MAS sidebands

tested 190817 using *SpinDynamica* 3.0.1 under *Mathematica* 11.0

code

init

```
Needs["SpinDynamica`"];
```

```
SpinDynamica version 3.0.1 loaded
```

ModifyBuiltIn: The following built-in routines have been modified in SpinDynamica:
{Chop, Dot, Duration, Exp, Expand, ExpandAll, NumericQ, Plus, Power, Simplify, Times, WignerD}.
Evaluate ??*symbol* to generate the additional definitions for *symbol*.

```
SetSpinSystem[1]
```

SetSpinSystem: the spin system has been set to $\{\{1, \frac{1}{2}\}\}$

SetBasis: the state basis has been set to ZeemanBasis$\left[\{\{1, \frac{1}{2}\}\}, \text{BasisLabels} \to \text{Automatic}\right]$.

CSA Hamiltonian in a rotating solid

```
ωCSA[t_, {ωaniso_, η_}, ΩPR_, {ωr_, βRL_}] :=
 ωCSA[t, {ωaniso, η}, ΩPR, {ωr, {0, βRL}}]
```

```
ωCSA[t_, {ωaniso_, η_}, ΩPR_, {ωr_, {αRL0_, βRL_}}] :=
 Chop@ExpToTrig[ωaniso ×
    {-η / Sqrt[6], 0, 1, 0, -η / Sqrt[6]}.WignerD[2, {{0}}][{ΩPR, {αRL0 - ωr t, βRL, 0}}]
  ]
```

```
ωCSA[t, {2 π, 0}, {0, π / 2, 0}, {2 π, ArcTan@Sqrt[2]}]
```

WignerD: The built-in function WignerD has been given extra functionality in SpinDynamica. Execute ?WignerD for more information.

For ?WignerD click <here>

$$\frac{3}{4}\pi\,\text{Cos}[4\pi t] - \frac{3}{4}\pi\,\text{Cos}[4\pi t]\,\text{Cos}\left[\frac{\text{ArcTan}\left[\sqrt{2}\right]}{2}\right]^4 + \frac{9}{2}\pi\,\text{Cos}[4\pi t]\,\text{Cos}\left[\frac{\text{ArcTan}\left[\sqrt{2}\right]}{2}\right]^2\text{Sin}\left[\frac{\text{ArcTan}\left[\sqrt{2}\right]}{2}\right]^2 - \frac{3}{4}\pi\,\text{Cos}[4\pi t]\,\text{Sin}\left[\frac{\text{ArcTan}\left[\sqrt{2}\right]}{2}\right]^4$$

```
ωCSA[t, {2 π, 0.5}, {0, π/2, 0}, {2 π, ArcTan@Sqrt[2]}]
```

$$2\pi\left(\frac{3}{8}\cos[4\pi t]-\frac{3}{8}\cos[4\pi t]\cos\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^4+\frac{9}{4}\cos[4\pi t]\cos\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^2\sin\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^2-\frac{3}{8}\cos[4\pi t]\sin\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^4-0.204124\left(\frac{1}{8}\sqrt{\frac{3}{2}}\cos[4\pi t]-\frac{1}{8}\sqrt{\frac{3}{2}}\cos[4\pi t]\cos\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^4-i\sqrt{2}\cos\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]\sin[2\pi t]\sin\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]+\frac{3}{4}\sqrt{\frac{3}{2}}\cos[4\pi t]\cos\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^2\sin\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^2-\frac{1}{8}\sqrt{\frac{3}{2}}\cos[4\pi t]\sin\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^4\right)-0.204124\left(\frac{1}{8}\sqrt{\frac{3}{2}}\cos[4\pi t]-\frac{1}{8}\sqrt{\frac{3}{2}}\cos[4\pi t]\cos\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^4+i\sqrt{2}\cos\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]\sin[2\pi t]\sin\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]+\frac{3}{4}\sqrt{\frac{3}{2}}\cos[4\pi t]\cos\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^2\sin\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^2-\frac{1}{8}\sqrt{\frac{3}{2}}\cos[4\pi t]\sin\left[\frac{\arctan\left[\sqrt{2}\right]}{2}\right]^4\right)\right)$$

```
HCSA[CSA_, ΩPR_, {ωr_, αβRL_}] :=
  PeriodicFunction[t, 2 π / ωr, Evaluate[ωCSA[t, CSA, ΩPR, {ωr, αβRL}] × opI["z"]]];
```

