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

```
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*.

2-spin-1/2 system

set up dipolar coupled 2-spin-1/2 system

```
SetSpinSystem[2]
```

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

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

```
H0 = Ω1 opI[1, "z"] + Ω2 opI[2, "z"] + d opT[{1, 2}, {2, 0}] Sqrt[6]
```

$$-\frac{1}{2}\,\mathrm{d}\,(\mathrm{I}_1^-\bullet\mathrm{I}_2^+ + \mathrm{I}_1^+\bullet\mathrm{I}_2^- - 4\,(\mathrm{I}_{1z}\bullet\mathrm{I}_{2z})) + \Omega1\,\mathrm{I}_{1z} + \Omega2\,\mathrm{I}_{2z}$$

```
parameters = {Ω1 → 2 π 5 × 10^3, Ω2 → 2 π (2 × 10^3), d → 2 π 10 × 10^3}
```

```
{Ω1 → 10 000 π, Ω2 → 4000 π, d → 20 000 π}
```

static spectrum with no decoupling

```
T = 40 × 10^-3; δt = 10 × 10^-6;
```

```
sig =
 Signal1D[{0, T, δt},
  BackgroundGenerator → (H0 /. parameters)
 ]
```

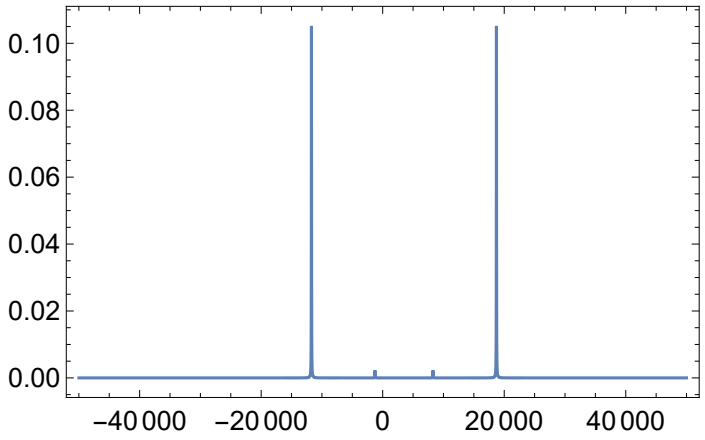
Signal1D: Using SignalCalculationMethod → Diagonalization

Signal1D: the last sampling point has been dropped in order to get an even number of points.

Signal1D: Using LineBroadening → 2π × 36.6468 rad s^{-1}.

```
Signal[ {0, 40. × 10^-3, 10. × 10^-6} , { Lorentzian ,<< 4 >>} ]
```

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



homonuclear decoupling examples

Lee-Goldburg decoupling

```
ωnut = 2 π 50 × 10^3
```

$100\,000\,\pi$

```
ωoff = ωnut / Sqrt[2]
```

$50\,000\,\sqrt{2}\,\pi$

```
τLG = N[2 π / (ωoff Sqrt[3])];
τLG // EngineeringForm
```

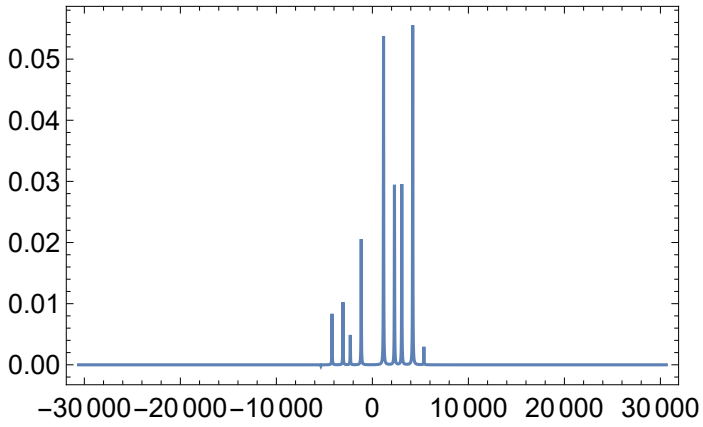
16.3299×10^{-6}

```
sig =
  Signal1D[{0, T, τLG},
   ωnut opI["x"] + ωoff opI["z"],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

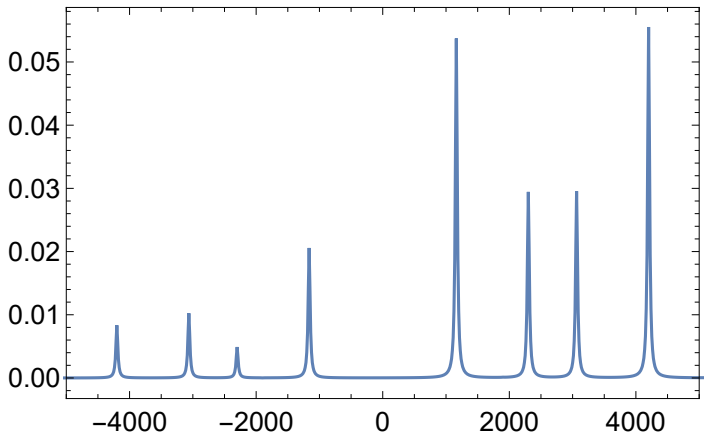
Signal1D: Using SignalCalculationMethod → Diagonalization

Signal1D: Using LineBroadening → $2\pi \times 36.6617$ rad s^{-1}.

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




```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```



the result is not very good. There are still large dipolar splittings

these are the expected peak positions:

```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

FSLG

```
ωnut = 2 π 50 × 10^3
```

$100\,000\,\pi$

```
ωoff = ωnut / Sqrt[2]
```

$50\,000\,\sqrt{2}\,\pi$

```
τLG = N[2 π / (ωoff Sqrt[3])];
τLG // EngineeringForm
```

16.3299×10^{-6}

```
FSLG = {{ωnut opI["x"] + ωoff opI["z"], τLG}, {-ωnut opI["x"] - ωoff opI["z"], τLG}};
```

```
T = 40 × 10^-3; δt = 10 × 10^-6;
```

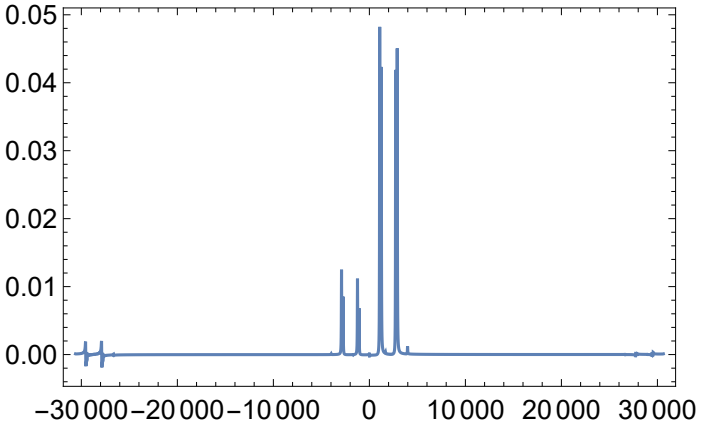
```
sig =
 Signal1D[{0, T, τLG},
  Repeat[FSLG],
  BackgroundGenerator → (H0 /. parameters)
 ]
```

