Notes on the extended grid

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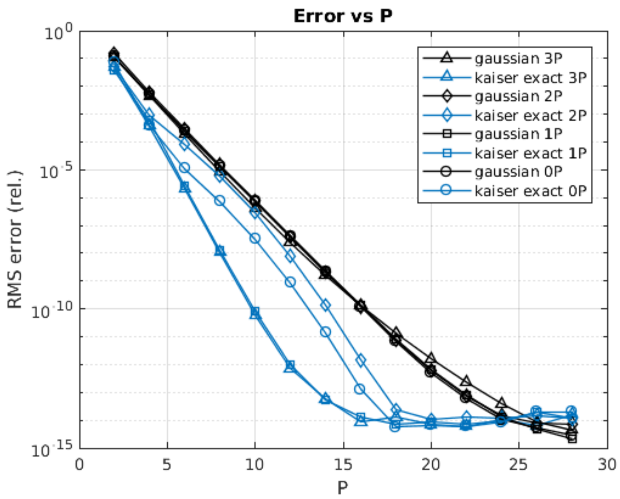
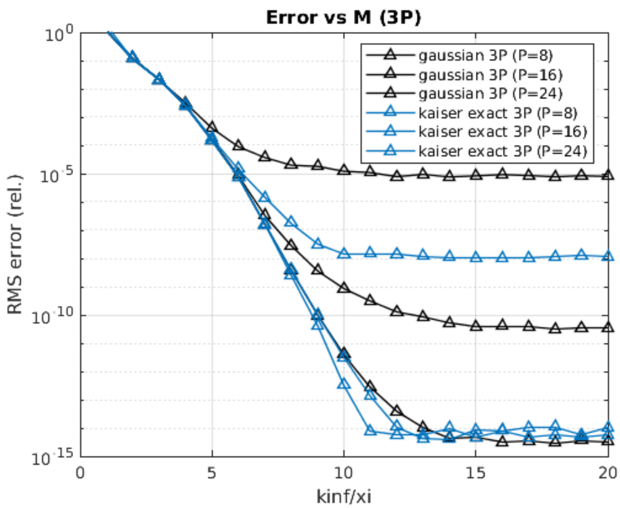
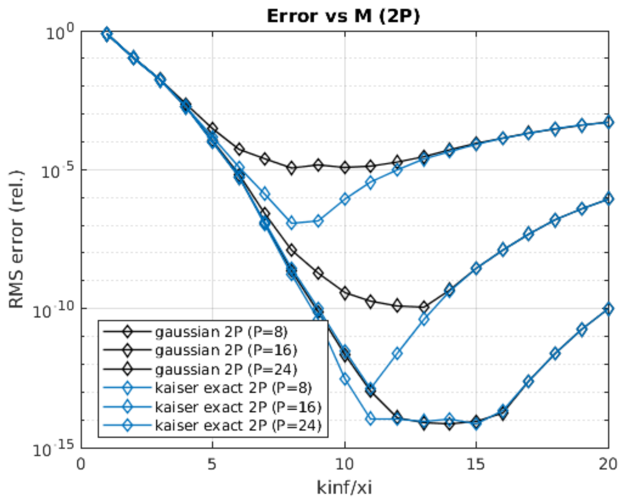
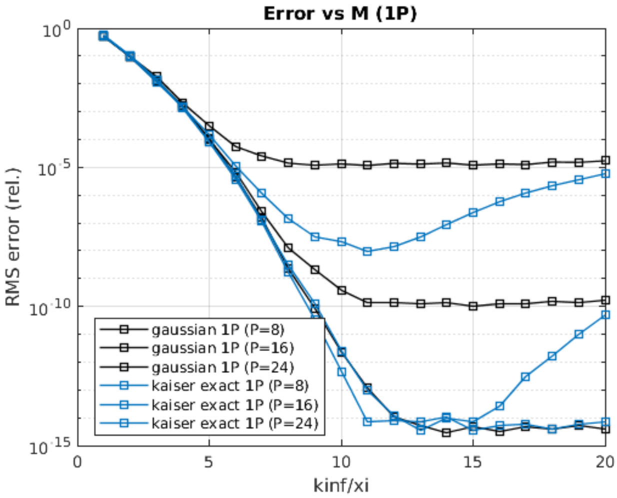
1 Baseline case

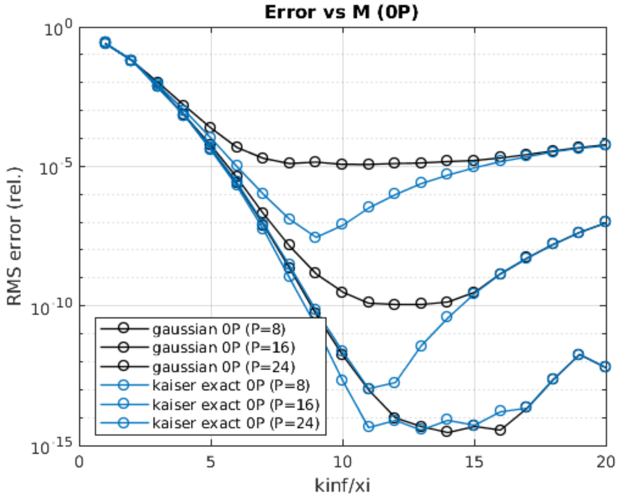
Plots produced by `../comp_fig5.m` and `../comp_figT1.m`, using 100 source particles in a cube of side length $L = 1$. For other parameters, see the scripts. In this baseline case, the grid size M is increased by P (the number of points in the window function's support) in the nonperiodic directions (this is needed to fit the window function without clipping or wrapping), and the side length is also increased to keep $h = L/M$ constant across all three directions.











Following Lindbo & Tornberg (2011),[1] we introduce the integer wavenumber $\kappa \in \{-M/2, \ldots, 0, \ldots, M/2\}$ and the scaled wavenumber $k = 2\pi\kappa/L$. The largest integer wavenumber is denoted by $\kappa_\infty = M/2$, and the corresponding k is $k_\infty = 2\pi(M/2)/L = \pi M/L$. In the first plot (Error vs P), ξ is selected as $\xi = \pi(M/L)/12$, which means that $k_\infty/\xi = 12$ in that plot. For smaller values of P, this is to the right of the "sweet spot" in 2P (third plot) and 0P (fifth plot). For some reason the error increase with k_∞/ξ is slower in 1P (fourth plot) than in 2P and 0P.

The reason that the error increases with k_∞/ξ when nonperiodic directions are present is explained in af Klinteberg, Saffar Shamshirgar, Tornberg (2017), section 5.3. For the Gaussian window function, this can be understood as the Gaussian $e^{-\xi^2 r^2/(1-\eta)}$ needing to be properly truncated when $\eta < 1$ (which is always the case in the first plot).[2]

2 The 0P fix

In af Klinteberg, Saffar Shamshirgar, Tornberg (2017), the suggested fix is to extend the box by

$$\delta_L = \begin{cases} hP & \text{if } \eta \geq 1, \\ \max(hP, \sqrt{2(1-\eta)m^2/\xi^2}) & \text{if } \eta < 1, \end{cases}$$

where $m = C\sqrt{\pi P}$ (where $C = 0.976$ in the 0P Stokes paper), i.e. $\tilde{L} = L + \delta_L$ is the side length of the extended box. This strategy is used for the Gaussian window in 0P electrostatics in the current code. For the Kaiser windows, we instead use

$$\delta_L = \max(hP, \sqrt{8(\beta/P)/\xi^2}),$$

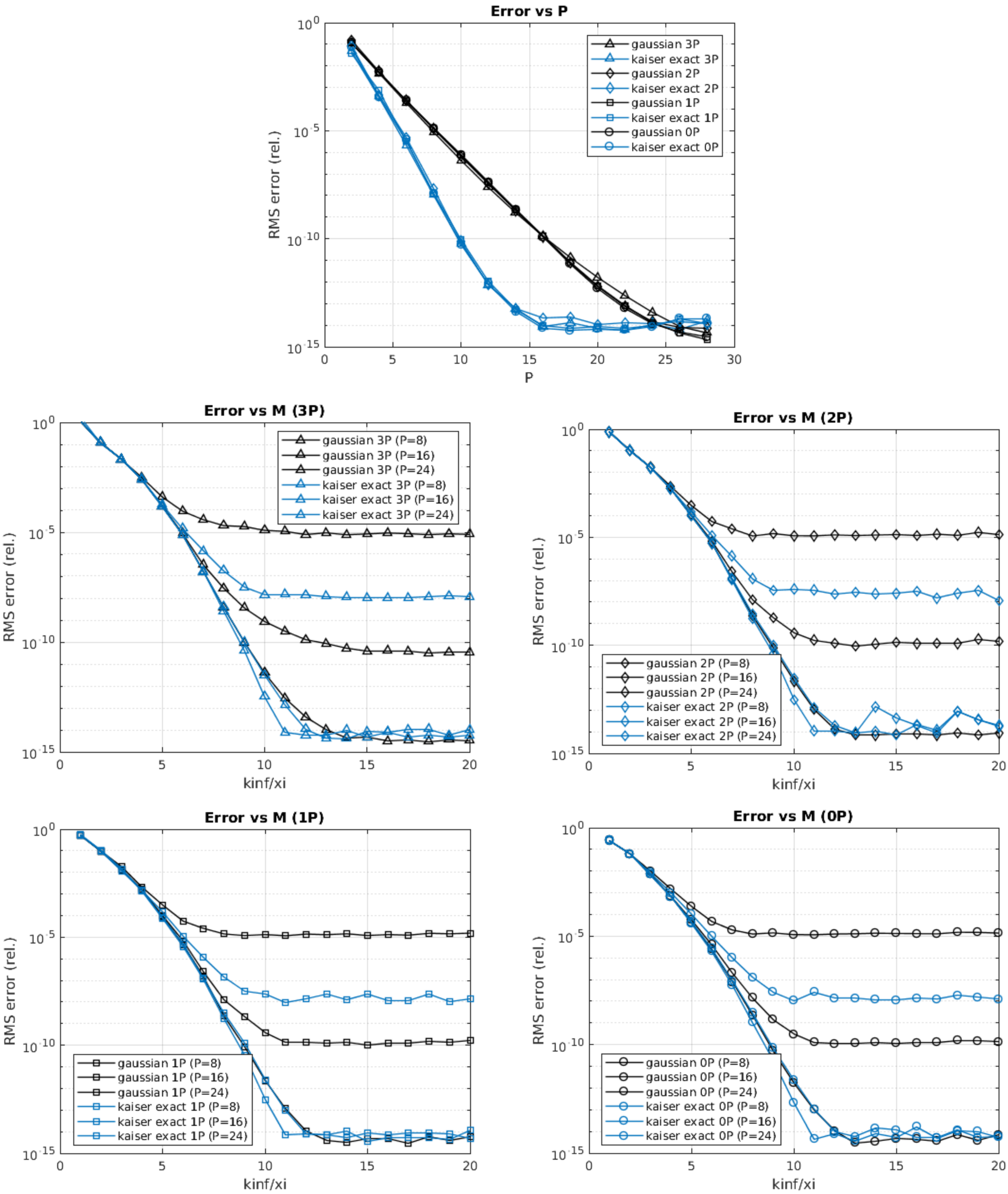
and since $\beta/P = 2.5$, this is actually $\delta_L = \max(hP, \sqrt{20}/\xi)$.

