RB-SFA: High Harmonic Generation in the Strong Field Approximation via *Mathematica*

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Usage and Examples

Loading the package

You can use this software

- · within the RB-SFA notebook itself by simply running the initialization cells of that notebook, or
- · from an external notebook by loading it as a package.

In the latter case, place a copy of the package file RB-SFA.m on the same directory as your notebook and run the loading command

```
Needs["RBSFA`", FileNameJoin[{NotebookDirectory[], "RB-SFA.m"}]]
```

You can also call the package from another directory by suitably modifying the directory call. If you plan on using this package in the long term you can use the File > Install prompt, in which case the package is simply loaded as Needs["RBSFA`"], though this is not particularly recommended. (A better choice is to include a soft link called RBSFA.m in your \$UserBaseDirectory/Applications/ directory to the file RB-SFA.m. This works just fine and is easy to undo if required.)

To print the version of the package in use, use the command

```
$RBSFAversion
```

```
RB-SFA v2.0.7, Thu 28 Apr 2016 21:03:45
```

There are also commands to get the \$RBSFAtimestamp directly, as well as the git \$RBSFAcommit hash and message.

Simple usage

For basic usage, simply call the main numerical integrator, makeDipoleList, with the vector potential you want to use, and provide any parameters you wish to specify using the FieldParameters option.

```
AbsoluteTiming  \begin{aligned} & \text{simpleDipole = makeDipoleList} [ \\ & \text{VectorPotential} \rightarrow \text{Function} \Big[ t, \Big\{ \frac{F}{\omega} \, \text{Sin}[\omega \, t], \, 0, \, 0 \Big\} \Big], \, \text{FieldParameters} \rightarrow \{ F \rightarrow 0.05, \, \omega \rightarrow 0.057 \} \Big]; \\ & \\ & \Big] \\ & \{ 3.01082, \, \text{Null} \} \end{aligned}
```

Calling the function with insufficient parameters will produce error messages:

$$makeDipoleList\Big[VectorPotential \rightarrow Function\Big[t, \Big\{\frac{F}{\omega} Sin[\omega t], 0, 0\Big\}\Big]\Big]$$

makeDipoleList::pot:

The vector potential A provided as VectorPotential \rightarrow Function $\left[t, \left\{\frac{F \sin[\omega t]}{\omega}, 0, 0\right\}\right]$ is incorrect or is missing FieldParameters.

Its usage as A[4.710127010714186`] returns $\left\{\frac{F \sin[4.71013 \omega]}{\omega}, 0, 0\right\}$ and should return a list of numbers.

\$Aborted

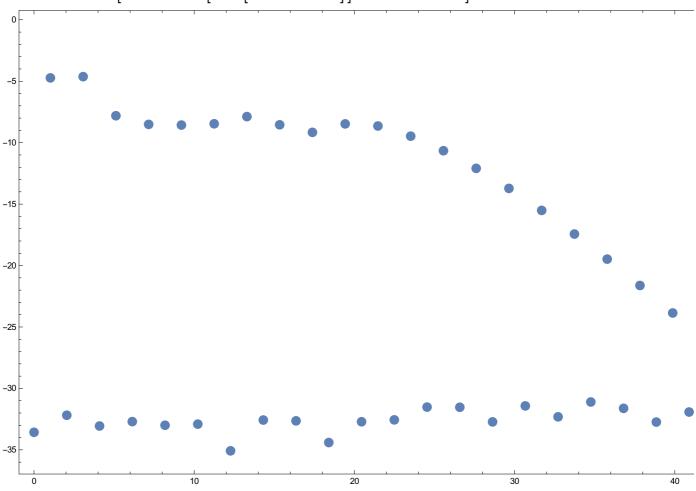
The symbol ω is taken to be the carrier frequency, and is set by default to $\omega = 0.057$ atomic units, corresponding to a wavelength of 800 nm. If the carrier frequency is changed, this must be specified on both the field parameters and the explicit option for the integrator, as

$$make \texttt{DipoleList} \Big[\texttt{VectorPotential} \rightarrow \texttt{Function} \Big[\texttt{t}, \, \Big\{ \frac{\texttt{F}}{\omega} \, \texttt{Sin} [\omega \, \texttt{t}] \,, \, 0 \,, \, 0 \Big\} \Big] \,, \\$$

