Initialize functions

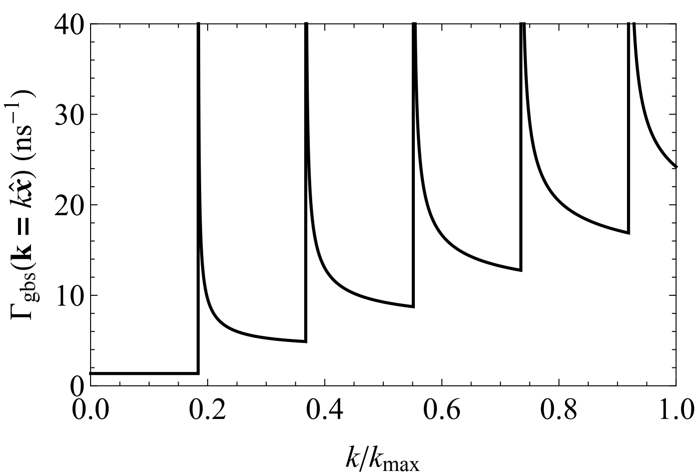
```
(*Ensure that variables are defined globally*)
SetOptions[EvaluationNotebook[], CellContext → "Global`"]
NotebookOpen[NotebookDirectory[] <> "GB-strain-scattering_init.nb"];
NotebookEvaluate[NotebookDirectory[] <> "GB-strain-scattering_init.nb"];
```

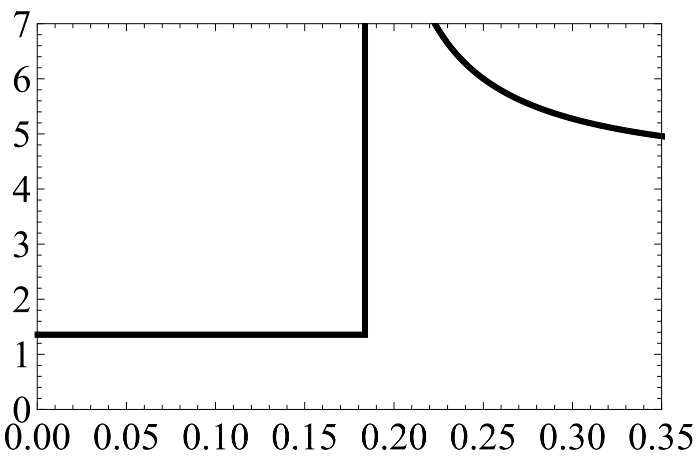
Define material values and phonon dispersion parameters

```
(*################################*)
(*### Material values for Si ###*)
(*################################*)

(*#### crystal properties ####*)
vs = 6084. (*[m/s] average speed of sound*);
V = 2 * 10^-29 (*[m^3] volume of atom*);
n = 2(*# atoms per primitive unit cell (N in paper)*);
γ = 1(*Gruneissen parameter*);
ν = 0.27(*Poisson's ratio*);
kmax = k0[V * n] // N(*[m^-1] edge of FBZ*);
ωD = vs kmax(*[s^-1] Debye frequency*);
disp = "Debye";
ωk[k_] := vs k (*Debye dispersion relation*);
vg[k_] := vs (*phonon group velocity*);

(*#### phonon-phonon ####*)
C1 = 2.69 * 10^-19 (*[s/K]*);
C2 = 167(*[K]*);

(*#### point defect ####*)
C3 = 1.81 * 10^-45 (*[s^3]*);

(*#### microstructure ####*)
b = (V n)^(1/3)(*[m] Burger's vector*);
dGS = 350 * 10^-9 (*[m] average grain size*);
n1D = 3 / dGS // N(*[m^-1] number density of GBs *);
d = 3 * 10^-9 (*[m] GB dislocation spacing (D in paper)*);
```

Diffraction peaks in $\Gamma_{gbs}(k)$

```
ΓMakeList[θ_, ϕ_] := Table[{ω / ωD, ΓGBS[ω / vs, θ, ϕ] * 10^-9}, {ω, 0, ωD, 10^10}];
(*θ=π/2 ϕ=0 is phonon incident normal to the GB.*)
ΓlistGBS = ΓMakeList[π / 2, 0];

ListPlot[{ΓlistGBS},
 PlotStyle → {Black},
 PlotRange → {{0, 1}, {0, 40}},
 Joined → True,
 FrameLabel → {"k / kmax", "Γgbs(k = k x̂) (ns^-1)"}]

ListPlot[{ΓlistGBS},
 Joined → True,
 FrameStyle → Directive[FontFamily → "Times New Roman", FontSize → 20, Black],
 PlotStyle → Directive[Black, Thickness[0.01]],
 PlotRange → {{0, 0.35}, {0, 7}}]
```