As can be seen in the plots below, these selections completely flatten the error curves (in plots 2–5) so that the error no longer grows with k_∞/ξ. Of course, δ_L is rounded up so that $\delta_M = \delta_L/h$ becomes an (even) integer, where $\tilde{M} = M + \delta_M$. We introduce

$$\begin{aligned} \delta_{M,\text{rem,Gauss}} &= 2 \times \text{ceil}(\sqrt{2(1-\eta)m^2/\xi^2}/(2h)), \\ \delta_{M,\text{rem,Kaiser}} &= 2 \times \text{ceil}(\sqrt{8(\beta/P)/\xi^2}/(2h)). \end{aligned}$$

[1] However, here M is the number of subintervals and is therefore even. (In the Lindbo & Tornberg paper, the same letter was used to denote number of grid points, which is odd.)

[2] The reason the error grows with k_∞/ξ is probably that the extension that we do, i.e. adding hP to the side length and P to the grid size, becomes more and more insufficient as h decreases.


Error vs P
RMS error (rel.)
P
gaussian 3P
kaiser exact 3P
gaussian 2P
kaiser exact 2P
gaussian 1P
kaiser exact 1P
gaussian 0P
kaiser exact 0P
Error vs M (3P)
gaussian 3P (P=8)
gaussian 3P (P=16)
gaussian 3P (P=24)
kaiser exact 3P (P=8)
kaiser exact 3P (P=16)
kaiser exact 3P (P=24)
kinf/xi
Error vs M (2P)
gaussian 2P (P=8)
gaussian 2P (P=16)
gaussian 2P (P=24)
kaiser exact 2P (P=8)
kaiser exact 2P (P=16)
kaiser exact 2P (P=24)
Error vs M (1P)
gaussian 1P (P=8)
gaussian 1P (P=16)
gaussian 1P (P=24)
kaiser exact 1P (P=8)
kaiser exact 1P (P=16)
kaiser exact 1P (P=24)
Error vs M (0P)
gaussian 0P (P=8)
gaussian 0P (P=16)
gaussian 0P (P=24)
kaiser exact 0P (P=8)
kaiser exact 0P (P=16)
kaiser exact 0P (P=24)

The following table shows $\delta_{M,\text{rem,Gauss}}$ and $\delta_{M,\text{rem,Kaiser}}$ as functions of P, for the setting in the first plot (Error vs P), where $M = 28$. This data is the same for all periodicities (but not applicable to 3P of course).

P	$\delta_{M,\text{rem,Gauss}}$	$\delta_{M,\text{rem,Kaiser}}$
2	14	18
4	18	18
6	22	18
8	24	18
10	26	18
12	28	18
14	28	18
16	30	18
18	30	18
20	30	18
22	30	18
24	30	18
26	28	18
28	28	18

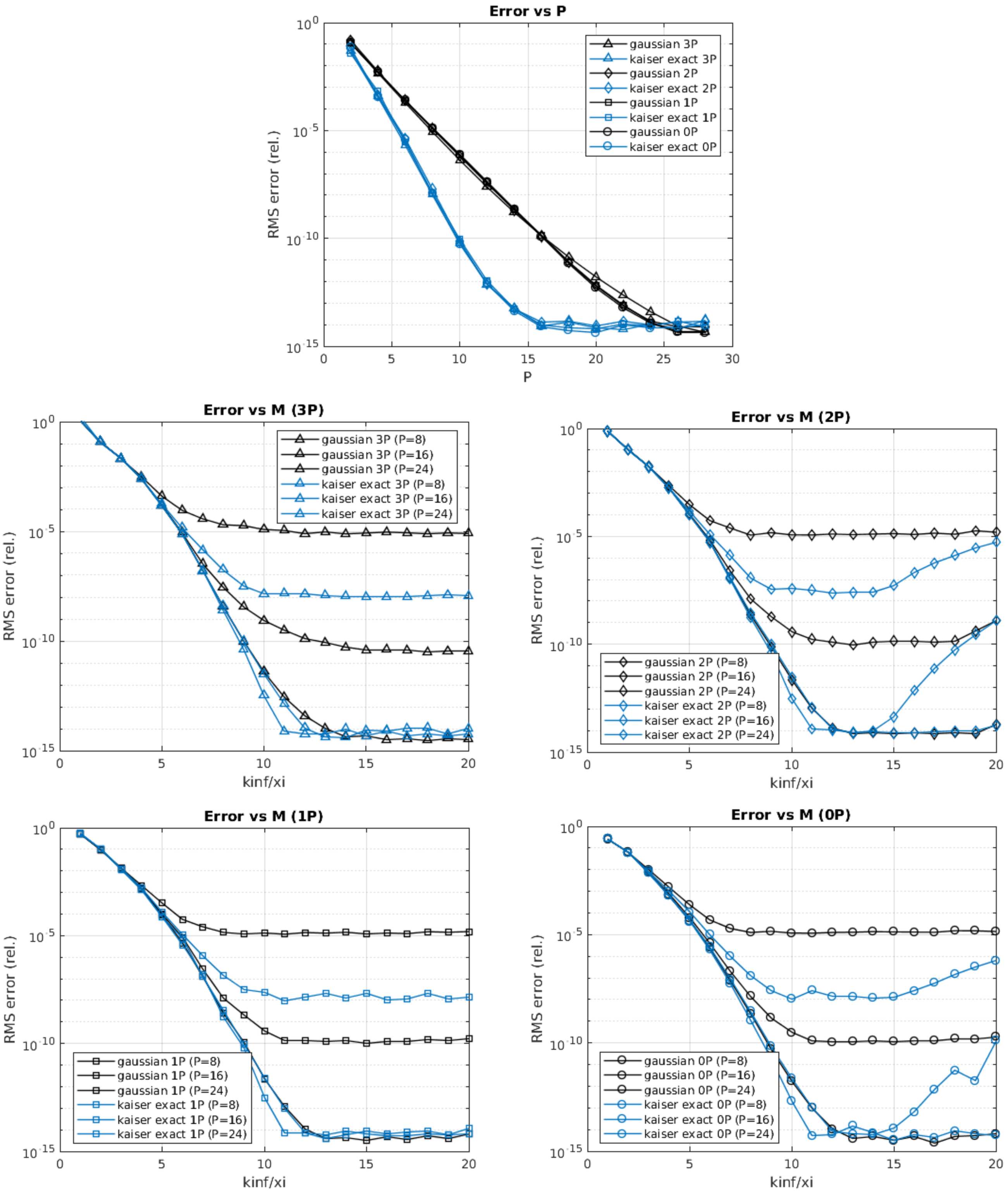
Note that $\delta_M = \max(P, \delta_{M,\text{rem}})$ for each window function. This means that the actual choices are as follows.

P	δ_M (Gauss)	δ_M (Kaiser)	$\tilde{M}$ (Gauss)	$\tilde{M}$ (Kaiser)	$\tilde{M}/M$ (Gauss)	$\tilde{M}/M$ (Kaiser)
2	14	18	42	46	1.5000	1.6429
4	18	18	46	46	1.6429	1.6429
6	22	18	50	46	1.7857	1.6429
8	24	18	52	46	1.8571	1.6429
10	26	18	54	46	1.9286	1.6429
12	28	18	56	46	2.0000	1.6429
14	28	18	56	46	2.0000	1.6429
16	30	18	58	46	2.0714	1.6429
18	30	18	58	46	2.0714	1.6429
20	30	20	58	48	2.0714	1.7143
22	30	22	58	50	2.0714	1.7857
24	30	24	58	52	2.0714	1.8571
26	28	26	56	54	2.0000	1.9286
28	28	28	56	56	2.0000	2.0000

Note that neither $\delta_{M,\text{rem,Gauss}}$ nor $\delta_{M,\text{rem,Kaiser}}$ changes when M/L changes (assuming $\xi \sim M/L$); they are functions only of P ($\delta_{M,\text{rem,Kaiser}}$ is even constant). This means that δ_M itself is a function only of P, not of M or anything else.

3 The 2P fix

The 2P fix is to always increase M by $P + 6$ in the nonperiodic directions, which corresponds to $\delta_M = P + 6$. This does not seem completely unreasonable in principle given that we observed above that δ_M is a function only of P in the 0P fix. The result is shown in the plots below. In the 1P case, this seems to be enough to completely flatten the curves, while in 2P and 0P it flattens the curves somewhat – enough to make the first plot look good (at $k_\infty/\xi = 12$).


