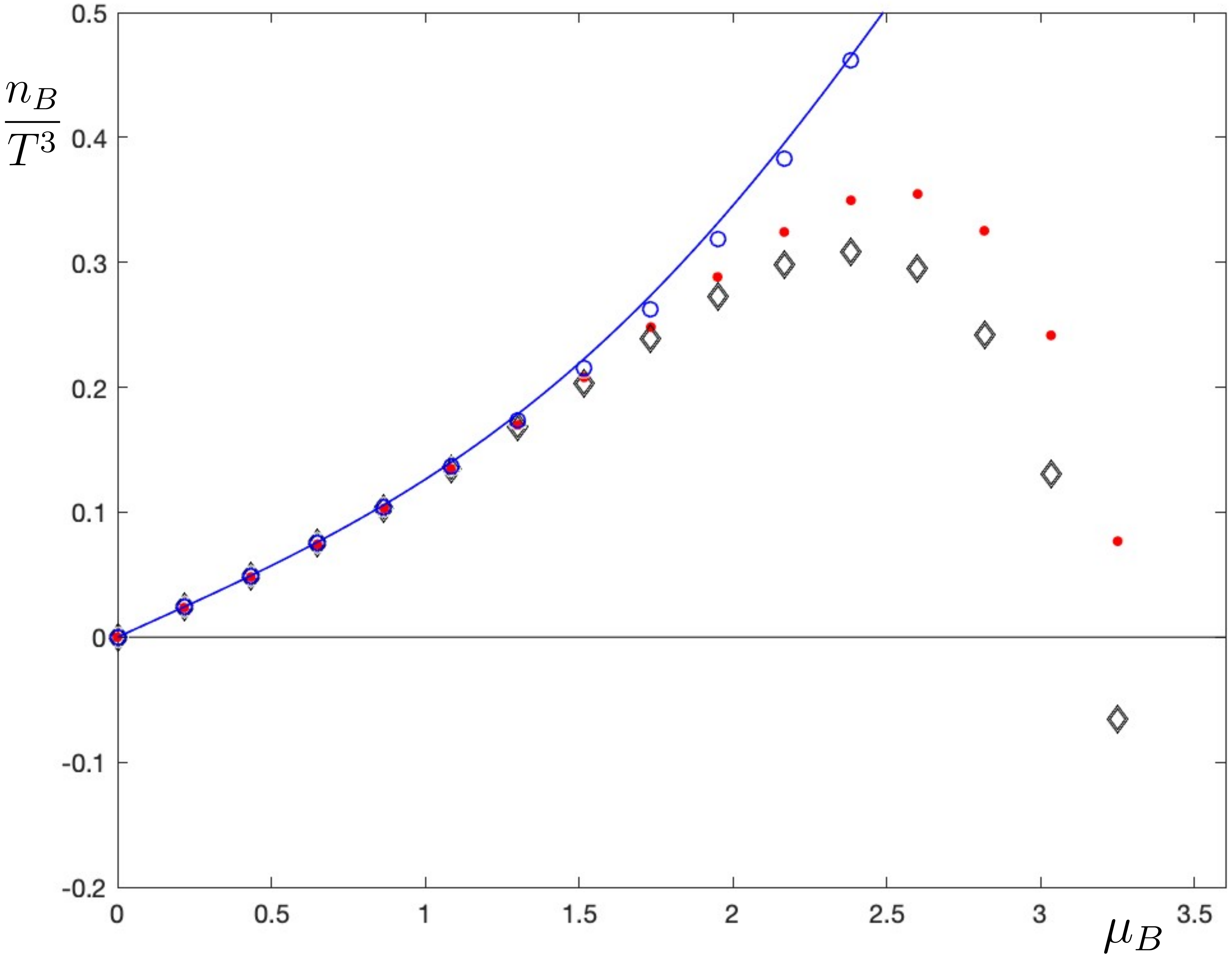

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