Signal1D: Using SignalCalculationMethod → COMPUTE

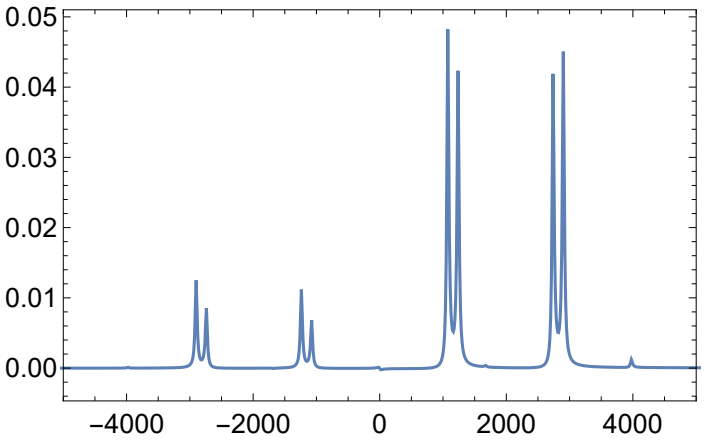
Signal1D: Using LineBroadening → $2\pi \times 36.6617$ rad s^{-1}.

```
Signal[ {0, 39.9837 × 10^-3, 16.3299 × 10^-6} , { Lorentzian ,<< 26 >>} ]
```

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




```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```




```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

this gives a good result with small splittings, and peaks in the expected position - although with a rather large image

WAHUHA or WHH4

```
τ = 5 × 10^-6
```

$$\frac{1}{200\,000}$$

```
WHH4 = {
    { None, τ},
    RotationSuperoperator[{π / 2, π}],
    {None, τ},
    RotationSuperoperator[{π / 2, 3 π / 2}],
    {None, 2 τ},
    RotationSuperoperator[{π / 2, π / 2}],
    {None, τ},
    RotationSuperoperator[{π / 2, 0}],
    {None, τ}
   };
```

```
sig =
  Signal1D[{0, T, EventDuration[WHH4] / 2},
   Repeat[WHH4],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

Signal1D: Using SignalCalculationMethod → COMPUTE

Signal1D: the last sampling point has been dropped in order to get an even number of points.

Signal1D: Using LineBroadening → $2\pi \times 36.633$ rad s^{-1}.

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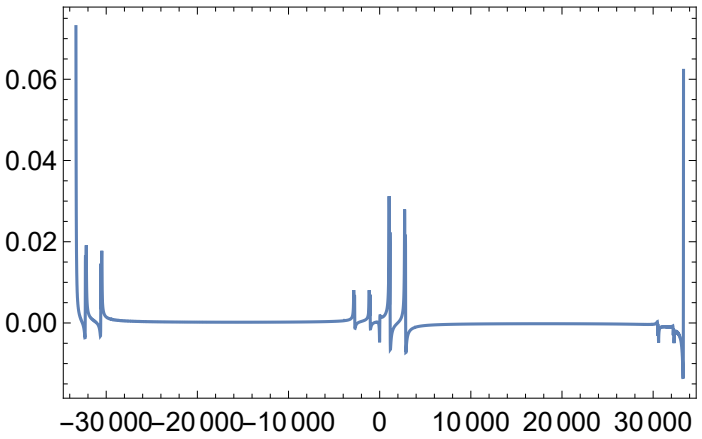


```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
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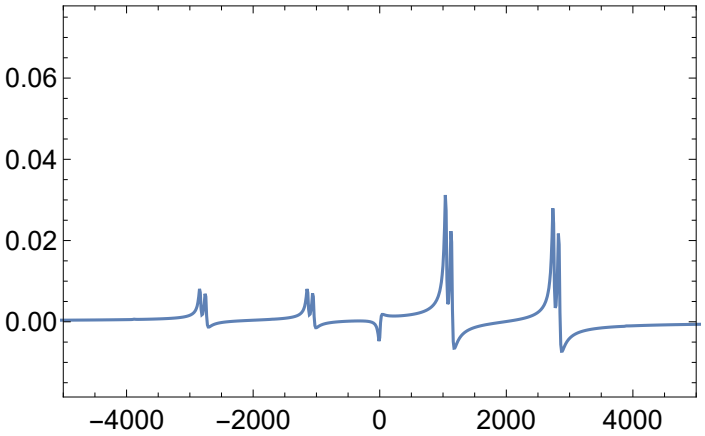

expected peak positions:

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N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

not a bad result, although there is a strong phase shift

3-spin-1/2 system

set up dipolar coupled 3-spin-1/2 system with random dipolar couplings

```
SetSpinSystem[3]
```

SetSpinSystem: the spin system has been set to $\{\{1, \frac{1}{2}\}, \{2, \frac{1}{2}\}, \{3, \frac{1}{2}\}\}$

SetBasis: the state basis has been set to ZeemanBasis$[\{\{1, \frac{1}{2}\}, \{2, \frac{1}{2}\}, \{3, \frac{1}{2}\}\}$, BasisLabels → Automatic$]$.

```
H0 = Ω1 opI[1, "z"] + Ω2 opI[2, "z"] + Ω3 opI[3, "z"] +
  Sum[d[j, k] opT[{j, k}, {2, 0}] Sqrt[6], {j, 2, 3}, {k, 1, j - 1}]
```

$$-\frac{1}{2} d[2, 1] \left(I_1^- \cdot I_2^+ + I_1^+ \cdot I_2^- - 4 \left(I_{1z} \cdot I_{2z}\right)\right) - \frac{1}{2} d[3, 1] \left(I_1^- \cdot I_3^+ + I_1^+ \cdot I_3^- - 4 \left(I_{1z} \cdot I_{3z}\right)\right) - \frac{1}{2} d[3, 2] \left(I_2^- \cdot I_3^+ + I_2^+ \cdot I_3^- - 4 \left(I_{2z} \cdot I_{3z}\right)\right) + \Omega 1\, I_{1z} + \Omega 2\, I_{2z} + \Omega 3\, I_{3z}$$

```
DipolarCouplings =
 Flatten@Table[d[j, k] → RandomReal[2 π {-5 × 10^3, 5 × 10^3}], {j, 2, 3}, {k, 1, j - 1}]
```

```
{d[2, 1] → -740.622, d[3, 1] → -9350.64, d[3, 2] → -10612.8}
```

```
parameters = {Ω1 → 2 π (5 × 10^3), Ω2 → 2 π (5 × 10^3), Ω3 → 2 π (2 × 10^3),
   Sequence @@ DipolarCouplings
 }
```

```
{Ω1 → 10000 π, Ω2 → 10000 π, Ω3 → 4000 π,
 d[2, 1] → -740.622, d[3, 1] → -9350.64, d[3, 2] → -10612.8}
```

```
H0 /. parameters
```

$$370.311 \left(I_1^- \cdot I_2^+ + I_1^+ \cdot I_2^- - 4 \left(I_{1z} \cdot I_{2z}\right)\right) + 4675.32 \left(I_1^- \cdot I_3^+ + I_1^+ \cdot I_3^- - 4 \left(I_{1z} \cdot I_{3z}\right)\right) + 5306.39 \left(I_2^- \cdot I_3^+ + I_2^+ \cdot I_3^- - 4 \left(I_{2z} \cdot I_{3z}\right)\right) + 10000 \pi I_{1z} + 10000 \pi I_{2z} + 4000 \pi I_{3z}$$

static spectrum with no decoupling

```
T = 40 × 10^-3; δt = 10 × 10^-6;
```

```
sig =
 Signal1D[{0, T, δt},
  BackgroundGenerator → (H0 /. parameters)
 ]
```

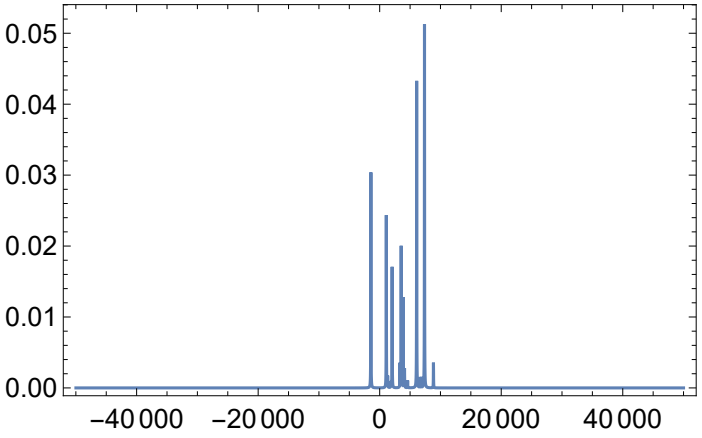
Signal1D: Using SignalCalculationMethod → Diagonalization

Signal1D: the last sampling point has been dropped in order to get an even number of points.