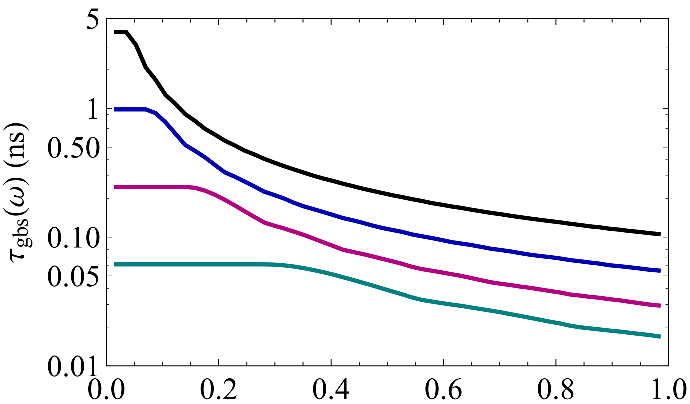
Calculating $\tau_{gbs}(\omega)^{-1}$

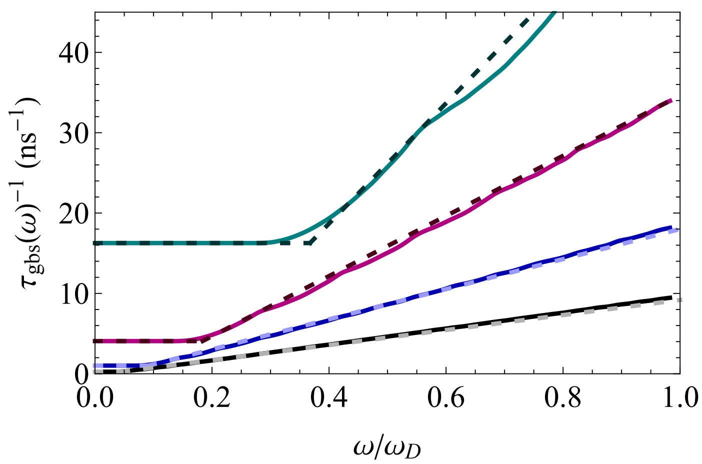
```
(*A convergence test was perfomed on δk by caluclating ϰL at different δk. δk=
 2*10^8 was found to be fully converged. This
  calculation takes ~20 min on most personal computers*)
Clear[d]
τGBSList = {disp};
δk = 2. * 10^8;
For[d = 1.0 * 10^-9, d ≤ 8.0 * 10^-9, d = d * 2.0,
 Print[d];
 τGBSListd = Table[{ω / vs, τGBSθϕIntegrate[ω / vs, 90]}, {ω, vs δk, ωD, vs δk}];
 AppendTo[τGBSList, {d, θcalc[b, d], τGBSListd}]
]
1. × 10^-9
2. × 10^-9
4. × 10^-9
8. × 10^-9
(*###############################*)
(*#### Exports τGBS results ###*)
(*###############################*)
Export[NotebookDirectory[] <> "CompResults/tauSTGB_results.m", τGBSList]
/Users/rileyhanus/Desktop/Papers/Phonon_diffraction/Scripts/FOR_DISTRIBUTION/
  CompResults/tauSTGB_results.m

(*################################################*)
(*#### Imports the last exported τGBS result ####*)
(*################################################*)
τGBSList = Import[NotebookDirectory <> "/CompResults/tauSTGB_results.m"];
```