Error vs P
RMS error (rel.)
P
gaussian 3P
kaiser exact 3P
gaussian 2P
kaiser exact 2P
gaussian 1P
kaiser exact 1P
gaussian 0P
kaiser exact 0P
Error vs M (3P)
gaussian 3P (P=8)
gaussian 3P (P=16)
gaussian 3P (P=24)
kaiser exact 3P (P=8)
kaiser exact 3P (P=16)
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kinf/xi
Error vs M (2P)
gaussian 2P (P=8)
gaussian 2P (P=16)
gaussian 2P (P=24)
kaiser exact 2P (P=8)
kaiser exact 2P (P=16)
kaiser exact 2P (P=24)
Error vs M (1P)
gaussian 1P (P=8)
gaussian 1P (P=16)
gaussian 1P (P=24)
kaiser exact 1P (P=8)
kaiser exact 1P (P=16)
kaiser exact 1P (P=24)
Error vs M (0P)
gaussian 0P (P=8)
gaussian 0P (P=16)
gaussian 0P (P=24)
kaiser exact 0P (P=8)
kaiser exact 0P (P=16)
kaiser exact 0P (P=24)

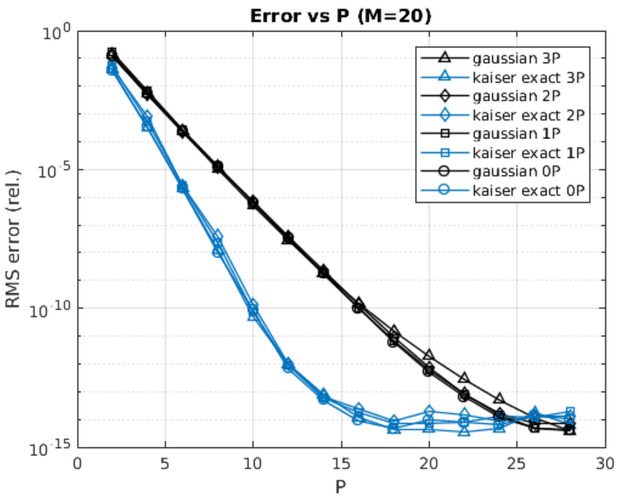
With $\delta_M = P + 6$, the choices look like this, independent of window function.

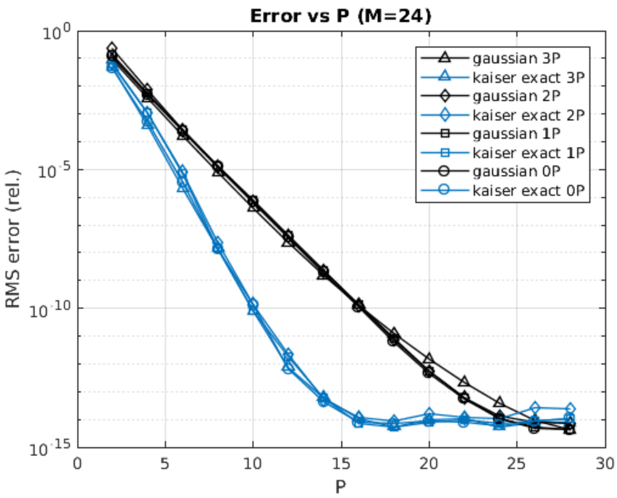
P	δ_M	$\tilde{M}$	$\tilde{M}/M$
2	8	36	1.2857
4	10	38	1.3571
6	12	40	1.4286
8	14	42	1.5000
10	16	44	1.5714
12	18	46	1.6429
14	20	48	1.7143
16	22	50	1.7857
18	24	52	1.8571
20	26	54	1.9286
22	28	56	2.0000
24	30	58	2.0714
26	32	60	2.1429
28	34	62	2.2143

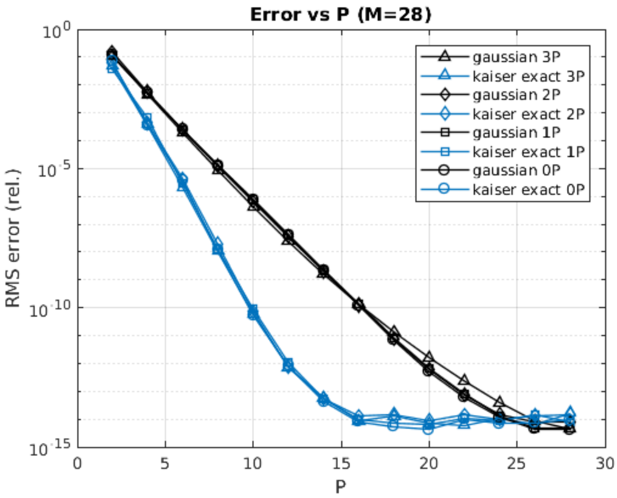
In this situation, the 2P fix results in a smaller δ_M than the 0P fix for $P < 24$ for the Gaussian window, and for $P < 12$ for the Kaiser window. Since both fixes seem to be working, one could simply pick the one with the smallest δ_M for a given P.

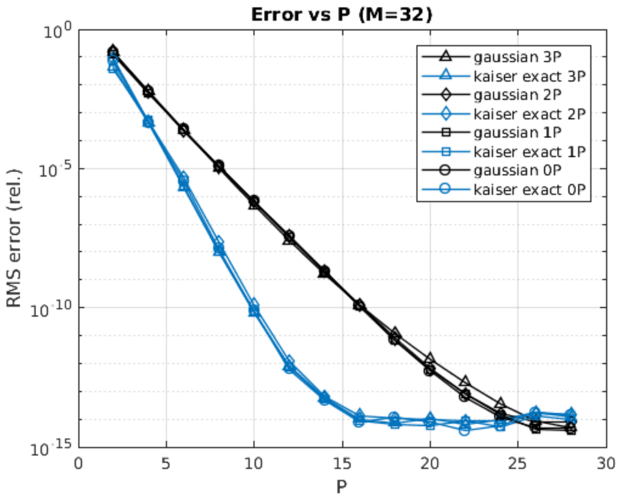
4 Variations

As the plots below show, the 2P fix ($\delta_M = P + 6$) seems to work for different original grid sizes (here tested with $M = 20, 24, 28, 32$), i.e. there is no strong dependence on M.

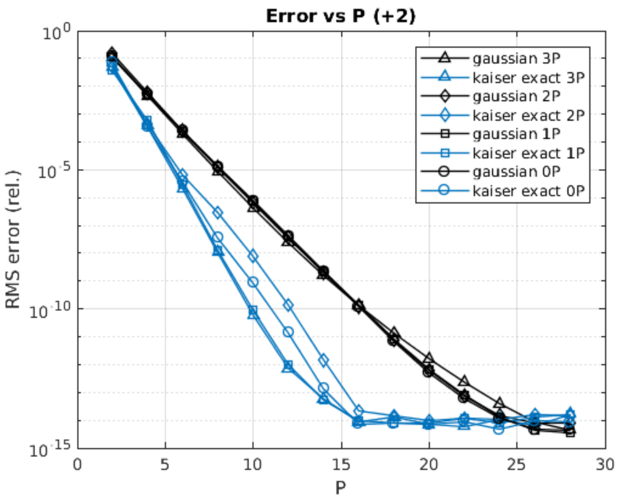


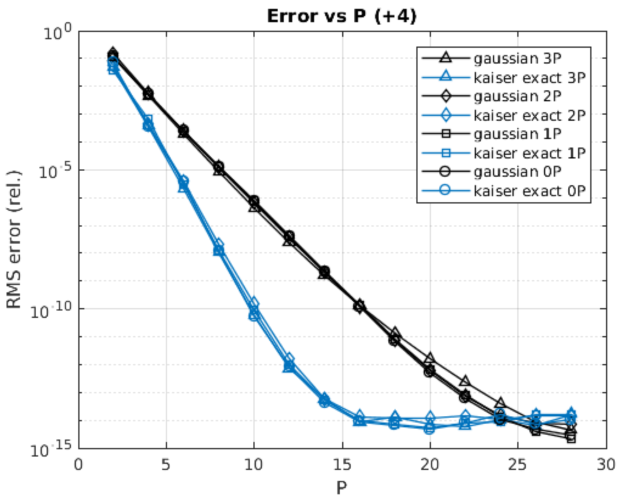


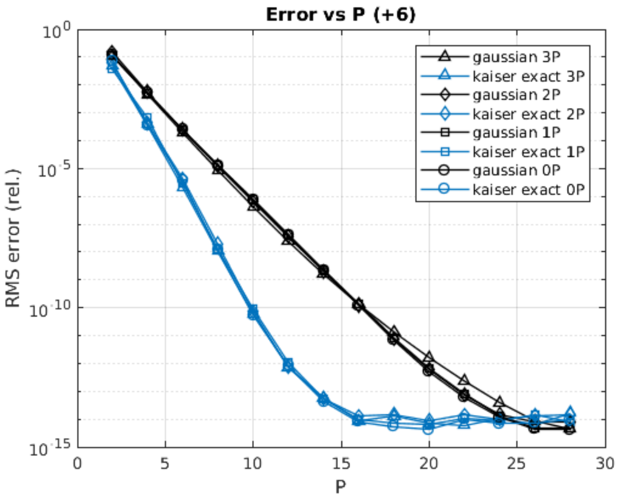


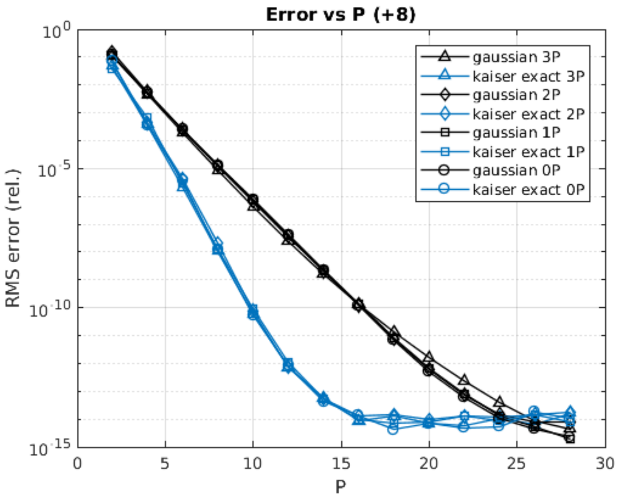


Next, we try different variants on the 2P fix, namely $\delta_M = P+2, P+4, P+6$ and $P+8$. It seems one could get away with $P+4$, but $P+6$ takes down the Kaiser 2P curve a bit more (compare for example at $P = 10$).