Signal1D: Using LineBroadening → $2\pi \times 36.6468$ rad s^{-1}.

```
Signal[ {0, 40. × 10^-3, 10. × 10^-6} , { Lorentzian ,<< 15 >>} ]
```

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



homonuclear decoupling examples

Lee-Goldburg decoupling

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ωnut = 2 π 50 × 10^3
```

$100\,000\,\pi$

```
ωoff = ωnut / Sqrt[2]
```

$50\,000\,\sqrt{2}\,\pi$

```
τLG = N[2 π / (ωoff Sqrt[3])]
τLG // EngineeringForm
```

```
0.0000163299
```

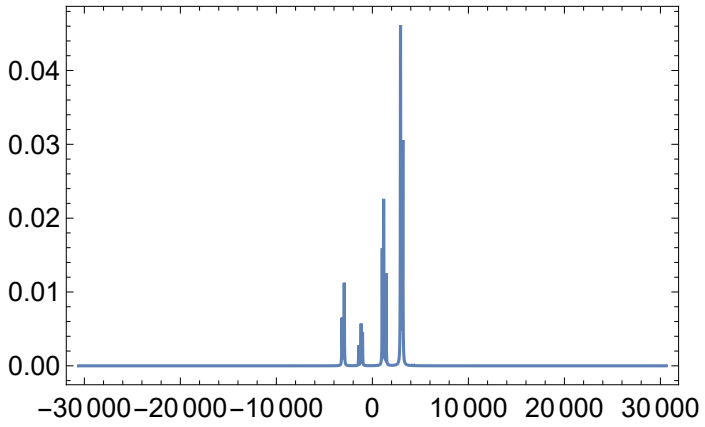
16.3299×10^{-6}

```
sig =
  Signal1D[{0, T, τLG},
   ωnut opI["x"] + ωoff opI["z"],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

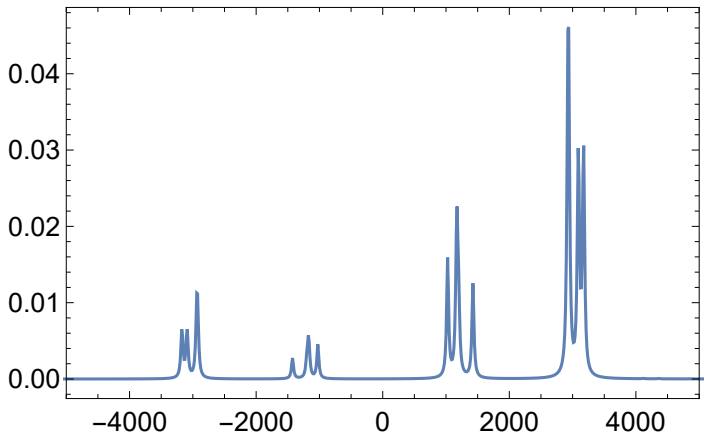
Signal1D: Using SignalCalculationMethod → Diagonalization

Signal1D: Using LineBroadening → $2\pi \times 36.6617$ rad s^{-1}.

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




```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```



the result is very poor. There are still large dipolar splittings

these are the expected peak positions:

```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

FSLG

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ωnut = 2 π 50 × 10^3
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ωoff = ωnut / Sqrt[2]
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```
τLG = N[2 π / (ωoff Sqrt[3])];
τLG // EngineeringForm
```

16.3299×10^{-6}

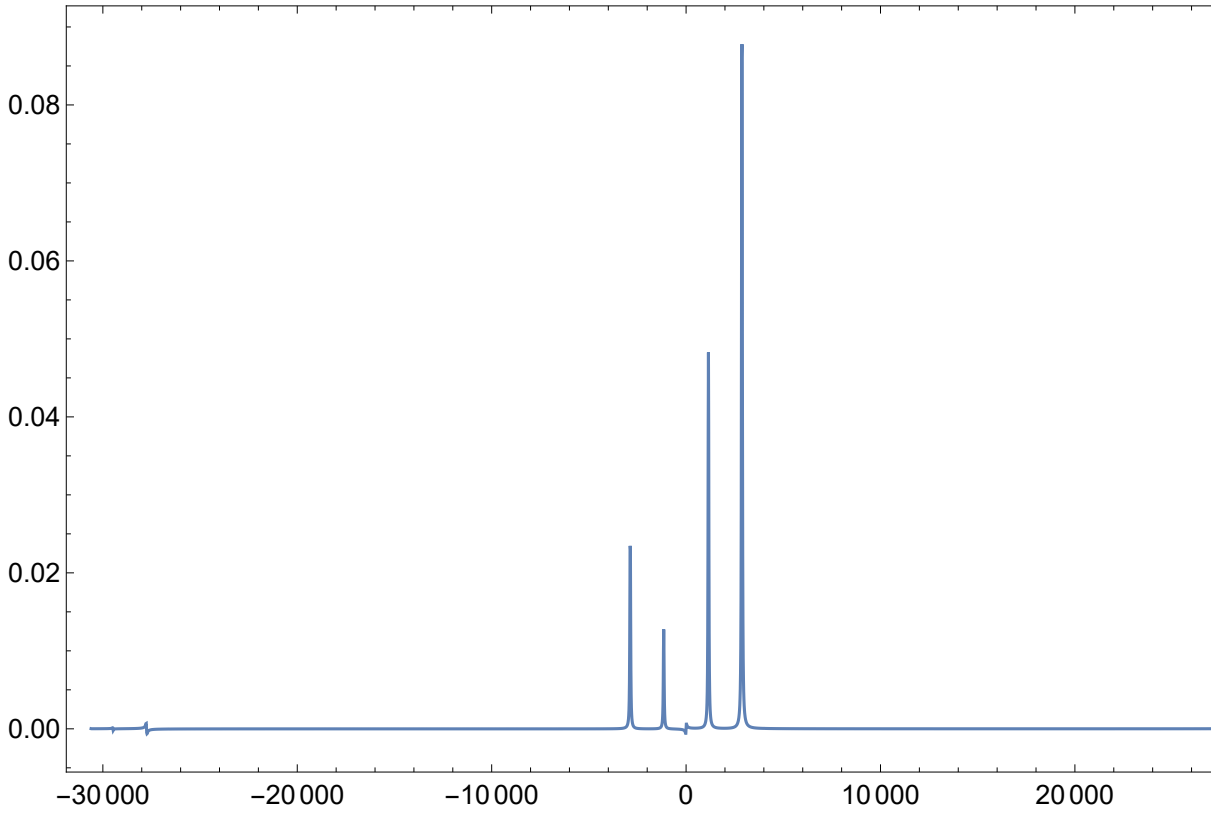
```
FSLG = {{ωnut opI["x"] + ωoff opI["z"], τLG}, {-ωnut opI["x"] - ωoff opI["z"], τLG}};
```