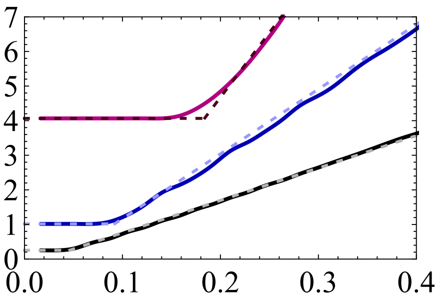
Plotting $\tau_{\text{gbs}}(\omega)$ for a STGB

```
"STGB"
Show[ListLogPlot[{τGBExtract[τGBSList, 2],
    τGBExtract[τGBSList, 3], τGBExtract[τGBSList, 4], τGBExtract[τGBSList, 5]},
  PlotStyle -> {Directive[RGBColor[0., 0.5, 0.5], Thickness[0.0075]],
    Directive[RGBColor[0.7, 0., 0.5], Thickness[0.0075]],
    Directive[RGBColor[0., 0, 0.7], Thickness[0.0075]],
    Directive[Black, Thickness[0.0075]]},
  FrameLabel → {Style["", 16], Style["τgbs(ω)  (ns)", 16]},
  PlotRange → {{0, 1}, {0.01, 5}},
  Joined → True,
  PlotRange → All]]
Show[
 ListPlot[{ΓGBExtract[τGBSList, 2],
   ΓGBExtract[τGBSList, 3], ΓGBExtract[τGBSList, 4], ΓGBExtract[τGBSList, 5]},
```

```
  PlotStyle -> {Directive[RGBColor[0., 0.5, 0.5], Thickness[0.0075]],
    Directive[RGBColor[0.7, 0., 0.5], Thickness[0.0075]],
    Directive[RGBColor[0., 0, 0.7], Thickness[0.0075]],
    Directive[Black, Thickness[0.0075]]},
  FrameLabel → {Style["ω/ωD", 16], Style["τgbs(ω)^-1 (ns^-1)", 16]},
  PlotRange → {{0, 1}, {0, 45}},
  Joined → True,
  InterpolationOrder → 3,
  PlotRange → All],
 Plot[{τinvEmp[ω * ωD, 1 * 10^-9, b, n1D] * 10^-9,
   τinvEmp[ω * ωD, 2 * 10^-9, b, n1D] * 10^-9, τinvEmp[ω * ωD, 4 * 10^-9, b, n1D] * 10^-9,
   τinvEmp[ω * ωD, 8 * 10^-9, b, n1D] * 10^-9}, {ω, 0, 1},
  PlotStyle → {Directive[Dashing[{.01, 0.03}],
     RGBColor[0, 0.2, 0.2], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.3, 0., 0.1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.6, 0.6, 1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], GrayLevel[0.7], Thickness[0.0075]]}]]

Show[
 ListPlot[{ΓGBExtract[τGBSList, 2], ΓGBExtract[τGBSList, 3],
   ΓGBExtract[τGBSList, 4], ΓGBExtract[τGBSList, 5]},
  PlotStyle -> {Directive[RGBColor[0., 0.5, 0.5], Thickness[0.01]],
    Directive[RGBColor[0.7, 0., 0.5], Thickness[0.01]],
    Directive[RGBColor[0., 0, 0.7], Thickness[0.01]],
    Directive[Black, Thickness[0.01]]},
  FrameLabel → {Style["", 16], Style["", 16]},
  PlotRange → {{0, 0.4}, {0, 7}},
  ImageSize → 250,
  Joined → True,
  InterpolationOrder → 3,
  PlotRange → All],
 Plot[{τinvEmp[ω * ωD, 1 * 10^-9, b, n1D] * 10^-9,
   τinvEmp[ω * ωD, 2 * 10^-9, b, n1D] * 10^-9, τinvEmp[ω * ωD, 4 * 10^-9, b, n1D] * 10^-9,
   τinvEmp[ω * ωD, 8 * 10^-9, b, n1D] * 10^-9}, {ω, 0, 1},
  PlotStyle → {Directive[Dashing[{.01, 0.03}],
     RGBColor[0, 0.2, 0.2], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.3, 0., 0.1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.6, 0.6, 1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], GrayLevel[0.7], Thickness[0.0075]]}]]

STGB
```