single-orientation MAS spectra

parameters

```
ωaniso = 2 π 40 × 10^3;  η = 0.5;
ΩPR = {0, π/2, 0};
βRL = ArcTan@Sqrt[2];
ωr = 10 × 2 π × 10^3;

T = 5 × 10^-3;  npoints = 1024;
```

default COMPUTE calculation (using periodicity)

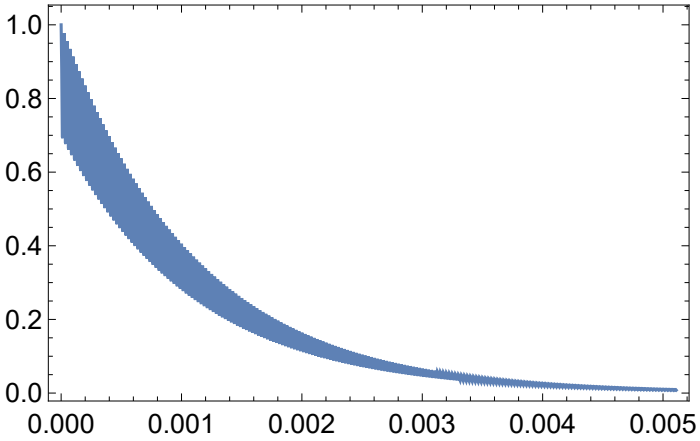
```
sig = Signal1D[{{2 π 200 × 10^3, "1k"}},
   BackgroundGenerator →
    HCSA[{ωaniso, η}, ΩPR, {ωr, βRL}],
   SignalCalculationMethod → "COMPUTE"
  ]
```

Signal1D: Using SignalCalculationMethod → COMPUTE

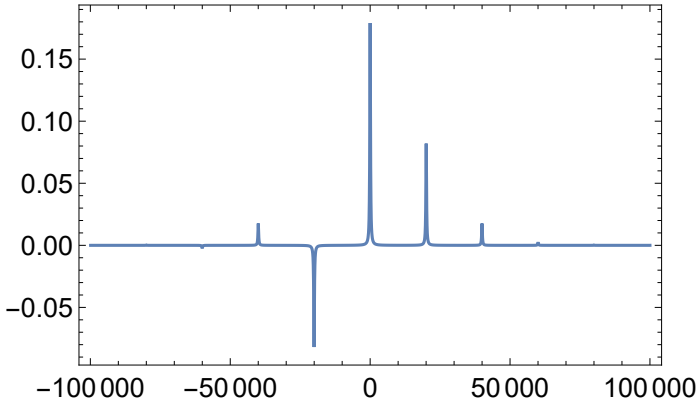
Signal1D: Using LineBroadening → 2π × 286.863 rad s^{-1}.

```
Signal[ {0, 5.11 × 10^-3, 5. × 10^-6} , { Lorentzian ,<< 20 >>} ]
```

```
ListPlot[Re@sig, Frame → True, Joined → True]
```




```
ListPlot[Re@FT@sig, Frame → True, Joined → True, PlotRange → All, Axes → None]
```