```
sig =
  Signal1D[{0, T, τLG},
   Repeat[FSLG],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

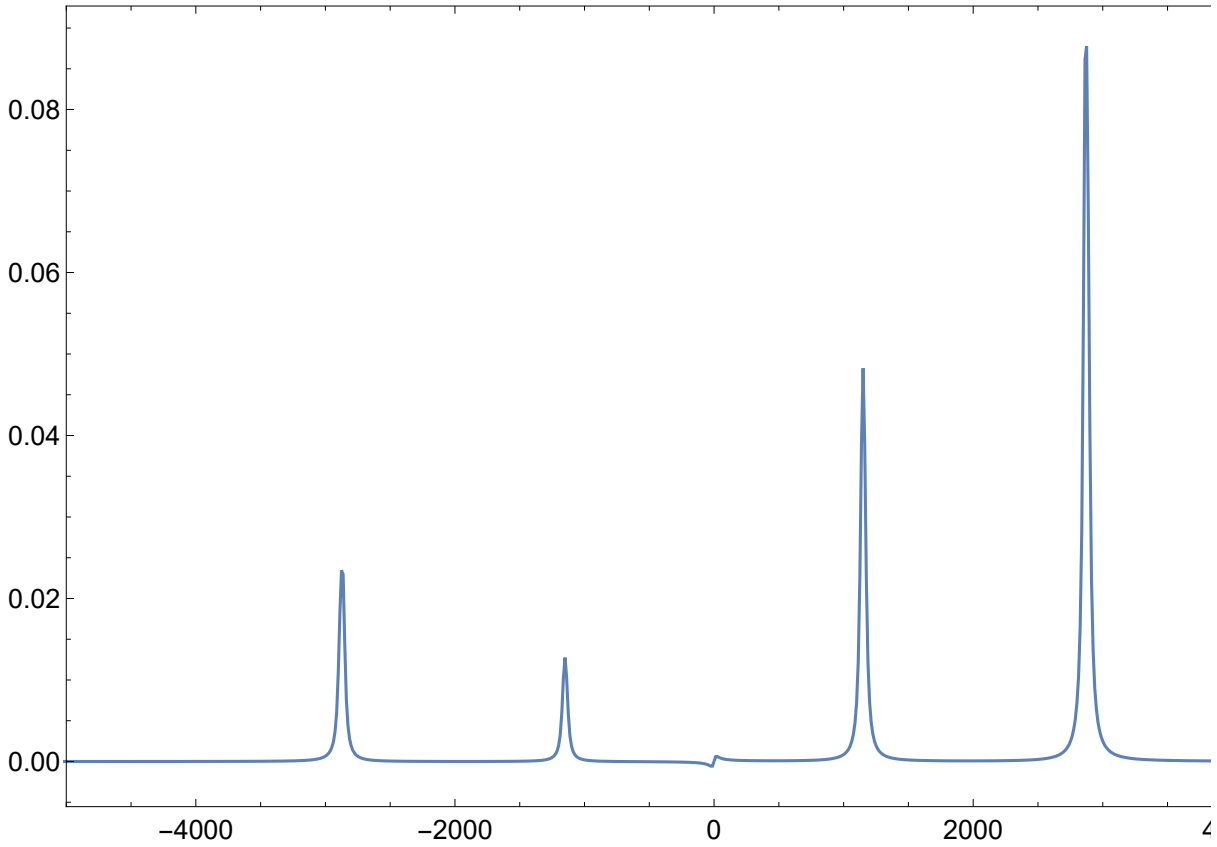
Signal1D: Using SignalCalculationMethod → COMPUTE

Signal1D: Using LineBroadening → $2\pi \times 36.6617$ rad s^{-1}.

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



```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```




```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

the peaks are in the expected positions, although with a rather large image.

WAHUHA or WHH4

```
τ = 5 × 10^-6
```

$$\frac{1}{200\,000}$$

```
WHH4 = {
    {None, τ},
    RotationSuperoperator[{π/2, π}],
    {None, τ},
    RotationSuperoperator[{π/2, 3π/2}],
    {None, 2τ},
    RotationSuperoperator[{π/2, π/2}],
    {None, τ},
    RotationSuperoperator[{π/2, 0}],
    {None, τ}
  };
```

```
sig =
  Signal1D[{0, T, EventDuration[WHH4] / 2},
   Repeat[WHH4],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

Signal1D: Using SignalCalculationMethod → COMPUTE

Signal1D: the last sampling point has been dropped in order to get an even number of points.

Signal1D: Using LineBroadening → $2\pi \times 36.633$ rad s^{-1}.

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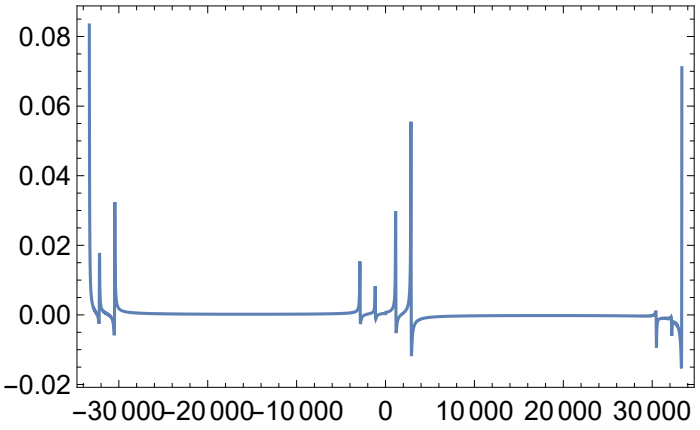
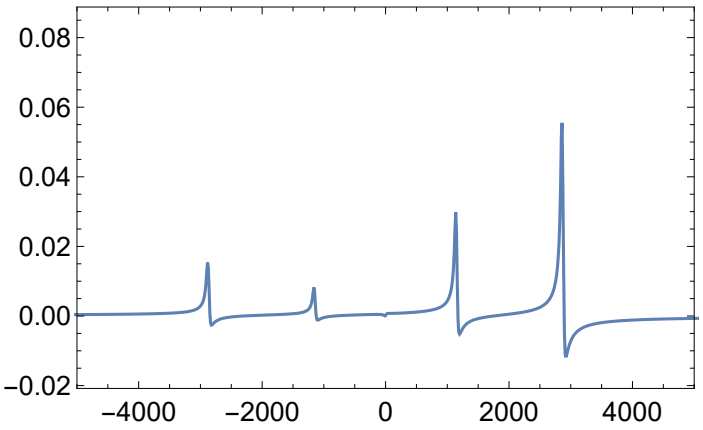



```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```



expected peak positions:

```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

not a bad result, although there is a strong phase shift

4-spin-1/2 system

set up dipolar coupled 4-spin-1/2 system with random dipolar couplings

```
SetSpinSystem[4]
```

SetSpinSystem: the spin system has been set to $\{\{1, \frac{1}{2}\}, \{2, \frac{1}{2}\}, \{3, \frac{1}{2}\}, \{4, \frac{1}{2}\}\}$

SetBasis: the state basis has been set to ZeemanBasis$[\{\{1, \frac{1}{2}\}, \{2, \frac{1}{2}\}, \{3, \frac{1}{2}\}, \{4, \frac{1}{2}\}\}$, BasisLabels → Automatic].