While $P+6$ seems optimal for the 2P case, it seems $P+4$ is enough for the 0P case, and in the 1P case it is sufficient to add only P.

5 The more complicated relation

Above, we used the simple relation

$$\xi = \frac{\pi}{12}\frac{M}{L}, \tag{1}$$

which is probably what we want to use when producing the Error-vs-P plots. However, in other circumstances, we like to use the more complicated relation

$$\frac{M}{L} = \frac{\sqrt{3}\xi}{\pi}\sqrt{W\left(\frac{4Q^{2/3}}{3L^2(\pi\xi\varepsilon_*^2)^{2/3}}\right)}, \tag{2}$$

where W is the Lambert W function and ε_* is an error tolerance (and $Q = \sum_{n=1}^{N} q_n^2$). This relation can also be inverted (i.e. solved for ξ), which yields

$$\xi = \frac{\pi}{\sqrt{2}}\frac{M}{L}\frac{1}{\sqrt{W\left(\frac{4Q}{\pi^2 L^2 \varepsilon_*^2 M}\right)}}. \tag{3}$$

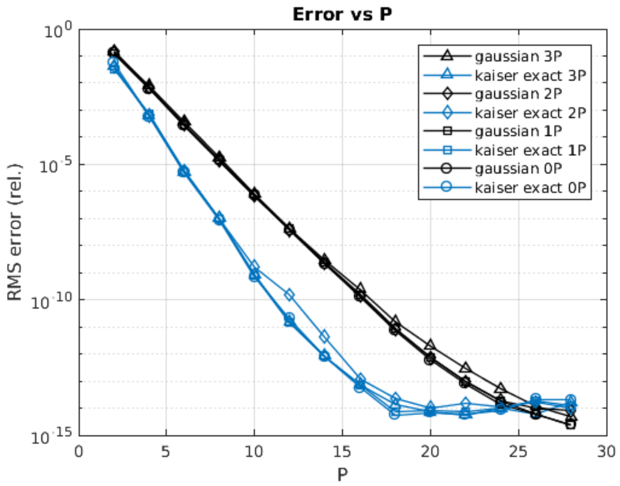
We have established a relation between P and the error tolerance, which is given by the table below.

$\varepsilon \geq 5\times 10^{-4}$	:	$P=4$
$\varepsilon \geq 5\times 10^{-6}$	:	$P=6$
$\varepsilon \geq 5\times 10^{-8}$	:	$P=8$
$\varepsilon \geq 1\times 10^{-10}$	:	$P=10$
$\varepsilon \geq 1\times 10^{-12}$	:	$P=12$
$\varepsilon \geq 1\times 10^{-13}$	:	$P=14$
$\varepsilon \geq 2\times 10^{-14}$	:	$P=16$

Here, $\varepsilon = 10\varepsilon_*$. This relation was based precisely on the Error-vs-P plots above. (This holds for the Kaiser windows, but we will use the same values for all windows.)

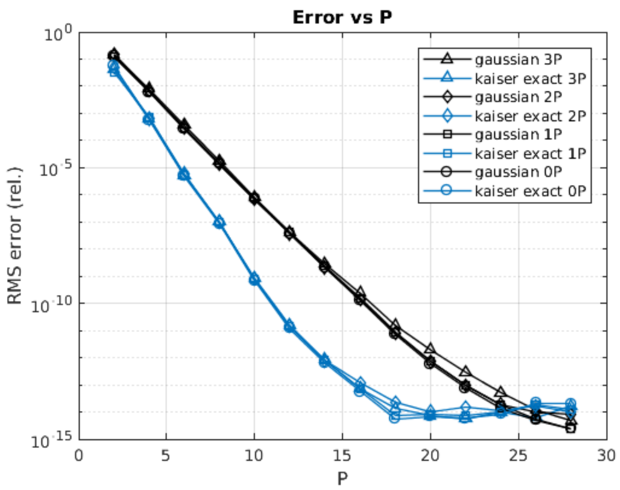
Below we present Error-vs-P plots where we use (3) rather than (1).

Baseline case



Comparing with the first plot on page 1, we see that the Kaiser error curves are a bit less steep (i.e. the error does not decay quite as fast), but the additional error coming from the free directions also seems to be quite a lot smaller. The reason for this latter phenomenon must be that we have changed k_∞/ξ, probably decreased it. Therefore we are less likely to end up in the bad part of the error curves. Recall that before, $k_\infty/\xi = 12$ always. Now the value depends on M as well as other parameters such as P (which sets ε_*), according to (3). For $P = 4$, we have $k_\infty/\xi = 5.6979$; for $P = 8$, we have $k_\infty/\xi = 8.2361$; for $P = 12$ we have $k_\infty/\xi = 10.4949$; and for $P = 16$ we have $k_\infty/\xi = 11.2040$. These values seem to be closer to the "sweet spot".

The 0P fix



As expected, the 0P fix solves the small remaining problem (only really visible for 2P). The table of δ_M for this case ($M = 28$) is found below.

P	δ_M (Gauss)	δ_M (Kaiser)	$\tilde{M}$ (Gauss)	$\tilde{M}$ (Kaiser)
2	6	10	34	38
4	8	10	36	38
6	10	12	38	40
8	14	12	42	40
10	18	14	46	42
12	22	16	50	44
14	24	16	52	44
16	26	16	54	44
18	28	18	56	46
20	28	20	56	48
22	28	22	56	50
24	28	24	56	52
26	28	26	56	54
28	26	28	54	56

This can be compared with the table on page 4; unsurprisingly, δ_M is smaller here than on page 4 (or at least never larger). Note that since ξ is determined by (3), it is no longer the case that ξ is directly proportional to M/L; rather, $\xi = C(M) \times M/L$, where the prefactor $C(M)$ is given by

$$C(M) = \frac{\pi}{\sqrt{2}} \frac{1}{\sqrt{W\left(\frac{4Q}{\pi^2 L^2 \varepsilon_*^2 M}\right)}}.$$

Here, Q depends on the particle system, and L on the box, so the prefactor depends on the problem. Furthermore, ε_*^2 is connected to P, so the prefactor depends on P. Lastly, the prefactor contains M, so even for the same problem and tolerance, the prefactor and thus δ_M may change when varying M. This seems to be very far from a simple rule such as $P + 6$. Note in particular that as $M \to \infty$, the value of the W function approaches zero (since $W(0) = 0$), and thus $C(M) \to \infty$. This in turn means that $\xi \to \infty$, and this is true even if M/L is fixed. As $\xi \to \infty$, we will have $\delta_{M,\text{rem}} \to 0$. This is in fact good news, since it means that δ_M will simply be equal to P in this situation. It would be far worse if $\delta_{M,\text{rem}}$ started to grow, but that can only happen if $\xi L/M \to 0$, which is equivalent to $C(M) \to 0$, which is in turn equivalent to

$$W\left(\frac{4Q}{\pi^2 L^2 \varepsilon_*^2 M}\right) \to \infty.$$

The W function is strictly increasing for nonnegative arguments, so the way to make this happen is if

$$\frac{4Q}{\pi^2 L^2 \varepsilon_*^2 M} \to \infty.$$

But this cannot happen for a fixed particle system and tolerance, since M cannot be selected arbitrarily small (it cannot be smaller than 2, and even that would be silly). Thus, δ_M cannot be larger than the value it takes for the smallest M one considers (for fixed Q, L, P and ε_*).

This leads us to the question: what *is* the smallest M that we can consider? Our main restriction is that $r_c \leq 1$, and the relation between r_c and ξ is

$$\xi = \frac{1}{r_c} \sqrt{W\left(\frac{1}{\varepsilon_*}\sqrt{\frac{Q}{2L^3}}\right)},$$

which means that the restriction is simply

$$\xi \geq \sqrt{W\left(\frac{1}{\varepsilon_*}\sqrt{\frac{Q}{2L^3}}\right)}.$$

The number in the right-hand side depends on the particle system (through Q and L) and the selected tolerance (through ε_*). For the test system that we use to compute the plots in this document, we have $Q = 31.4433$ and $L = 1$. The tolerance is related to P through the table on page 8. The lower bound for ξ in this case is shown below.

P	Lower bound for ξ
2	3.01255
4	3.01255
6	3.64671
8	4.19788
10	4.85252
12	5.28958
14	5.49597
16	5.63603
18	5.94532
20	5.94532
22	5.94532
24	5.94532
26	5.94532
28	5.94532

Plugging this into (2), we get M at the bounding value (first unrounded, then rounded):

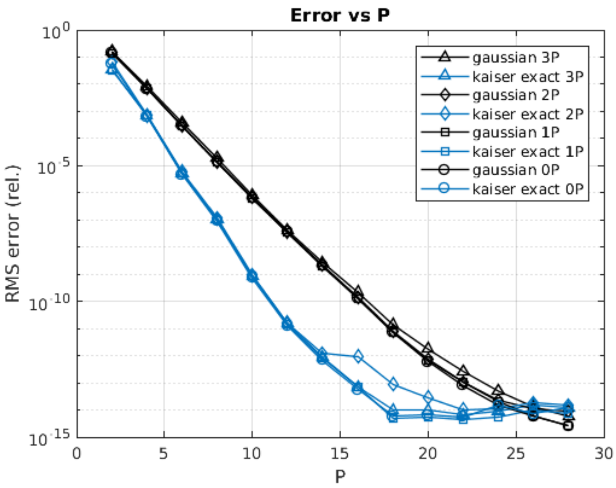
P	M for ξ as in the table above	Rounded up to even number
2	5.71089	6
4	5.71089	6
6	8.39782	10
8	11.1495	12
10	14.9207	16
12	17.7423	18
14	19.1593	20
16	20.1518	22
18	22.432	24
20	22.432	24
22	22.432	24
24	22.432	24
26	22.432	24
28	22.432	24

I don't know if this is the smallest M (if ξ increases in (2), are we sure that M also increases?), but I would guess this is pretty much the smallest. The corresponding values for δ_M are shown in the table below.