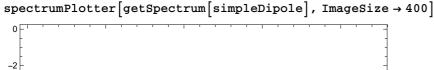
FieldParameters \rightarrow {F \rightarrow 0.05, $\omega \rightarrow$ 0.0456}, CarrierFrequency \rightarrow 0.0456

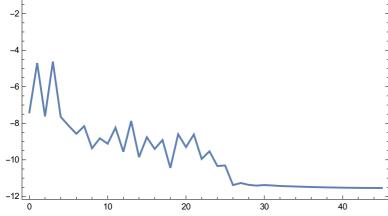
To see the spectrum, use the getSpectrum and the spectrumPlotter commands, such as

spectrumPlotter[getSpectrum[Most[simpleDipole]], Joined → False]



Note here the use of Most on the dipole when a monochromatic field is indicated. This ensures that the signal is actually periodic (i.e. it eliminates repetition between the initial and final points, which are separated by exactly one period). If this is not done, the spectrum is much noisier:



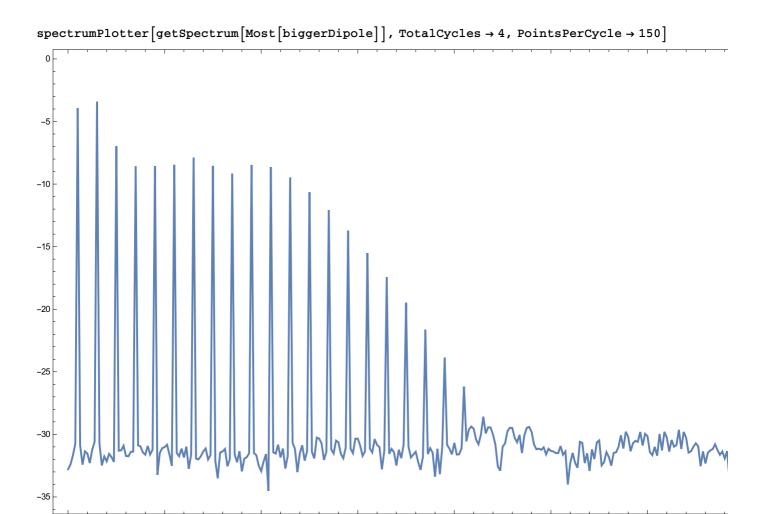


The default options are built for a periodic pulse for which simple functions of the vector potential can be integrated analytically, and for which only a single period of integration is necessary. More periods can be specified using the TotalCycles option. Similarly, the PointsPerCycle option controls the number of points per period.

```
AbsoluteTiming
```

```
\label{eq:pole_pole} \mbox{biggerDipole} = \mbox{makeDipoleList} \Big[ \mbox{VectorPotential} \rightarrow \mbox{Function} \Big[ \mbox{t}, \left\{ \frac{\mbox{F}}{\omega} \mbox{Sin}[\omega \mbox{ t}] \,, \, 0 \,, \, 0 \right\} \Big] \,,
         FieldParameters \rightarrow {F \rightarrow 0.05, \omega \rightarrow 0.057}, TotalCycles \rightarrow 4, PointsPerCycle \rightarrow 150];
{27.772, Null}
```

To get a correct spectrum plot, give these settings to the spectrum plotter.



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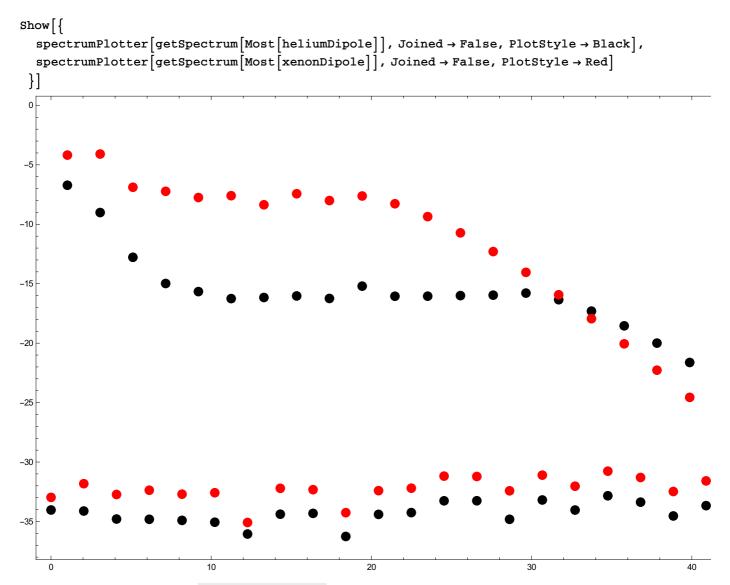
You can specify a Target chemical species using the option