force direct calculation method

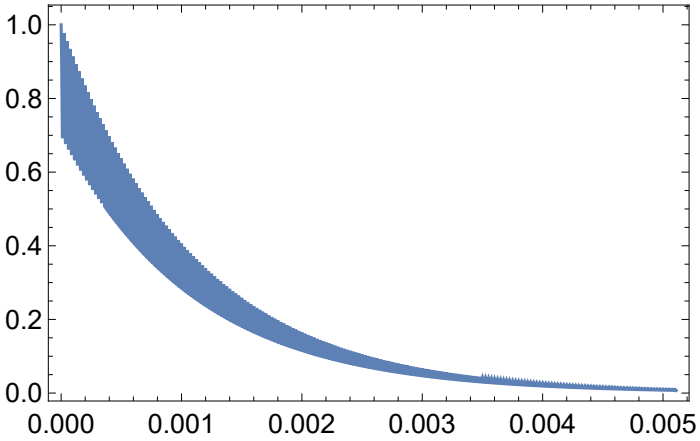
```
sig = Signal1D[{{2 π 200 × 10^3, "1k"}},
   BackgroundGenerator →
    HCSA[{ωaniso, η}, ΩPR, {ωr, βRL}],
   SignalCalculationMethod → "Direct"
  ]
```

Signal1D: Using SignalCalculationMethod → Direct

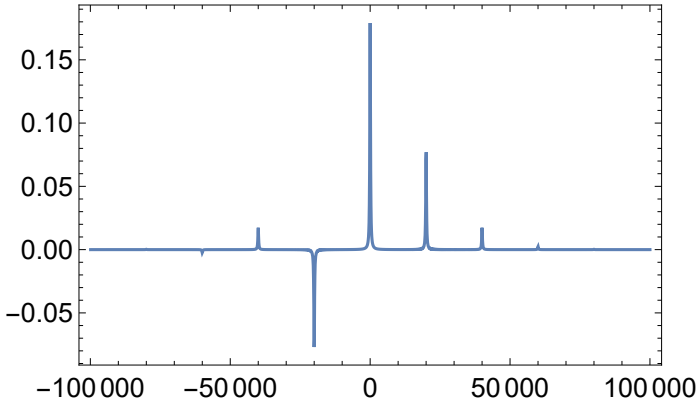
Signal1D: Using LineBroadening → 2π × 286.863 rad s^{-1}.

```
Signal[ {0, 5.11 × 10^-3, 5. × 10^-6} , << 1023 >>]
```

```
ListPlot[Re@sig, Frame → True, Joined → True]
```




```
ListPlot[Re@FT@sig, Frame → True, Joined → True, PlotRange → All, Axes → None]
```



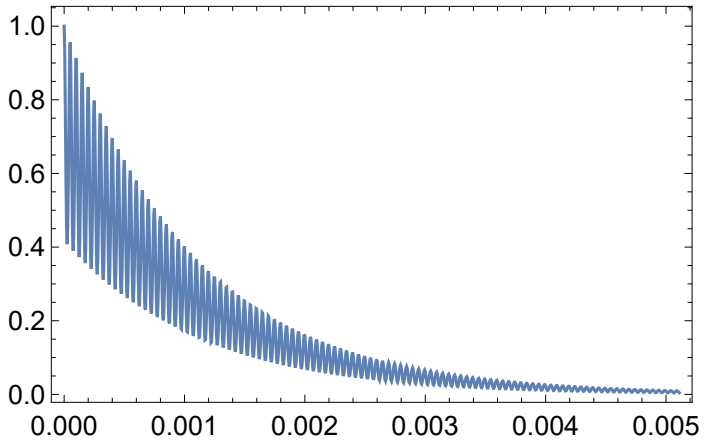
COMPUTE calculation with implicit γ-average

```
sig = Signal1D[{{2 π 200 × 10^3, "1k"}},
    BackgroundGenerator →
     HCSA[{ωaniso, η}, ΩPR, {ωr, βRL}],
    CarouselAverage → True
   ];
```