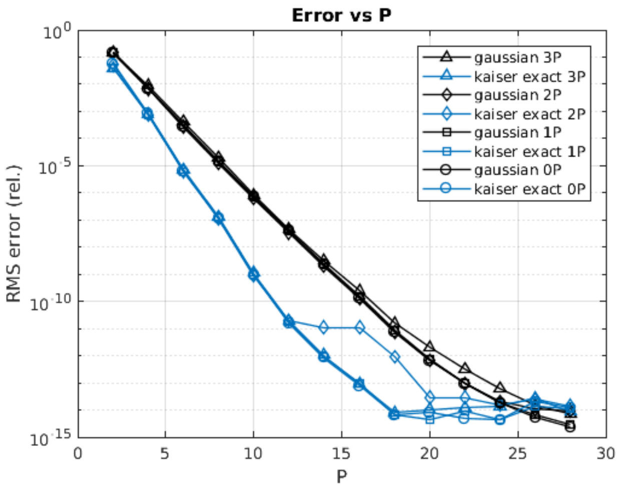
P	M	δ_M (Gauss)	δ_M (Kaiser)	$\tilde{M}$ (Gauss)	$\tilde{M}$ (Kaiser)
2	6	6	10	12	16
4	6	8	10	14	16
6	10	12	12	22	22
8	12	14	12	26	24
10	16	20	14	36	30
12	18	22	16	40	34
14	20	24	16	44	36
16	22	26	16	48	38
18	24	28	18	52	42
20	24	28	20	52	44
22	24	28	22	52	46
24	24	28	24	52	48
26	24	28	26	52	50
28	24	28	28	52	52

These should be the largest values of δ_M, and therefore also the largest ratios $\tilde{M}/M$. It seems the Error-vs-P plot still looks okay with these choices (although $M = 6$ is a silly choice of course). Finally, I check the Error-vs-P plot for $M = 32$, and it looks like this:

The 0P fix, M=32

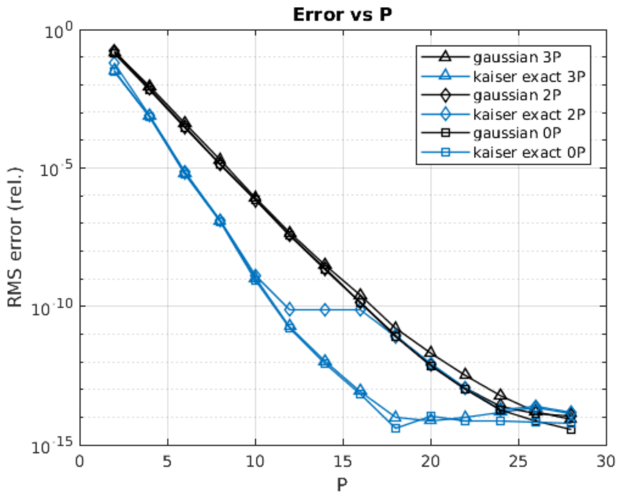


The 0P fix, M=36



Not sure why the 2P Kaiser curve behaves strange for P between 16 and 22. Whatever happens seems to become even worse for $M = 36$. Maybe δ_M becomes too small somehow? I notice that for $M = 40$, a bug prevents the 1P code from running (this could be in the direct summation though). The other codes can run, and the result is shown below:

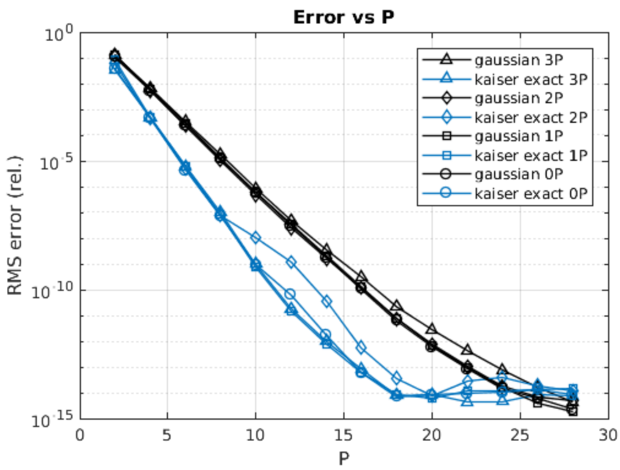
The 0P fix, M=40



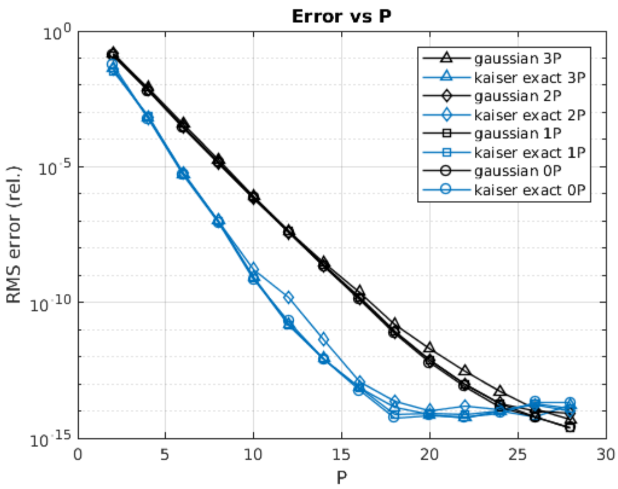
Strange, the Kaiser 2P curve flattens out completely and then joins the Gaussian curves. And δ_M is more or less the same as its maximum value (table on page 12), just the maximum minus 2 in some cases. I don't really see how this would explain the problem, but it is still possible that δ_M is too small.

Anyway, time to move on to the 2P fix, i.e. $\delta_M = P + k$ for some constant k (we try $k = 2, 4, 6, 8$). We will try this fix for $M = 16$, $M = 28$, $M = 32$ and possibly some larger values of M as well. First of all, we note that the baseline case itself becomes worse for $M = 16$ than for $M = 28$:

Baseline case, M=16

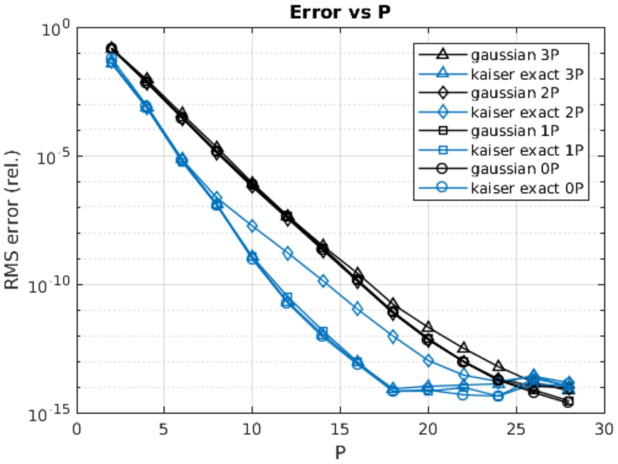


Baseline case, M=28

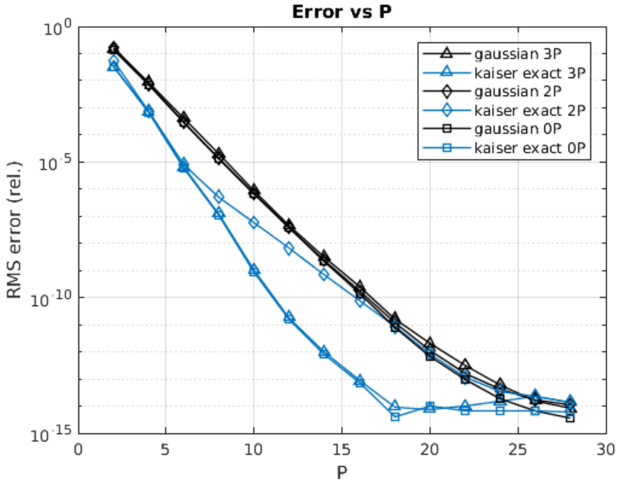


One can't help but wonder what happens to the baseline case for $M = 36$ and $M = 40$:

Baseline case, M=36



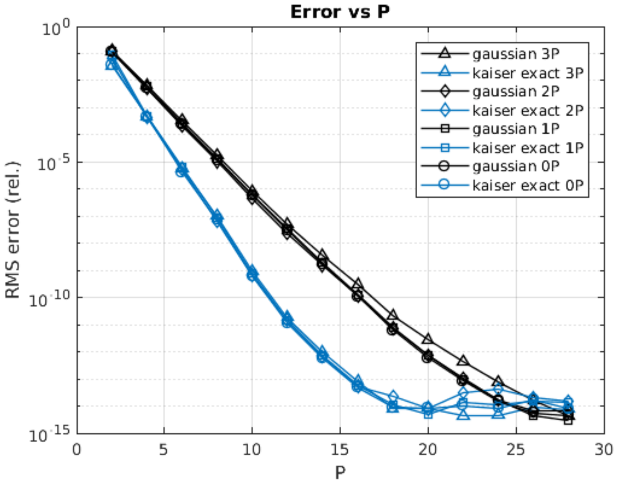
Baseline case, M=40



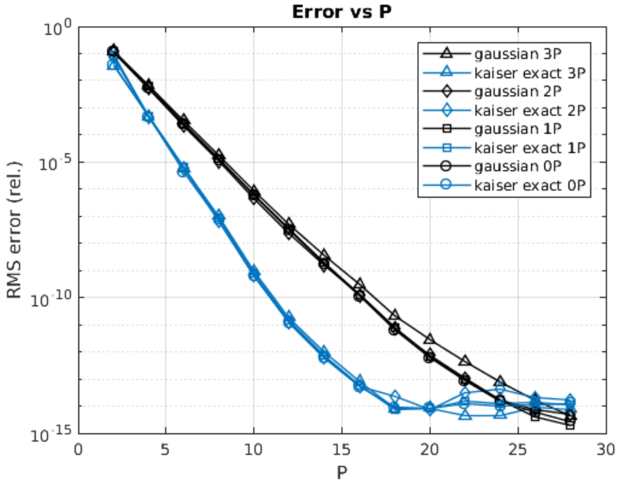
Something strange clearly happens to the 2P case. It could be that some other unrelated error also appears, which cannot be decreased by increasing δ_M?