? Target

Target is an option for makeDipoleList which specifies chemical species producing the HHG emission, pulling the ionization potential from the Wolfram ElementData curated data set.

```
i.e. using the syntax
```

```
AbsoluteTiming
 \text{heliumDipole} = \text{makeDipoleList} \Big[ \text{VectorPotential} \rightarrow \text{Function} \Big[ \text{t, } \Big\{ \frac{\text{F}}{\omega} \, \text{Sin} [\omega \, \text{t], } 0, \, 0 \Big\} \Big],
      FieldParameters \rightarrow {F \rightarrow 0.05, \omega \rightarrow 0.057}, Target \rightarrow "Helium" |;
 xenonDipole = makeDipoleList[VectorPotential \rightarrow Function[t, \left\{\frac{F}{\omega} \sin[\omega t], 0, 0\right\}],
      FieldParameters \rightarrow {F \rightarrow 0.05, \omega \rightarrow 0.057}, Target \rightarrow "Xenon" ;
{8.04619, Null}
```



For convenience, the function getlonizationPotential gives a public-facing access to this functionality, via ? getIonizationPotential

getIonizationPotential[Target] returns the ionization potential of an atomic target, e.g. "Hydrogen", in atomic units. getIonizationPotential[Target,q] returns the ionization potential of the q-th ion of the specified Target, in atomic units.

```
so that e.g.
```

```
{"H", #, UnitConvert Quantity[#, "Hartrees"], "Electronvolts"]} &[
 getIonizationPotential["Hydrogen"]]
{"He^+", \#, UnitConvert[Quantity[\#, "Hartrees"], "Electronvolts"]} &[
 getIonizationPotential["Helium", 1]]
H, 0.49971, 13.598 eV
{He<sup>+</sup>, 1.9998, 54.418 eV }
```

An ionization potential can also be specified directly:

? IonizationPotential

IonizationPotential is an option for makeDipoleList which specifies the ionization potential Ip of the target.

To see the available options for this function (and others), use

Options [makeDipoleList]

```
\{ 	ext{PointsPerCycle} 
ightarrow 90, 	ext{TotalCycles} 
ightarrow 1, 	ext{CarrierFrequency} 
ightarrow 0.057,
 VectorPotential \rightarrow Automatic, FieldParameters \rightarrow \{\}, VectorPotentialGradient \rightarrow None,
 Preintegrals \rightarrow Analytic, ReportingFunction \rightarrow Identity, Gate \rightarrow SineSquaredGate \begin{bmatrix} 1 \\ - \end{bmatrix},
nGate \rightarrow \frac{3}{2}, \epsilon Correction \rightarrow 0.1, IonizationPotential \rightarrow 0.5,
 Target → Automatic, DipoleTransitionMatrixElement → hydrogenicDTME,
 \texttt{PointNumberCorrection} \rightarrow \texttt{0, Verbose} \rightarrow \texttt{0, IntegrationPointsPerCycle} \rightarrow \texttt{Automatic} \Big\}
```

All options have suitable information messages.

? VectorPotential

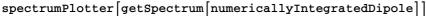
VectorPotential is an option for makeDipole list which specifies the field's vector potential. Usage should be VectorPotential→A, where A[t]//.pars must yield a list of numbers for numeric t and parameters indicated by FieldParameters pars.