```
H0 = Ω1 opI[1, "z"] + Ω2 opI[2, "z"] + Ω3 opI[3, "z"] + Ω4 opI[4, "z"] +
   Sum[d[j, k] opT[{j, k}, {2, 0}] Sqrt[6], {j, 2, 3}, {k, 1, j - 1}]
```

$$-\frac{1}{2} d[2, 1] \left(I_1^- \cdot I_2^+ + I_1^+ \cdot I_2^- - 4 \left(I_{1z} \cdot I_{2z}\right)\right) - \frac{1}{2} d[3, 1] \left(I_1^- \cdot I_3^+ + I_1^+ \cdot I_3^- - 4 \left(I_{1z} \cdot I_{3z}\right)\right) - \frac{1}{2} d[3, 2] \left(I_2^- \cdot I_3^+ + I_2^+ \cdot I_3^- - 4 \left(I_{2z} \cdot I_{3z}\right)\right) + \Omega 1\, I_{1z} + \Omega 2\, I_{2z} + \Omega 3\, I_{3z} + \Omega 4\, I_{4z}$$

```
DipolarCouplings =
 Flatten@Table[d[j, k] → RandomReal[2 π {-5 × 10^3, 5 × 10^3}], {j, 2, 4}, {k, 1, j - 1}]
```

```
{d[2, 1] → -29758.1, d[3, 1] → -28133.6, d[3, 2] → 1946.3,
 d[4, 1] → 4429.44, d[4, 2] → -349.795, d[4, 3] → 22305.5}
```

```
parameters =
 {Ω1 → 2 π (5 × 10^3), Ω2 → 2 π (5 × 10^3), Ω3 → 2 π (2 × 10^3), Ω4 → 2 π (2 × 10^3),
  Sequence @@ DipolarCouplings
 }
```

```
{Ω1 → 10000 π, Ω2 → 10000 π, Ω3 → 4000 π, Ω4 → 4000 π,
 d[2, 1] → -29758.1, d[3, 1] → -28133.6, d[3, 2] → 1946.3,
 d[4, 1] → 4429.44, d[4, 2] → -349.795, d[4, 3] → 22305.5}
```

```
H0 /. parameters
```

$$14879.1 \left(I_1^- \cdot I_2^+ + I_1^+ \cdot I_2^- - 4 \left(I_{1z} \cdot I_{2z}\right)\right) + 14066.8 \left(I_1^- \cdot I_3^+ + I_1^+ \cdot I_3^- - 4 \left(I_{1z} \cdot I_{3z}\right)\right) - 973.148 \left(I_2^- \cdot I_3^+ + I_2^+ \cdot I_3^- - 4 \left(I_{2z} \cdot I_{3z}\right)\right) + 10000 \pi I_{1z} + 10000 \pi I_{2z} + 4000 \pi I_{3z} + 4000 \pi I_{4z}$$

static spectrum with no decoupling

```
T = 40 × 10^-3; δt = 10 × 10^-6;
```

```
sig =
 Signal1D[{0, T, δt},
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```

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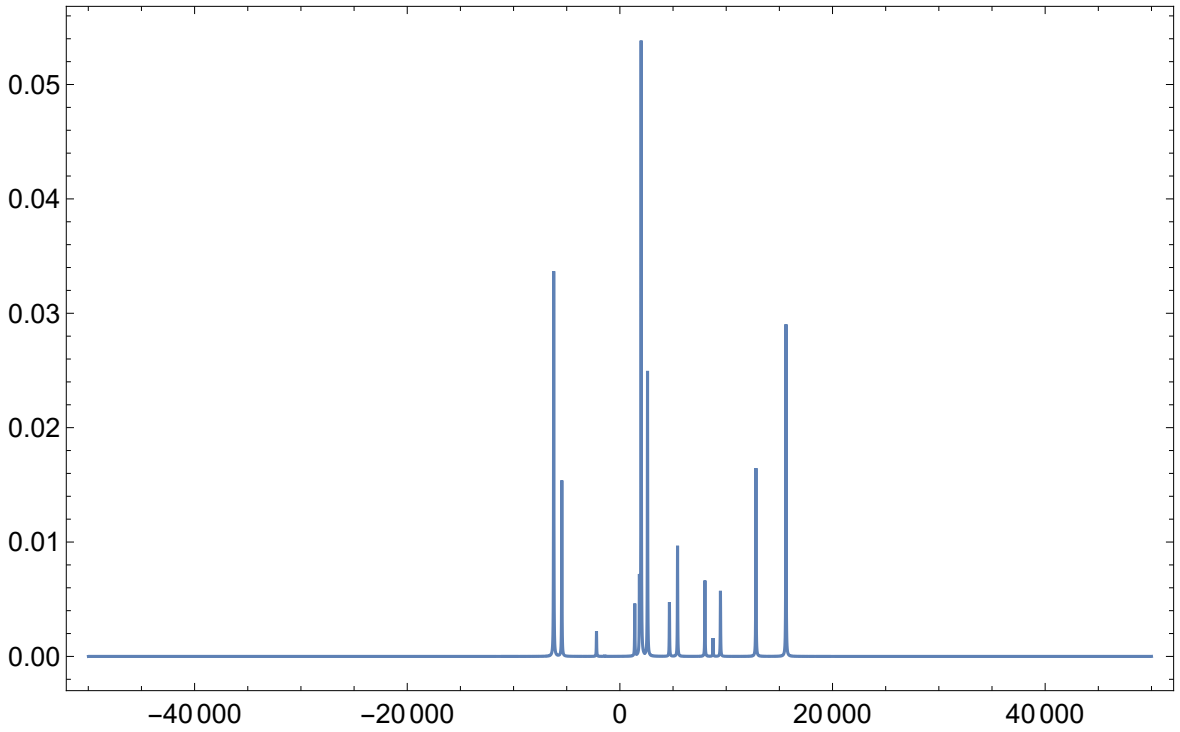
Signal1D: Using LineBroadening → $2\pi \times 36.6468$ rad s^{-1}.

```
Signal[ {0, 40. × 10^-3, 10. × 10^-6} , { Lorentzian ,<< 34 >>} ]
```

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



homonuclear decoupling examples

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τLG = N[2 π / (ωoff Sqrt[3])]
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16.3299×10^{-6}

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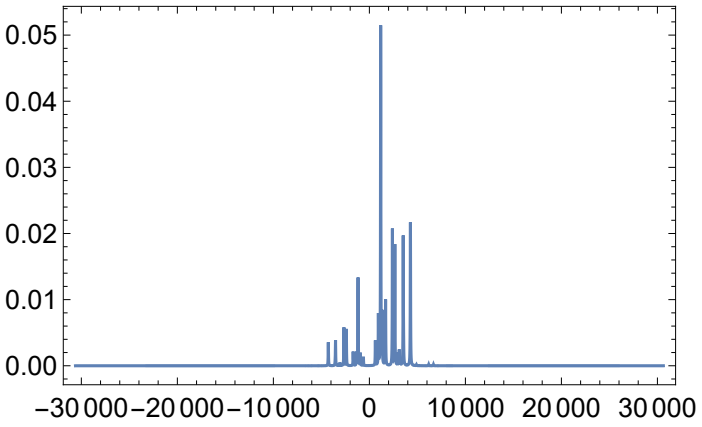
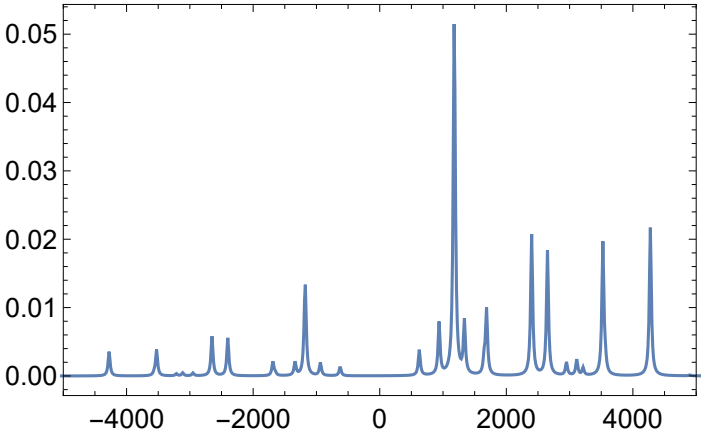



```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```



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16.3299×10^{-6}

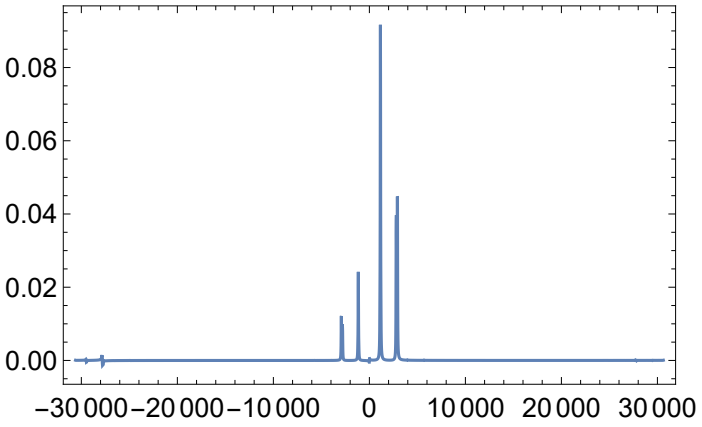
```
FSLG = {{ωnut opI["x"] + ωoff opI["z"], τLG}, {-ωnut opI["x"] - ωoff opI["z"], τLG}};
```