Moving on, it's time to check $\delta_M = P + k$ for $M = 16$.

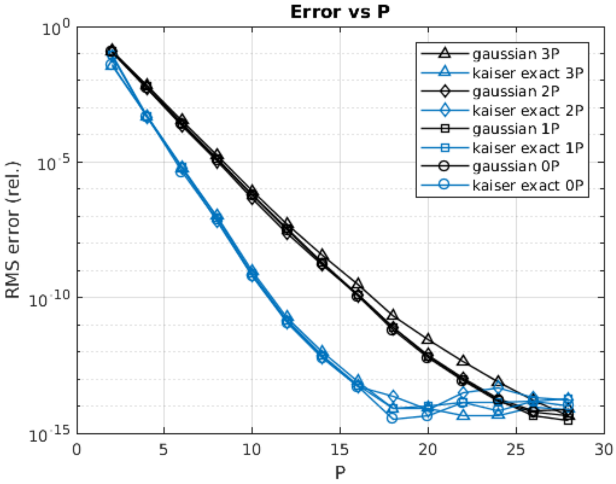
P+2, M=16



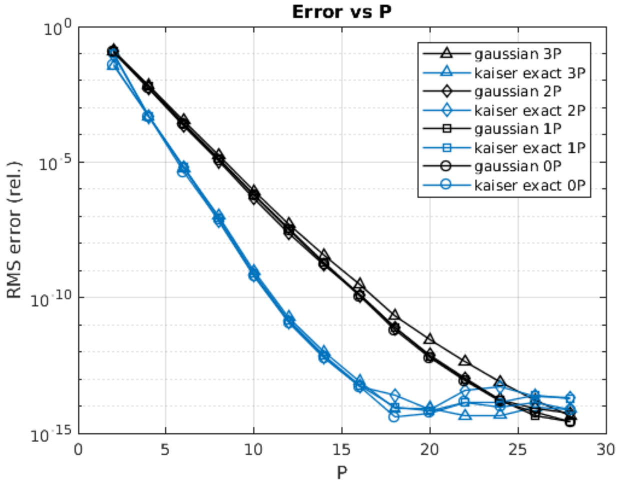
P+4, M=16



P+6, M=16



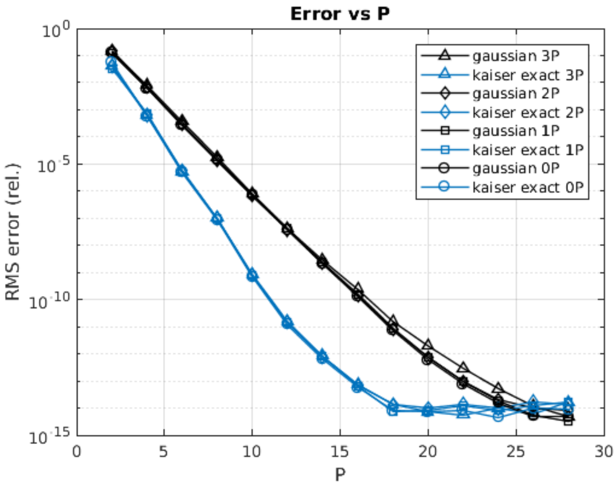
P+8, M=16



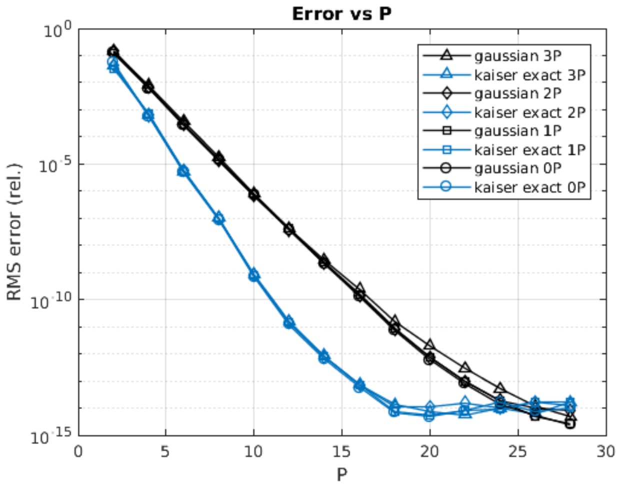
We see that for $M = 16$, it is enough to choose $\delta_M = P + 2$.

Now for $M = 28$:

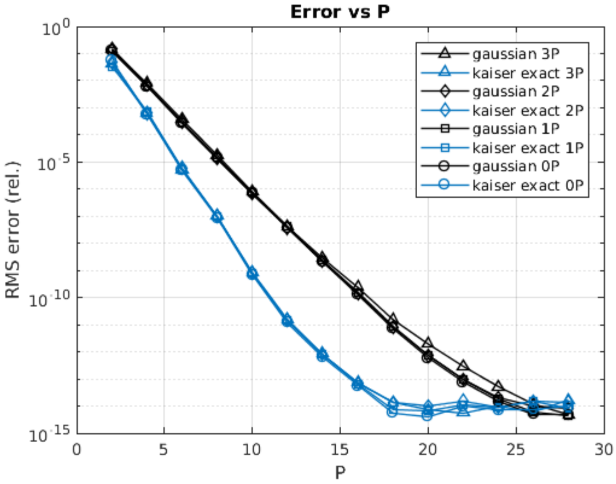
P+2, M=28



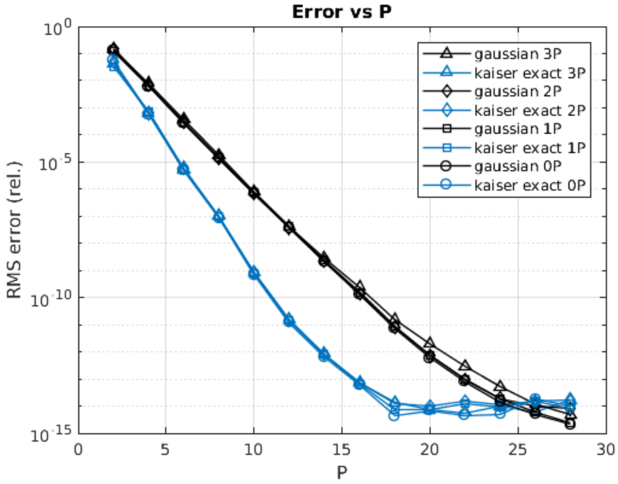
P+4, M=28



P+6, M=28



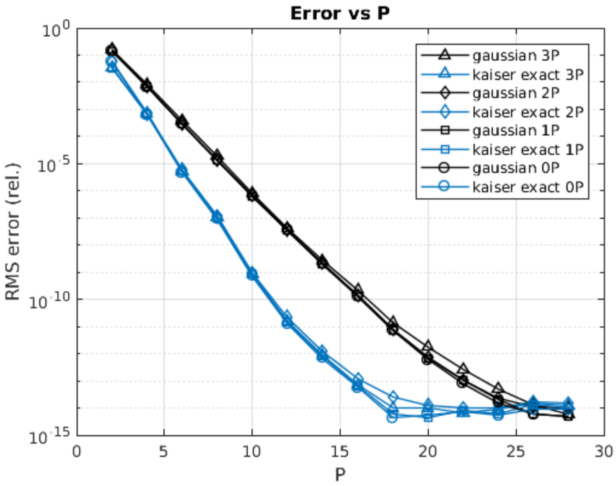
P+8, M=28



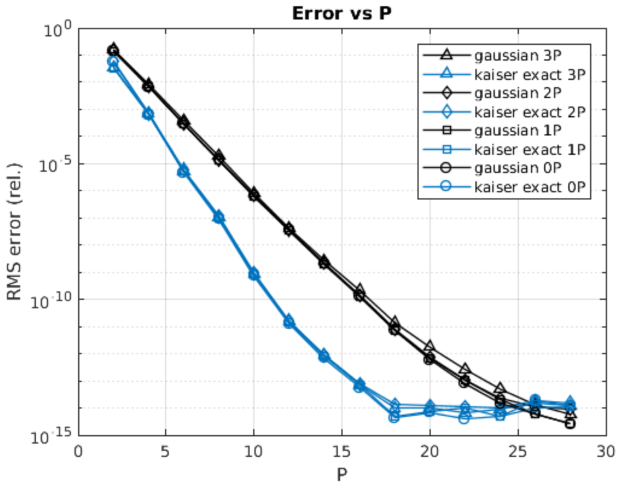
It seems $P+2$ is enough here as well.