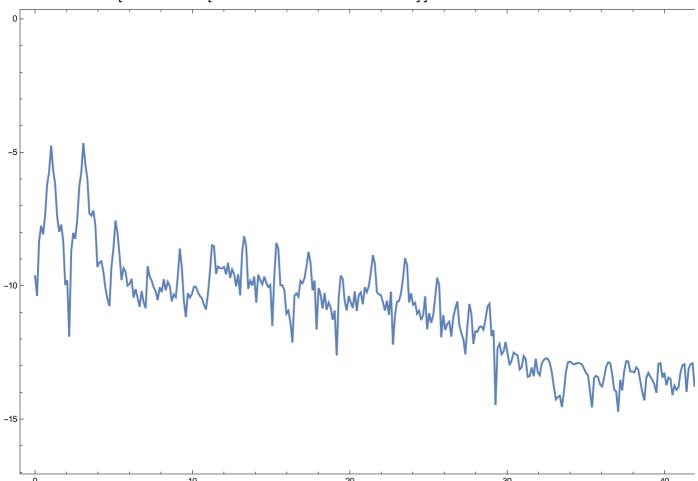
Using numerical integration for the preintegrals

Dipole case

To simulate a pulse with an envelope, it can be convenient to perform the preintegrals numerically, using the option Preintegrals→"Numeric". These cases are generally slower but mainly because they require many more periods of integration.

```
AbsoluteTiming
 numericallyIntegratedDipole =
    makeDipoleList \Big[ VectorPotential \rightarrow Function \Big[ t, \Big\{ \frac{F}{\omega} envelope[t] Sin[\omega t], 0, 0 \Big\} \Big] \Big]
      , FieldParameters \rightarrow \{\omega \rightarrow 0.057, F \rightarrow 0.055, envelope \rightarrow cosPowerFlatTop[0.057, 8, 16]\}
      , TotalCycles → 8
      , Preintegrals → "Numeric"
{20.4918, Null}
```





When using flat top pulses, and other waveforms that depend on Piecewise functions, it is possible that the function will return errors caused by an Indeterminate derivative being evaluated at the corners of the envelope.

```
AbsoluteTiming
  flatTopPulseDipole =
     makeDipoleList[VectorPotential \rightarrow Function[t, \left\{\frac{F}{\omega} \text{ envelope[t] Sin}[\omega t], 0, 0\right\}],
        \texttt{FieldParameters} \rightarrow \left\{ \omega \rightarrow \texttt{0.057}, \; \texttt{F} \rightarrow \texttt{0.055}, \; \texttt{envelope} \rightarrow \texttt{flatTopEnvelope}[\texttt{0.057}, \; \texttt{8}, \; \texttt{2}] \right\},
        TotalCycles → 8, Preintegrals → "Numeric"];
{21.6107, Null}
```

In these cases, use a numeric test to diagnose what's happened

```
Tally[flatTopPulseDipole /. _?NumberQ \rightarrow \checkmark]
\{\{\{\langle , \vee, \vee \rangle, 721\}\}
```

and if the function is returning non-numeric values, it can help to fiddle with the PointNumberCorrection option.

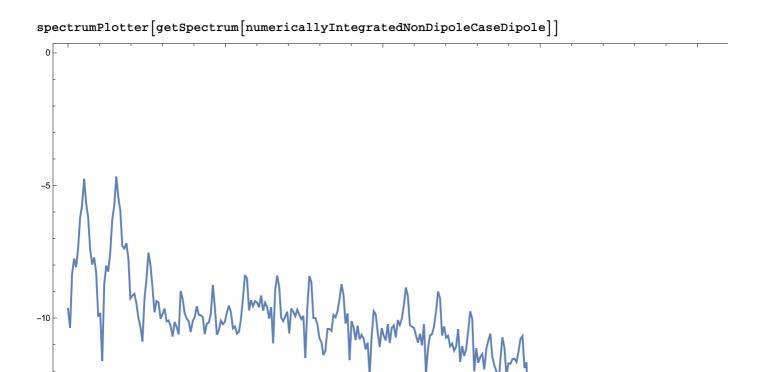
? PointNumberCorrection

PointNumberCorrection is an option for makeDipoleList and timeAxis which specifies an extra number of points to be integrated over, which is useful to prevent Indeterminate errors when a Piecewise envelope is being differentiated at the boundaries.