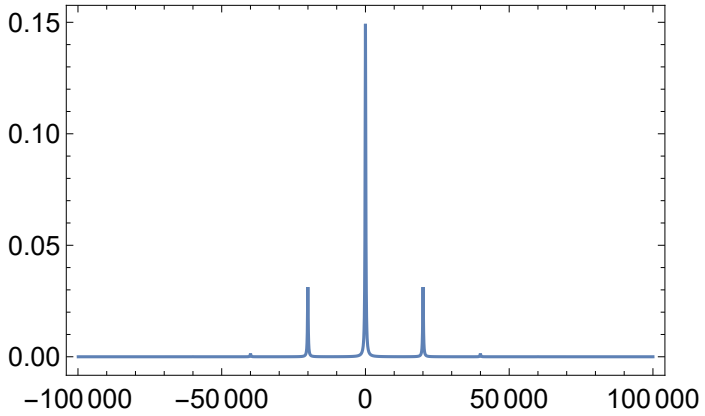
Signal1D: Using SignalCalculationMethod → COMPUTE

Signal1D: Using LineBroadening → 2π × 286.863 rad s^{-1}.

```
ListPlot[Re@sig, Frame → True, Joined → True]
```




```
ListPlot[Re@FT@sig, Frame → True, Joined → True, PlotRange → All, Axes → None]
```



powder-average MAS spectra

parameters

```
Clear[ΩPR];
```

```
ωaniso = 2 π 40 × 10^3;  η = 0.5;
βRL = ArcTan@Sqrt[2];
ωr = 10 × 2 π × 10^3;
T = 5 × 10^-3;  npoints = 1024;
```

simulations

10 Lebedev angles: COMPUTE

```
sig = Signal1D[{{2 π 200 × 10^3, "1k"}},
   BackgroundGenerator →
    HCSA[{ωaniso, η}, ΩPR, {ωr, βRL}],
   CarouselAverage → True,
   EnsembleAverage → {ΩPR, OrientationsAndWeights["Leboct10"]}
  ]
```

```
Predefined orientational sampling schemes:
 {Leboct10, Leboct16, Leboct19, Leboct22, Leboct31, Leboct37, Leboct46,
  Leboct85, POLYTOPE12, POLYTOPE60, Randomαβ, Randomαβγ, Randomβ, REPULSION100,
  REPULSION150, REPULSION168, REPULSION232, REPULSION376, REPULSION700,
  Stepαβ, Stepβ, ZCW1154, ZCW144, ZCW200, ZCW300, ZCW50, ZCW538, ZCW6044}
 Execute OrientationalSamplingScheme[scheme] for the usage message of a sampling scheme.
```

Signal1D: Using SignalCalculationMethod → COMPUTE

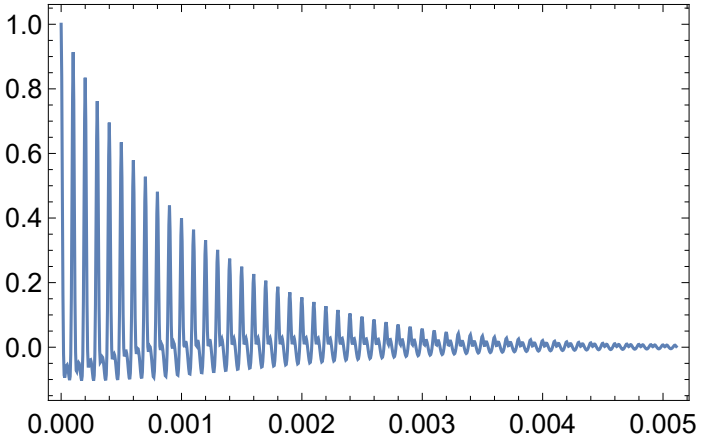
Signal1D: Using LineBroadening → $2\pi \times 286.863$ rad s^{-1}.

Get: Cannot open CloudObjectLoader`.