Next is $M = 32$:

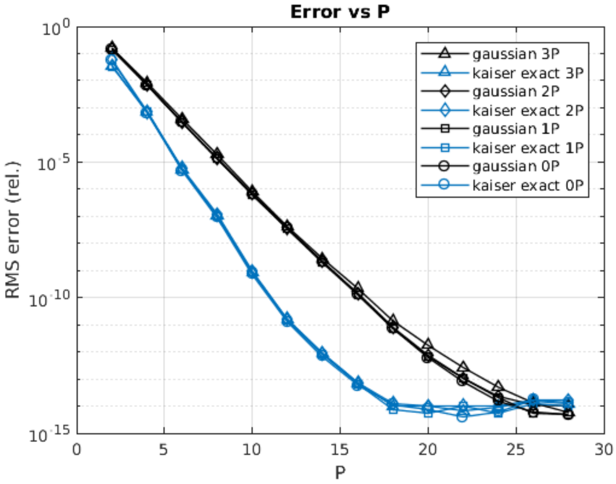
P+2, M=32



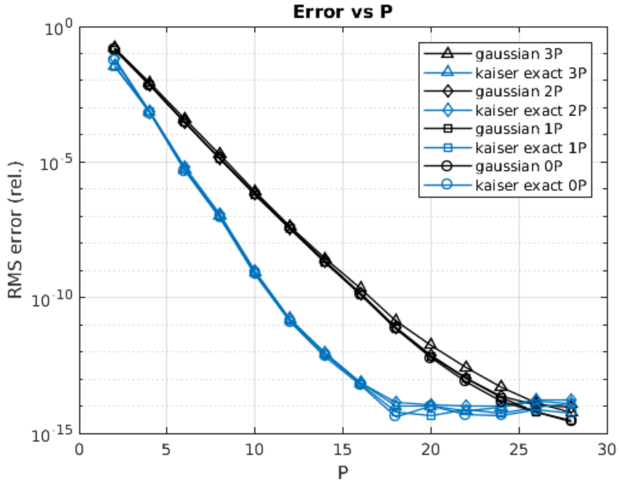
P+4, M=32



P+6, M=32



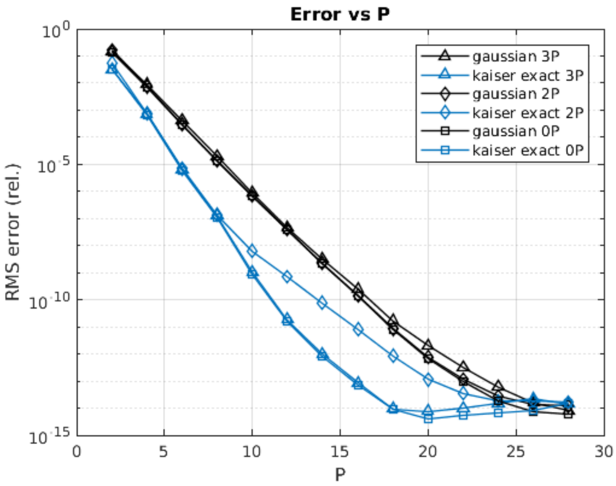
P+8, M=32



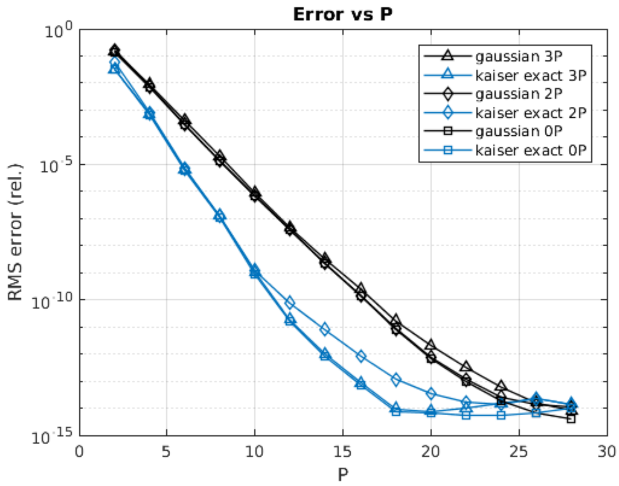
For $M = 32$ it seems $P + 4$ is the best choice; $P + 2$ isn't quite enough.

Finally we try $M = 40$:

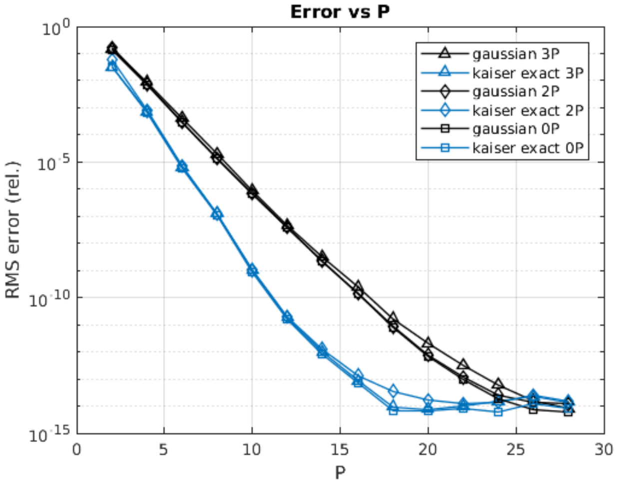
P+2, M=40



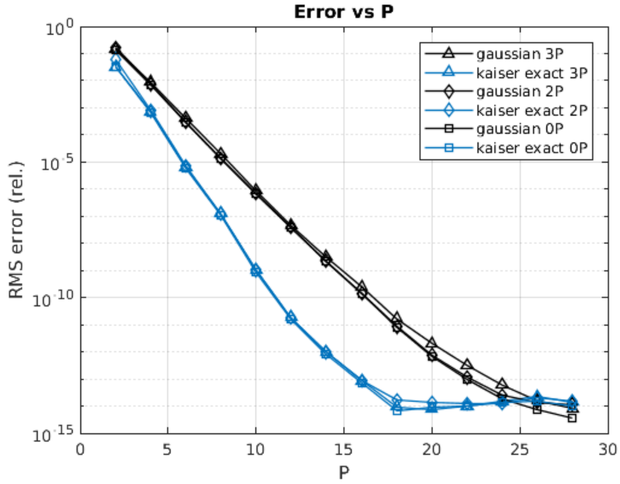
P+4, M=40



P+6, M=40



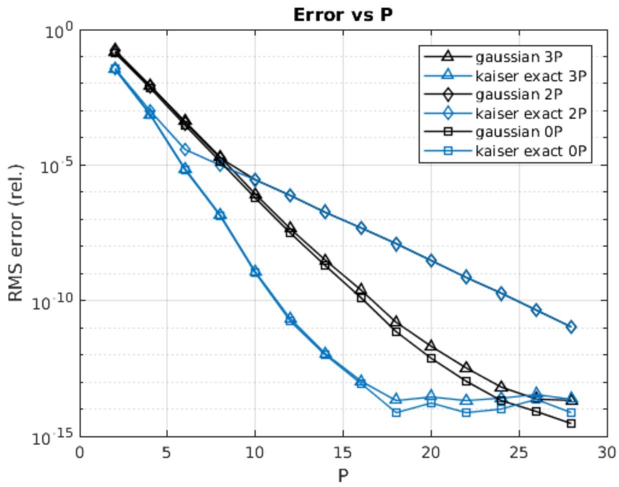
P+8, M=40



Here it seems one has to go up to $P + 8$. On the other hand, this fixes the problem better than the 0P fix.

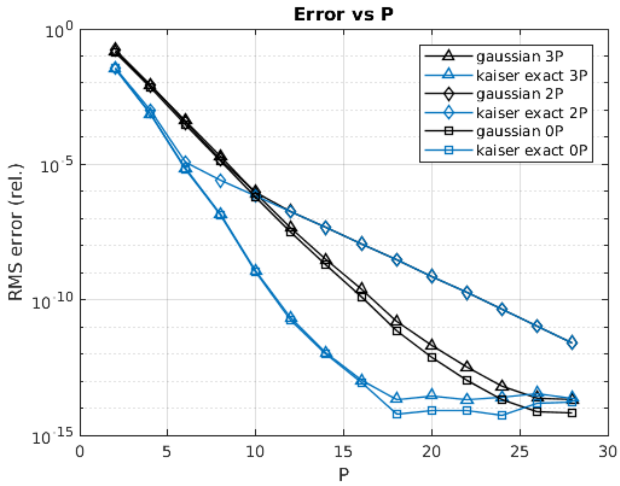
I will try to run with $M = 64$ as well, since it seems a bit like the problem becomes worse and worse as M grows. If that's the case, one might be worried that not even $P + 8$ would be enough for large enough M. Results (1P cannot be ran for $M = 64$ either due to the bug):

Baseline case, M=64

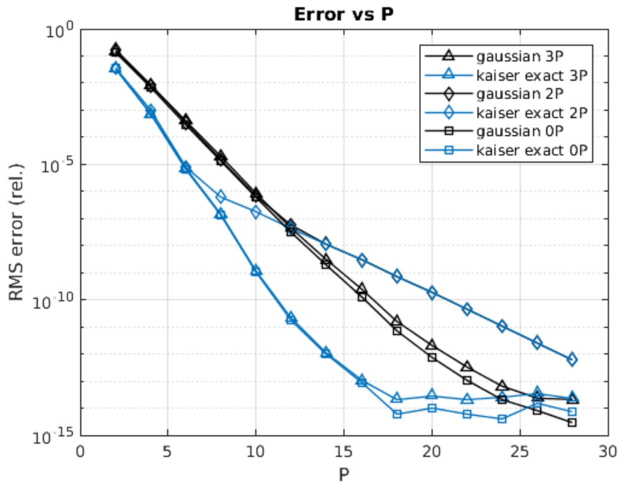


Note that both window functions are affected by the bad behaviour. However, it only happens in the 2P case (but of course, we cannot see the 1P case here).