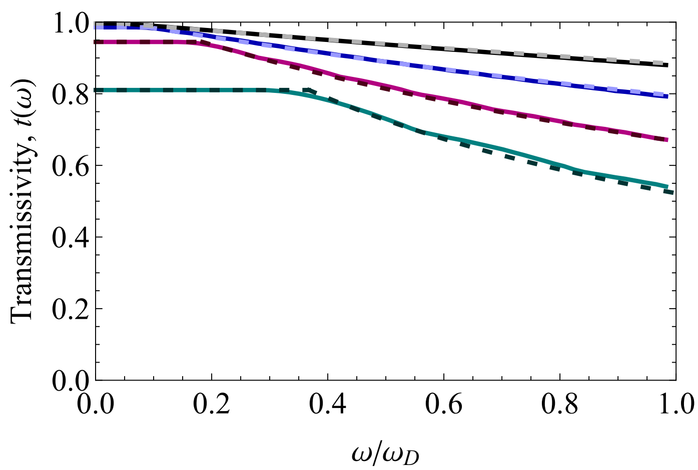






Convert $\tau(\omega)$ to $t(\omega)$ and plot

```
Show[ListPlot[{tGBExtract[τGBSList, 2], tGBExtract[τGBSList, 3],
    tGBExtract[τGBSList, 4], tGBExtract[τGBSList, 5]},
  PlotRange → {{0, 1}, {0., 1}},
  FrameLabel → {"ω/ωD", "Transmissivity,  t(ω)"},
  Joined → True,
  PlotStyle -> {Directive[RGBColor[0., 0.5, 0.5], Thickness[0.0075]],
    Directive[RGBColor[0.7, 0., 0.5], Thickness[0.0075]],
    Directive[RGBColor[0., 0, 0.7], Thickness[0.0075]],
    Directive[Black, Thickness[0.0075]]}],
 Plot[{tEmp[ω * ωD, 1 * 10^-9, b, n1D], tEmp[ω * ωD, 2 * 10^-9, b, n1D],
    tEmp[ω * ωD, 4 * 10^-9, b, n1D], tEmp[ω * ωD, 8 * 10^-9, b, n1D]}, {ω, 0, 1},
  PlotStyle → {Directive[Dashing[{.01, 0.03}],
      RGBColor[0, 0.2, 0.2], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.3, 0., 0.1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.6, 0.6, 1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], GrayLevel[0.7], Thickness[0.0075]]}]]
```



Calculating κ_L

```
Timing[
 ϰTList = {disp};
 For[i = 2, i ≤ 5, i++,
  Print[τGBSList[[i, 1]] // N];
  ϰT = {};
  For[T = 5, T ≤ 500, T = T * 1.1,
   AppendTo[ϰT, {T, ϰLCalc[τTotCalc[τGBSList[[i, 3]], T], T]}]];
  AppendTo[ϰTList, {τGBSList[[i, 1]] // N, τGBSList[[i, 2]], ϰT}]]]
```