```
sig =
  Signal1D[{0, T, τLG},
   Repeat[FSLG],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

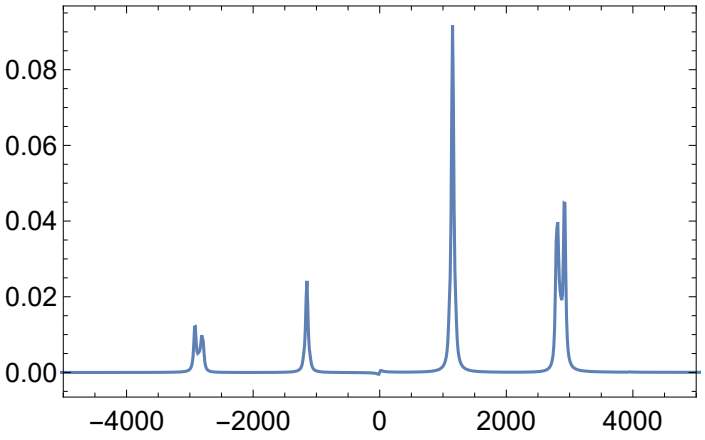
Signal1D: Using SignalCalculationMethod → COMPUTE

Signal1D: Using LineBroadening → $2\pi \times 36.6617$ rad s^{-1}.

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




```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```




```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

the peaks are in the expected positions, although with a rather large image.

WAHUHA or WHH4

```
τ = 5 × 10^-6
```

$$\frac{1}{200\,000}$$

```
WHH4 = {
    { None, τ},
    RotationSuperoperator[{π / 2, π}],
    {None, τ},
    RotationSuperoperator[{π / 2, 3 π / 2}],
    {None, 2 τ},
    RotationSuperoperator[{π / 2, π / 2}],
    {None, τ},
    RotationSuperoperator[{π / 2, 0}],
    {None, τ}
   };
```

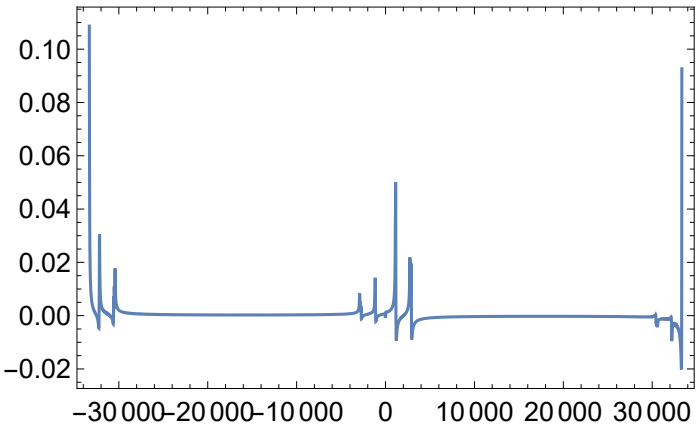
```
sig =
  Signal1D[{0, T, EventDuration[WHH4] / 2},
   Repeat[WHH4],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

Signal1D: Using SignalCalculationMethod → COMPUTE

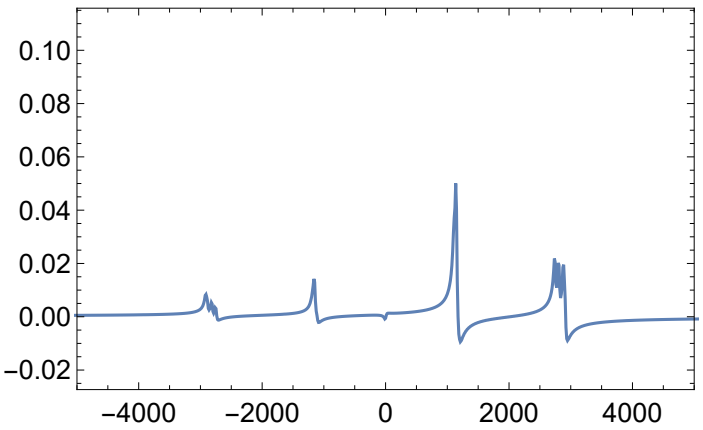
Signal1D: the last sampling point has been dropped in order to get an even number of points.

Signal1D: Using LineBroadening → $2\pi \times 36.633$ rad s^{-1}.

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




```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```



expected peak positions:

```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

not a bad result, although there is a strong phase shift

5-spin-1/2 system

set up dipolar coupled 5-spin-1/2 system with random dipolar couplings

```
SetSpinSystem[5]
```

SetSpinSystem: the spin system has been set to $\{\{1, \frac{1}{2}\}, \{2, \frac{1}{2}\}, \{3, \frac{1}{2}\}, \{4, \frac{1}{2}\}, \{5, \frac{1}{2}\}\}$

SetBasis: the state basis has been set to ZeemanBasis$[\{\{1, \frac{1}{2}\}, \{2, \frac{1}{2}\}, \{3, \frac{1}{2}\}, \{4, \frac{1}{2}\}, \{5, \frac{1}{2}\}\}$, BasisLabels → Automatic].