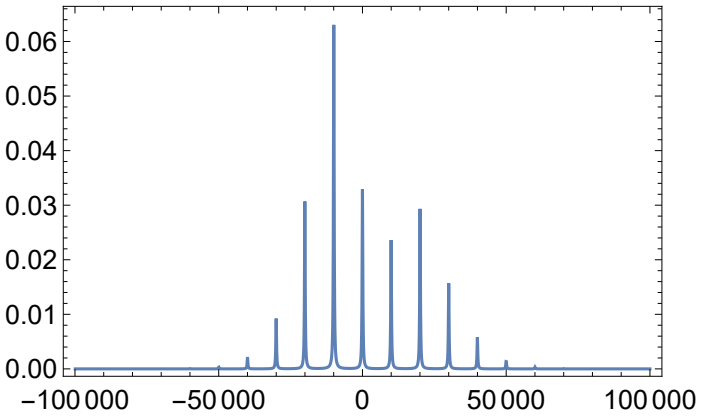
SetOperatorBasis: the operator basis has been set to ShiftAndZOperatorBasis[{{1, $\frac{1}{2}$}}, Sorted → CoherenceOrder].

```
Signal[ {0, 5.11 × 10^-3, 5. × 10^-6} , { Lorentzian ,<< 167 >>} ]
```

```
ListPlot[Re@sig, Frame → True, Joined → True]
```



```
ListPlot[Re@FT@sig, Frame → True, Joined → True, PlotRange → All, Axes → None]
```



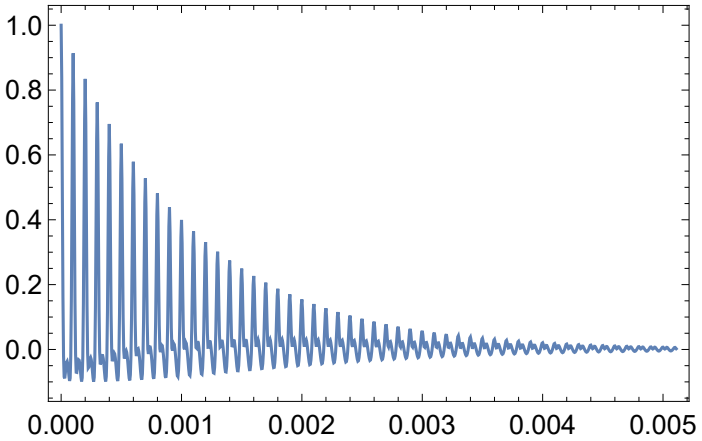
85 Lebedev angles

```
sig = Signal1D[{{2 π 200 × 10^3, "1k"}},
    BackgroundGenerator →
     HCSA[{ωaniso, η}, ΩPR, {ωr, βRL}],
    CarouselAverage → True,
    EnsembleAverage → {ΩPR, OrientationsAndWeights["Leboct85"]}
   ];
```

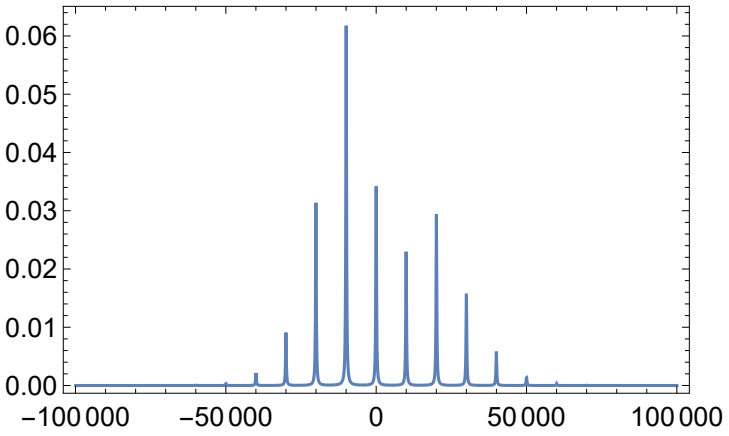
Signal1D: Using SignalCalculationMethod → COMPUTE

Signal1D: Using LineBroadening → $2\pi \times 286.863$ rad s^{-1}.

```
ListPlot[Re@sig, Frame → True, Joined → True]
```



```
ListPlot[Re@FT@sig, Frame → True, Joined → True, PlotRange → All, Axes → None]
```



Note that the simulation with only 10 Lebedev angles is almost the same as the one with Lebedev 85 angles.