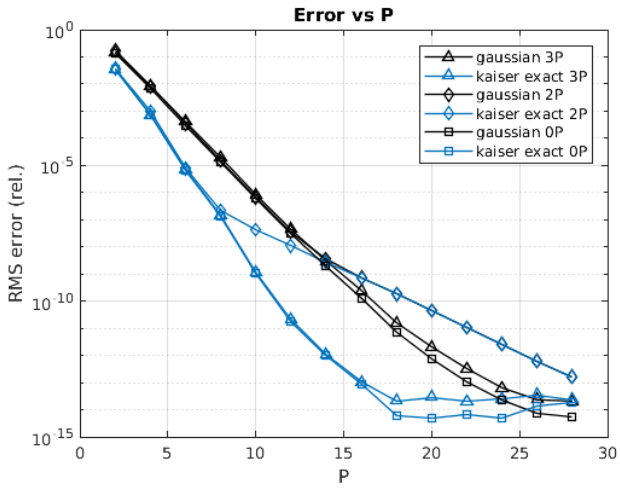
P+2, M=64



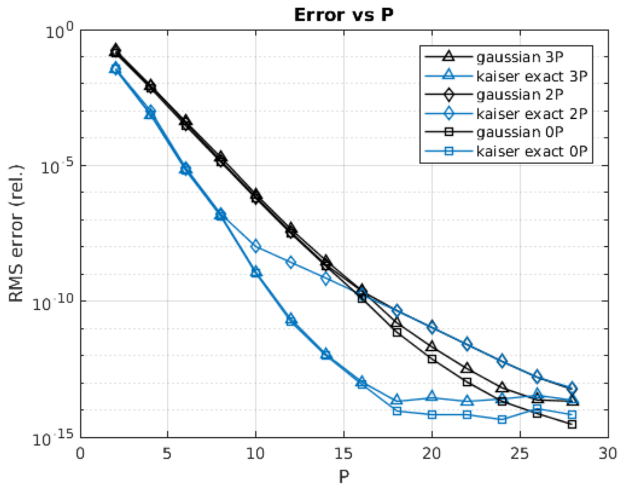
P+4, M=64



P+6, M=64



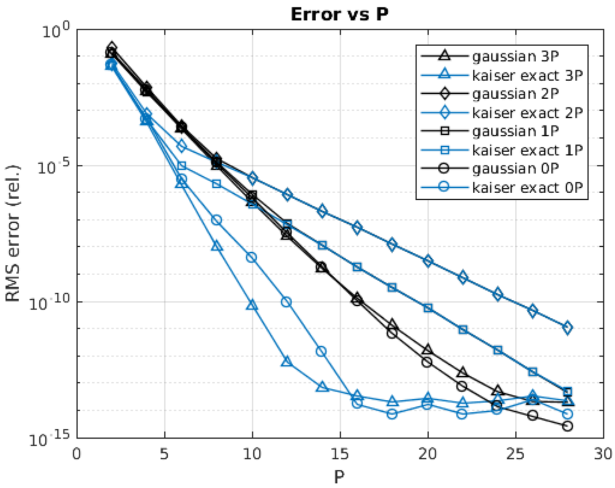
P+8, M=64



This seems to confirm the worries. We probably need to either understand why this happens only for 2P and fix it, or adapt the rule $P+k$ so that k depends on M.

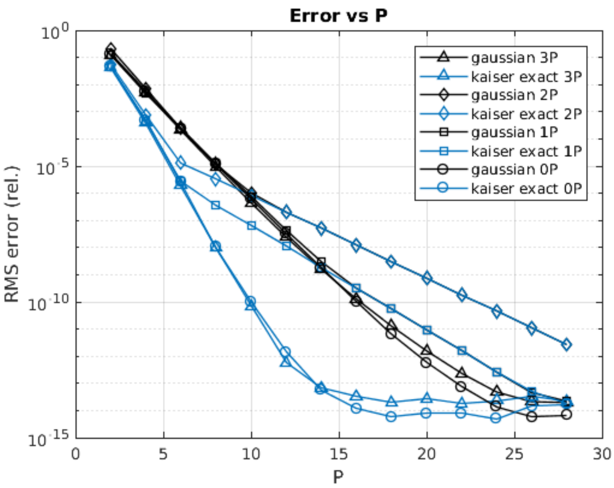
This section was about the more complicated relation between ξ and M, but the last results begs the question if $M = 64$ looks bad also using the simpler relation (1). Therefore we finish with a battery of such tests.

Baseline case ($\xi = \pi(M/L)/12$), M=64

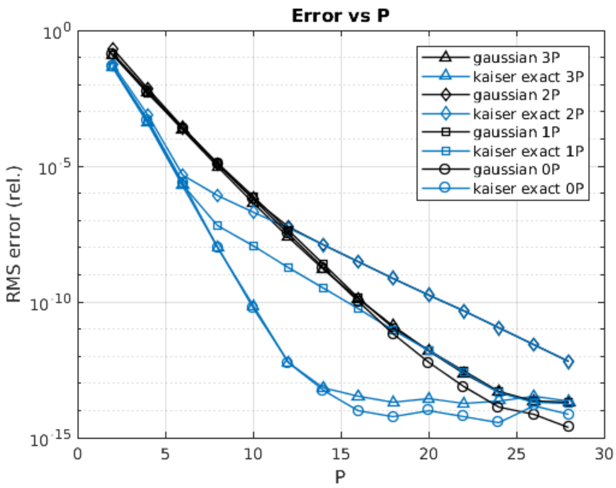


Interestingly, the 1P code worked in this case. So the error must be related to the relation between M and ξ. It seems the 2P error was not very affected by changing relation, but for the 0P code, the error went up. Now we can also see that the 1P code has an error between the 2P and 0P codes.

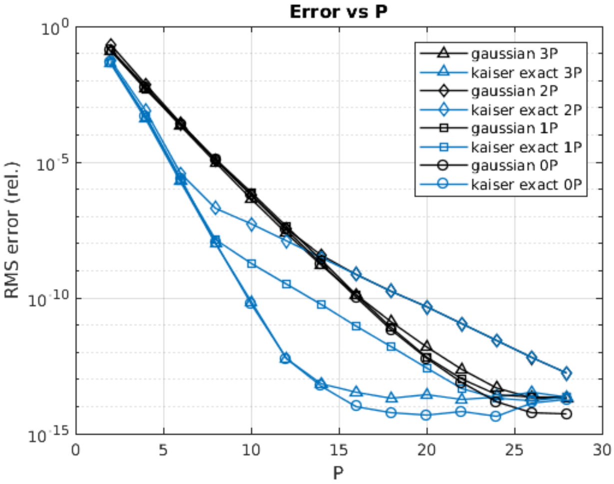
($\xi = \pi(M/L)/12$) **P+2, M=64**



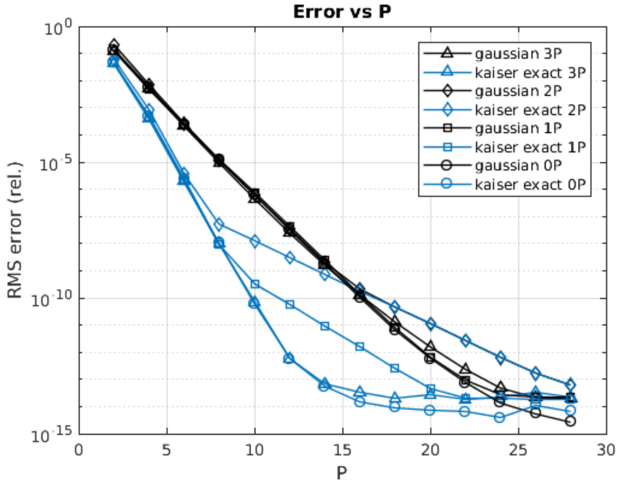
($\xi = \pi(M/L)/12$) **P+4, M=64**



($\xi = \pi(M/L)/12$) **P+6, M=64**



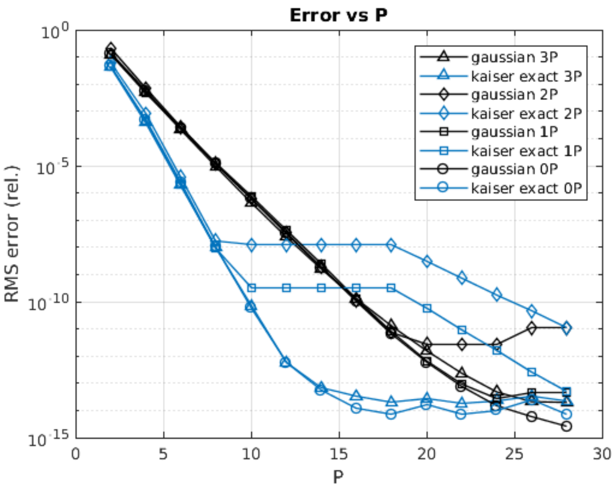
($\xi = \pi(M/L)/12$) **P+8, M=64**



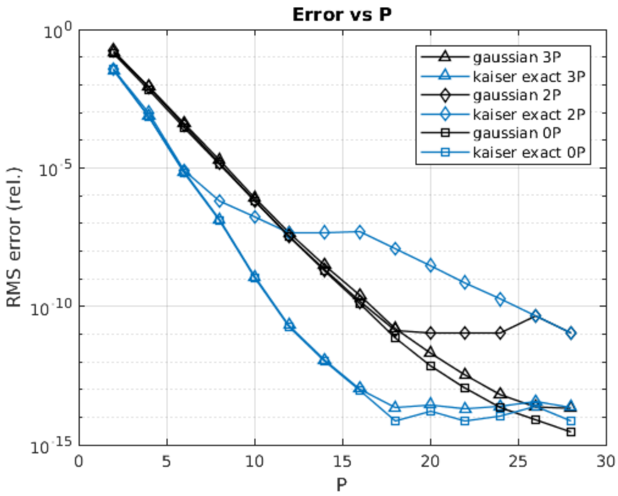
Here the results seem rather similar to those shown on page 19. So the problems with $M = 64$ seems to hold for both M-ξ-relations. Then it might be enough to do tests with the simple relation; it seems this captures all problems already (we just didn't try large enough M before).

We will also try the 0P fix for $M = 64$, both using the simple and complicated relations between M and ξ.

($\xi = \pi(M/L)/12$) **0P fix, M=64**



(Complicated M-ξ-relation) 0P fix, M=64



We see that the 0P fix is also not enough for $M = 64$. This is expected. It seems that δ_M really should depend on M somehow, but it doesn't in the 0P fix (not in the right way at least).

6 Finding out how much is needed

We return to the simple relation between M and ξ, i.e. (1), and investigate how large k in $\delta_M = P + k$ needs to be to remove the bulge in the error curve, as a function of M and the periodicity.

7 Timing tests

TODO: These are done, and I will do no more timing. But write down the conclusion here (which I think was to use $P+4$ or $P+6$ and then round up M to the nearest multiple of 4).

([The only reason to complicate the simplest rule (which is to use $\delta_M = P+6$ in all cases) would be if it makes a difference to the runtime.])