$1. \times 10^{-9}$

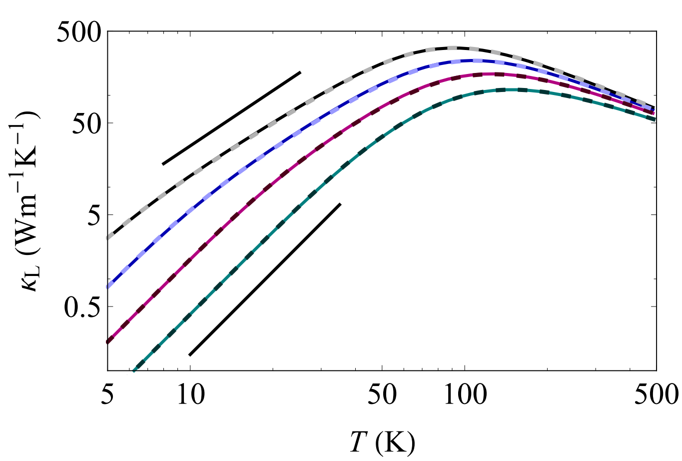
$2. \times 10^{-9}$

$4. \times 10^{-9}$

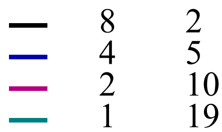
$8. \times 10^{-9}$

{0.287243, Null}

```
Show[
 ListLogLogPlot[{κTList[[2, 3]], κTList[[3, 3]], κTList[[4, 3]], κTList[[5, 3]]},
  FrameLabel → {Style["T (K)"], Style["κL (Wm^-1K^-1)", SingleLetterItalics → False]},
  FrameTicks → Automatic,
  Joined → True,
  PlotStyle →
   {RGBColor[0., 0.5, 0.5], RGBColor[0.7, 0., 0.5], RGBColor[0., 0, 0.7], Black},
  PlotRange → {{5, 500}, {0.1, 500}},
  ImageSize → 350],
 LogLogPlot[
  {κL[T, (τinvEmp[ω, 1 * 10^-9, b, n1D] + τppModel[ω, T, C1, C2]^-1 + τPD[ω, C3]^-1)^-1,
     vs, ω / vs, {ω, 0, ωD}],
   κL[T, (τinvEmp[ω, 2 * 10^-9, b, n1D] + τppModel[ω, T, C1, C2]^-1 + τPD[ω, C3]^-1)^-1,
     vs, ω / vs, {ω, 0, ωD}],
   κL[T, (τinvEmp[ω, 4 * 10^-9, b, n1D] + τppModel[ω, T, C1, C2]^-1 + τPD[ω, C3]^-1)^-1,
     vs, ω / vs, {ω, 0, ωD}],
   κL[T, (τinvEmp[ω, 8 * 10^-9, b, n1D] + τppModel[ω, T, C1, C2]^-1 + τPD[ω, C3]^-1)^-1,
     vs, ω / vs, {ω, 0, ωD}]}, {T, 5, 500},
  PlotStyle → {Directive[Dashing[{.01, 0.03}],
      RGBColor[0, 0.2, 0.2], Thickness[0.0075]],
     Directive[Dashing[{.01, 0.03}], RGBColor[0.3, 0., 0.1], Thickness[0.0075]],
     Directive[Dashing[{.01, 0.03}], RGBColor[0.6, 0.6, 1], Thickness[0.0075]],
     Directive[Dashing[{.01, 0.03}], GrayLevel[0.7], Thickness[0.0075]]}],
 ListLogLogPlot[{T2[18, {Tref, 8, 25}], T3[0.15, {Tref, 10, 35}]}, Joined → True]]
```



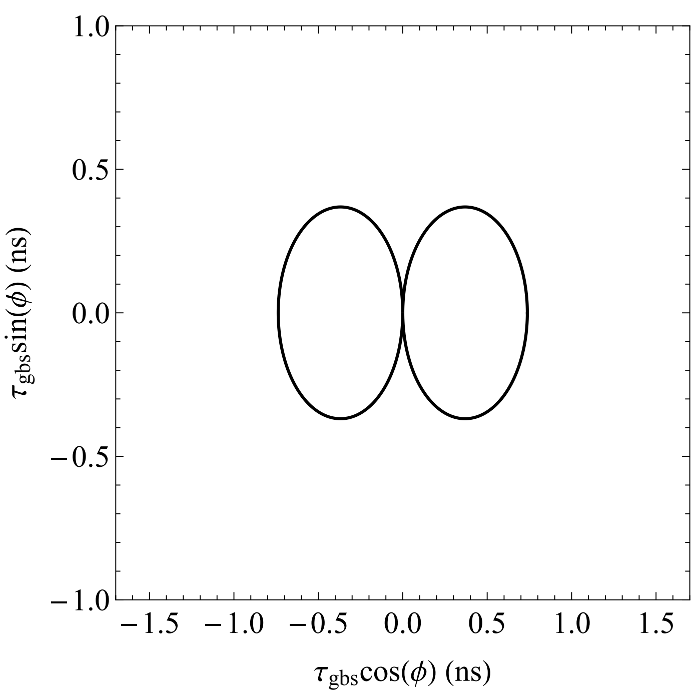
```
LineLegend[{Directive[Black, Thickness[0.0075]],
  Directive[RGBColor[0., 0, 0.7], Thickness[0.0075]],
  Directive[RGBColor[0.7, 0., 0.5], Thickness[0.0075]],
  Directive[RGBColor[0., 0.5, 0.5], Thickness[0.0075]]},
 {Style["     8        2", FontFamily → "Times New Roman", 18],
  Style["     4        5", FontFamily → "Times New Roman", 18],
  Style["     2        10", FontFamily → "Times New Roman", 18],
  Style["     1        19", FontFamily → "Times New Roman", 18]}, Spacings → 0.3]
```