Nondipole case

The numerical Preintegrals can be used in the nondipole case but they're obviously much slower. The number of preintegrals to find numerically increases from two in the dipole case ($\int A(\tau) d\tau$ and $\int A(\tau)^2 d\tau$) to eight with the nondipole contributions, three of them parametrized by t'. The main load, however, is not in numerically calculating these integrals via NDSolve constructs, but rather in the added strain of accessing the preintegrals as Interpolating : Function objects once they've been calculated, from the main integration loop.

```
DateString[]
AbsoluteTiming
 numericallyIntegratedNonDipoleCaseDipole = makeDipoleList
      VectorPotential \rightarrow Function[t, \left\{\frac{F}{\omega} \text{ envelope[t] Sin}[\omega \text{ t], 0, 0}\right\}],
      VectorPotentialGradient →
        Function [t, \{0, 0, 0\}, \{0, 0, 0\}, \{-\frac{k F}{\omega}\}  envelope[t] Sin[\omega t], 0, 0\}],
      \texttt{FieldParameters} \rightarrow \left\{\omega \rightarrow \texttt{0.057, F} \rightarrow \texttt{0.055, envelope} \rightarrow \texttt{cosPowerFlatTop[0.057, 8, 16], model} \right\}
          k \rightarrow \omega \omega, \alpha \rightarrow 1/20
       , TotalCycles → 8, Preintegrals → "Numeric"
     |;
DateString[]
Beep[]
Wed 17 Feb 2016 12:38:15
{73.411, Null}
Wed 17 Feb 2016 12:39:29
```



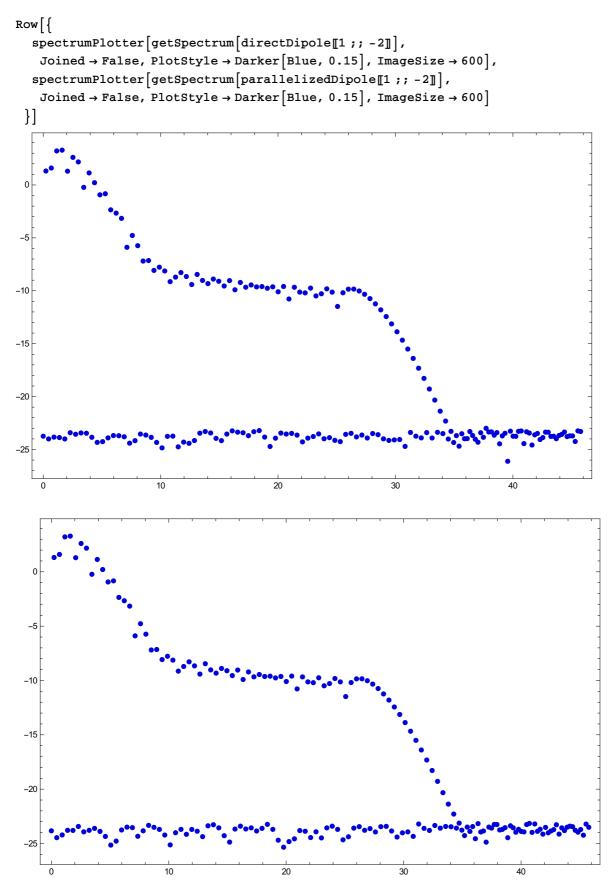
Parallelization

-15

Parallelizing single instances

For faster evaluation of a single instance, it is possible to parallelize the evaluation, by adding the option RunInParal. lel → True.

```
AbsoluteTiming [directDipole = makeDipoleList [VectorPotential \rightarrow Function [t, \left\{\frac{F}{\omega} \operatorname{Sin}[\omega t], 0, 0\right\}],
          \texttt{FieldParameters} \rightarrow \left\{\texttt{F} \rightarrow \sqrt{\texttt{10}} \ \texttt{0.05}, \ \omega \rightarrow \texttt{0.057}\right\}, \ \texttt{PointsPerCycle} \rightarrow \texttt{400}, \ \texttt{RunInParallel} \rightarrow \texttt{False} \ ]; \ ]
AbsoluteTiming parallelizedDipole = makeDipoleList
          \mbox{VectorPotential} \rightarrow \mbox{Function} \Big[ \mbox{t,} \Big\{ \frac{\mbox{F}}{\mbox{$\omega$}} \mbox{Sin} [\mbox{$\omega$} \mbox{t]} \,, \, 0 \,, \, 0 \Big\} \Big] \,,
          \texttt{FieldParameters} \rightarrow \left\{\texttt{F} \rightarrow \sqrt{10} \ \texttt{0.05}, \ \omega \rightarrow \texttt{0.057}\right\}, \ \texttt{PointsPerCycle} \rightarrow \texttt{400}, \ \texttt{RunInParallel} \rightarrow \texttt{True} \ ]; \ ]
{48.6612, Null}
{17.2579, Null}
```