```
H0 = Ω1 opI[1, "z"] + Ω2 opI[2, "z"] + Ω3 opI[3, "z"] + Ω4 opI[4, "z"] + Ω5 opI[5, "z"] +
  Sum[d[j, k] opT[{j, k}, {2, 0}] Sqrt[6], {j, 2, 5}, {k, 1, j - 1}]
```

$$-\frac{1}{2} d[2, 1] (I_1^- \bullet I_2^+ + I_1^+ \bullet I_2^- - 4 (I_{1z} \bullet I_{2z})) - \frac{1}{2} d[3, 1] (I_1^- \bullet I_3^+ + I_1^+ \bullet I_3^- - 4 (I_{1z} \bullet I_{3z})) - \frac{1}{2} d[4, 1] (I_1^- \bullet I_4^+ + I_1^+ \bullet I_4^- - 4 (I_{1z} \bullet I_{4z})) - \frac{1}{2} d[5, 1] (I_1^- \bullet I_5^+ + I_1^+ \bullet I_5^- - 4 (I_{1z} \bullet I_{5z})) - \frac{1}{2} d[3, 2] (I_2^- \bullet I_3^+ + I_2^+ \bullet I_3^- - 4 (I_{2z} \bullet I_{3z})) - \frac{1}{2} d[4, 2] (I_2^- \bullet I_4^+ + I_2^+ \bullet I_4^- - 4 (I_{2z} \bullet I_{4z})) - \frac{1}{2} d[5, 2] (I_2^- \bullet I_5^+ + I_2^+ \bullet I_5^- - 4 (I_{2z} \bullet I_{5z})) - \frac{1}{2} d[4, 3] (I_3^- \bullet I_4^+ + I_3^+ \bullet I_4^- - 4 (I_{3z} \bullet I_{4z})) - \frac{1}{2} d[5, 3] (I_3^- \bullet I_5^+ + I_3^+ \bullet I_5^- - 4 (I_{3z} \bullet I_{5z})) - \frac{1}{2} d[5, 4] (I_4^- \bullet I_5^+ + I_4^+ \bullet I_5^- - 4 (I_{4z} \bullet I_{5z})) + Ω1 I_{1z} + Ω2 I_{2z} + Ω3 I_{3z} + Ω4 I_{4z} + Ω5 I_{5z}$$

```
DipolarCouplings =
 Flatten@Table[d[j, k] → RandomReal[2 π {-5 × 10^3, 5 × 10^3}], {j, 2, 5}, {k, 1, j - 1}]
```

```
{d[2, 1] → -20028.5, d[3, 1] → -13804.8, d[3, 2] → -18999.4,
 d[4, 1] → -11951.5, d[4, 2] → 6576.55, d[4, 3] → -29600.4, d[5, 1] → 14317.7,
 d[5, 2] → -10281.3, d[5, 3] → -17589.5, d[5, 4] → -27621.8}
```

```
parameters = {Ω1 → 2 π (5 × 10^3), Ω2 → 2 π (5 × 10^3),
  Ω3 → 2 π (2 × 10^3), Ω4 → 2 π (2 × 10^3), Ω5 → 2 π (2 × 10^3),
  Sequence @@ DipolarCouplings
 }
```

```
{Ω1 → 10000 π, Ω2 → 10000 π, Ω3 → 4000 π, Ω4 → 4000 π, Ω5 → 4000 π,
 d[2, 1] → -20028.5, d[3, 1] → -13804.8, d[3, 2] → -18999.4,
 d[4, 1] → -11951.5, d[4, 2] → 6576.55, d[4, 3] → -29600.4, d[5, 1] → 14317.7,
 d[5, 2] → -10281.3, d[5, 3] → -17589.5, d[5, 4] → -27621.8}
```

```
H0 /. parameters
```

$$10\,014.3\,(I_1^-\cdot I_2^+ + I_1^+\cdot I_2^- - 4\,(I_{1z}\cdot I_{2z})) + 6902.38\,(I_1^-\cdot I_3^+ + I_1^+\cdot I_3^- - 4\,(I_{1z}\cdot I_{3z})) +$$
$$5975.77\,(I_1^-\cdot I_4^+ + I_1^+\cdot I_4^- - 4\,(I_{1z}\cdot I_{4z})) - 7158.84\,(I_1^-\cdot I_5^+ + I_1^+\cdot I_5^- - 4\,(I_{1z}\cdot I_{5z})) +$$
$$9499.71\,(I_2^-\cdot I_3^+ + I_2^+\cdot I_3^- - 4\,(I_{2z}\cdot I_{3z})) - 3288.28\,(I_2^-\cdot I_4^+ + I_2^+\cdot I_4^- - 4\,(I_{2z}\cdot I_{4z})) +$$
$$5140.65\,(I_2^-\cdot I_5^+ + I_2^+\cdot I_5^- - 4\,(I_{2z}\cdot I_{5z})) + 14\,800.2\,(I_3^-\cdot I_4^+ + I_3^+\cdot I_4^- - 4\,(I_{3z}\cdot I_{4z})) +$$
$$8794.75\,(I_3^-\cdot I_5^+ + I_3^+\cdot I_5^- - 4\,(I_{3z}\cdot I_{5z})) + 13\,810.9\,(I_4^-\cdot I_5^+ + I_4^+\cdot I_5^- - 4\,(I_{4z}\cdot I_{5z})) +$$
$$10\,000\,\pi\,I_{1z} + 10\,000\,\pi\,I_{2z} + 4000\,\pi\,I_{3z} + 4000\,\pi\,I_{4z} + 4000\,\pi\,I_{5z}$$

static spectrum with no decoupling

```
T = 40 × 10^-3; δt = 10 × 10^-6;
```

```
sig =
 Signal1D[{0, T, δt},
  BackgroundGenerator → (H0 /. parameters)
 ]
```

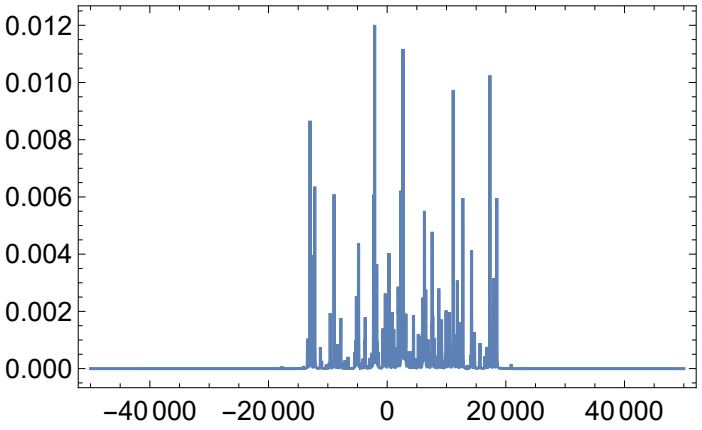
Signal1D: Using SignalCalculationMethod → Diagonalization

Signal1D: the last sampling point has been dropped in order to get an even number of points.

Signal1D: Using LineBroadening → $2\pi \times 36.6468$ rad s^{-1}.

Signal[$\{0, 40. \times 10^{-3}, 10. \times 10^{-6}\}$, { Lorentzian ,<< 210 >>}]

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



homonuclear decoupling examples

Lee-Goldburg decoupling

```
ωnut = 2 π 50 × 10^3
```

$100\,000\,\pi$

```
ωoff = ωnut / Sqrt[2]
```

$50\,000\,\sqrt{2}\,\pi$

```
τLG = N[2 π / (ωoff Sqrt[3])]
τLG // EngineeringForm
```

```
0.0000163299
```

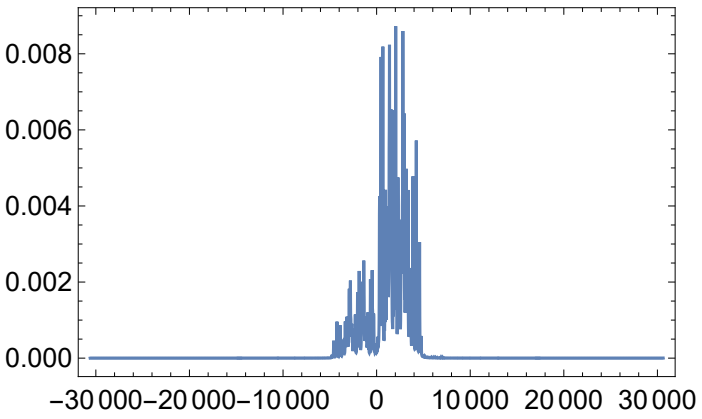
16.3299×10^{-6}

```
sig =
  Signal1D[{0, T, τLG},
   ωnut opI["x"] + ωoff opI["z"],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