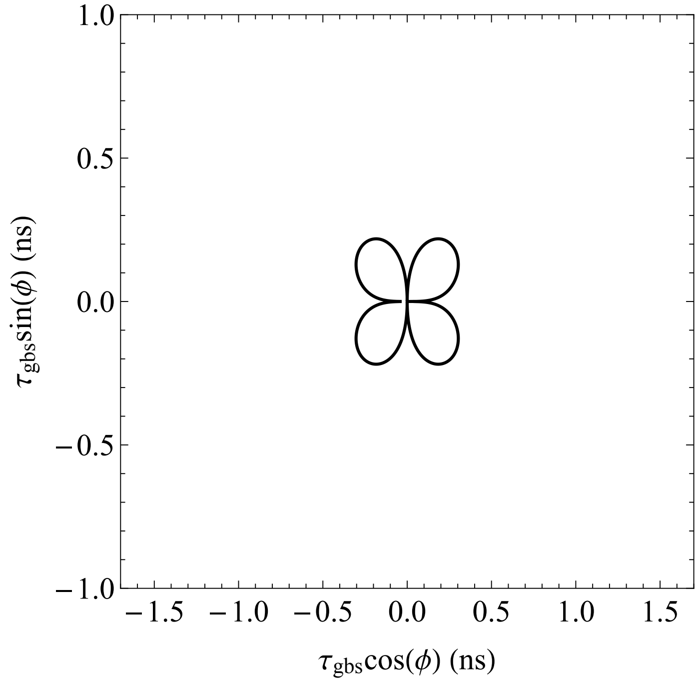
Supplemental:
Pole plots of Γ^{-1}(k)

```
For[i = 1, i ≤ 4, i++,
 Print["k=" <> ToString[i] <> "π/d"];
 Print[τPolarPlot[i π / d]]]
```

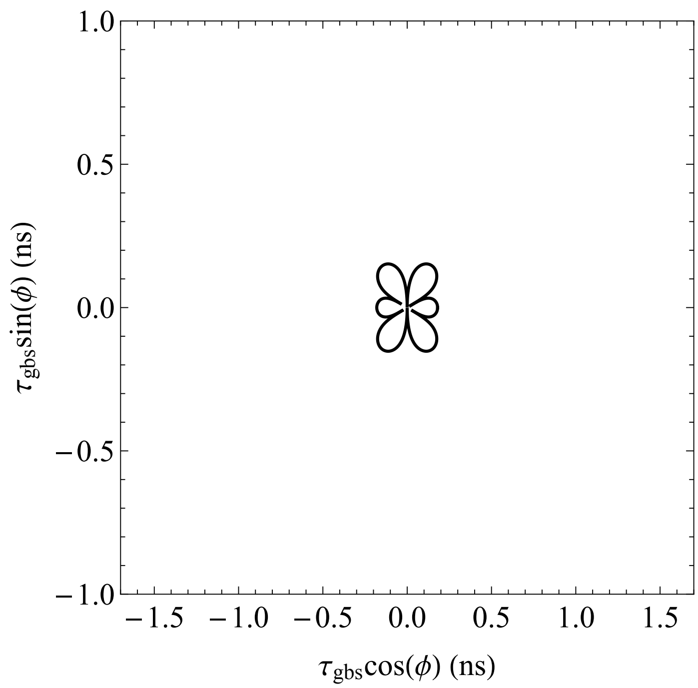
k=1 $\frac{\pi}{d}$



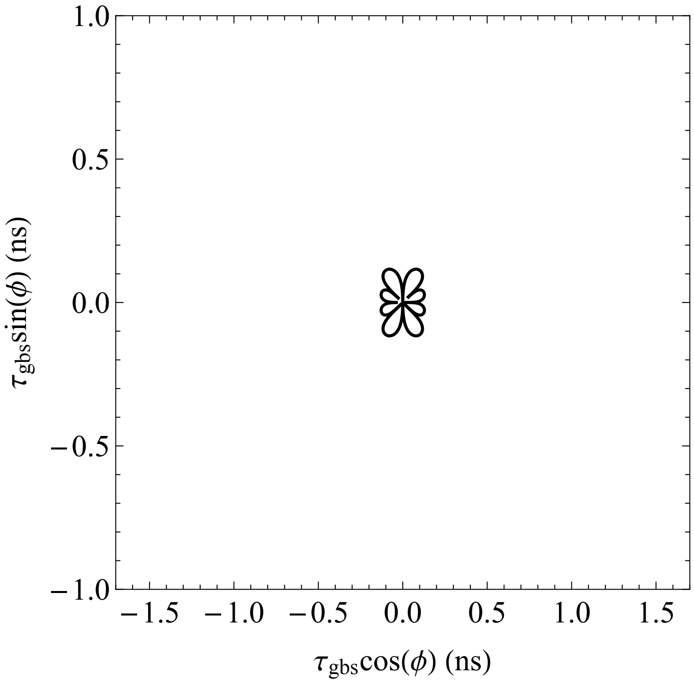
k=2 $\frac{\pi}{d}$



$k = 3\frac{\pi}{d}$



$k = 4\frac{\pi}{d}$


1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
$\tau_{gbs}\sin(\phi)$ (ns)
$\tau_{gbs}\cos(\phi)$ (ns)