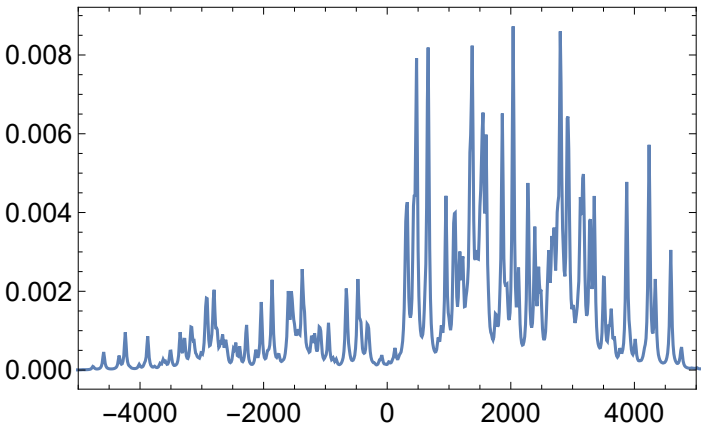
Signal1D: Using SignalCalculationMethod → Diagonalization

Signal1D: Using LineBroadening → $2\pi \times 36.6617$ rad s^{-1}.

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




```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```



the result is very poor. There are still large dipolar splittings

these are the expected peak positions:

```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

FSLG

```
ωnut = 2 π 50 × 10^3
```

$100\,000\,\pi$

```
ωoff = ωnut / Sqrt[2]
```

$50\,000\,\sqrt{2}\,\pi$

```
τLG = N[2 π / (ωoff Sqrt[3])];
τLG // EngineeringForm
```

16.3299×10^{-6}

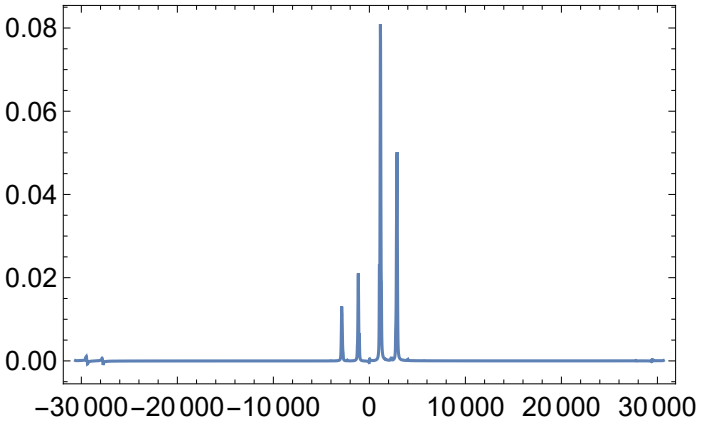
```
FSLG = {{ωnut opI["x"] + ωoff opI["z"], τLG}, {-ωnut opI["x"] - ωoff opI["z"], τLG}};
```

```
sig =
  Signal1D[{0, T, τLG},
   Repeat[FSLG],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

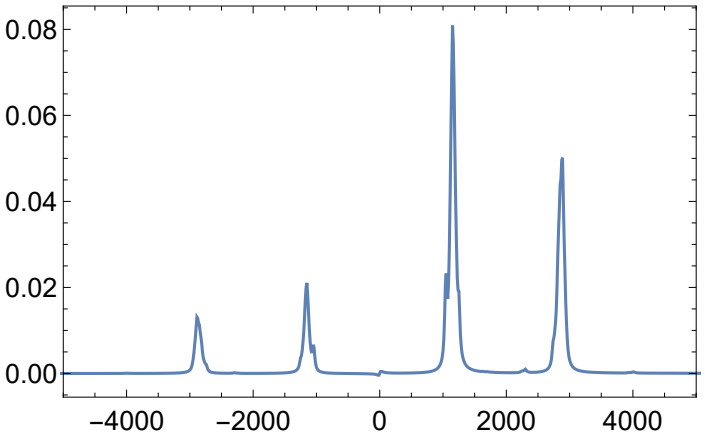
Signal1D: Using SignalCalculationMethod → COMPUTE

Signal1D: Using LineBroadening → $2\pi \times 36.6617$ rad s^{-1}.

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



```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```




```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

the peaks are in the expected positions, although with a rather large image.

WAHUHA or WHH4

```
τ = 5 × 10^-6
```

$$\frac{1}{200\,000}$$

```
WHH4 = {
    {None, τ},
    RotationSuperoperator[{π/2, π}],
    {None, τ},
    RotationSuperoperator[{π/2, 3π/2}],
    {None, 2τ},
    RotationSuperoperator[{π/2, π/2}],
    {None, τ},
    RotationSuperoperator[{π/2, 0}],
    {None, τ}
   };
```

```
sig =
  Signal1D[{0, T, EventDuration[WHH4] / 2},
   Repeat[WHH4],
   BackgroundGenerator → (H0 /. parameters)
  ];
```

Signal1D: Using SignalCalculationMethod → COMPUTE

Signal1D: the last sampling point has been dropped in order to get an even number of points.

Signal1D: Using LineBroadening → $2\pi \times 36.633$ rad s^{-1}.

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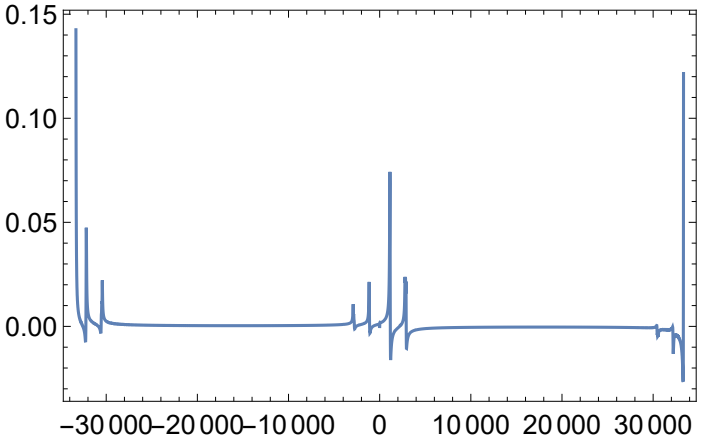
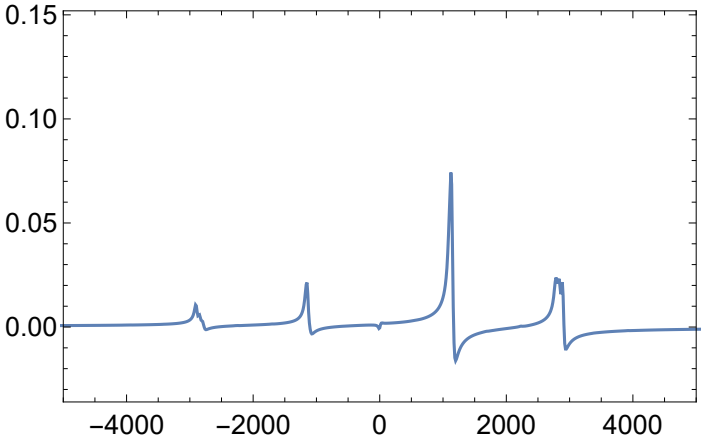



```
ListPlot[Re@FT@sig, Frame → True, Joined → True,
 PlotRange → {{-5000, 5000}, All}, Axes → None]
```



expected peak positions:

```
N[{2 × 10^3, 4 × 10^3} / Sqrt[3]]
```

```
{1154.7, 2309.4}
```

not a bad result, although there is a strong phase shift