Unfortunately, the in-package single-instance parallelization can be unstable on occasion; this is probably due to a bug in ParallelTable (which can, under enough load, return different results to Table, in which case results typically differ run-to-run) that has proven so far very difficult to diagnose.

In such cases, the RunInParallel option takes a third possibility - an explicit set of commands, {TableCommand, SumCommand}, to use in the iteration.

? RunInParallel

RunInParallel is an option for makeDipoleList which controls whether each RB-SFA instance is parallelized. It accepts False as the (Automatic) option, True, to parallelize each instance, or a pair of functions (TableCommand, SumCommand} to use for the iteration and summing, which could be e.g. {Inactive[ParallelTable], Inactive[Sum]}.

This is meant to be used by changing those commands to dud versions which can be sprung up later. The ideal use case (in v10 and up) is via Inactive commands, which return as

```
makeDipoleList[VectorPotential \rightarrow Function[t, \left\{\frac{F}{\omega} \sin[\omega t], 0, 0\right\}],
               FieldParameters \rightarrow \left\{ F \rightarrow \sqrt{10} \ 0.05, \ \omega \rightarrow 0.057 \right\}, Gate \rightarrow (1 \ \&), PointsPerCycle \rightarrow 400
                  , RunInParallel → {Inactive[ParallelTable], Inactive[Sum]}
        /. {RBSFA`Private`t \rightarrow t, RBSFA`Private`\tau \rightarrow \tau}
 ParallelTable [0.275578 \text{ Sum}] [\{(56.7185 + 0.i)\}
                                                       e^{-i\left(-\frac{(-48.6654\cos[0.057\,t]+48.6654\cos[0.057\,(t-\tau)])^2}{(0.-0.1\,i)+\tau}+\frac{1}{2}\,\tau\,\left(1.+\frac{(-48.6654\cos[0.057\,t]+48.6654\cos[0.057\,(t-\tau)])^2}{((0.-0.1\,i)+\tau)^2}\right)+\frac{1}{2}\,\left(7.69468\,\left(0.5\,t-4.38596\sin[0.114\,t]+\frac{1}{2}\right)^{3/2}\left(-\left((-48.6654\cos[0.057\,t]+48.6654\cos[0.057\,t]+48.6654\cos[0.057\,(t-\tau)]\right)\right)\right)}
                                                                                                      ((0.-0.1i)+\tau))+2.77393 \sin[0.057t]
                                                           \left(\text{0.-}\left(\text{(0.+0.56941 i)}\right) \, \text{Cos[0.057 (t-\tau)]} \, \left(\text{-((-48.6654} \, \text{Cos[0.057} \, \text{t]} + 48.6654 \, \text{cos[0.057}) \right)\right) + 48.6654 \, \text{Cos[0.057]} + 48.6654 \, \text{Cos[0.0
                                                                                                                                                                  \texttt{Cos[0.057 (t-\tau)]) / ((0.-0.1 i) + \tau)) + 2.77393 \, \texttt{Sin[0.057 (t-\tau)]))} /
                                                                                   \left(1. + \left(-\left(\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0.-0.1 i\right) + \tau\right)\right) + \left(1. + \left(-\left(\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right)\right) / \left(\left(0.-0.1 i\right) + \tau\right)\right)\right)
                                                                                                                                 2.77393 Sin[0.057 (t - \tau)])<sup>2</sup>)<sup>3</sup>)
                                          \left(\texttt{1.} + \left(-\left(\left(-48.6654\, \texttt{Cos} \left[\texttt{0.057}\, \texttt{t}\right] + 48.6654\, \texttt{Cos} \left[\texttt{0.057}\, \left(\texttt{t} - \tau\right)\right]\right)\,/\, \left(\left(\texttt{0.} - \texttt{0.1}\, \dot{\texttt{i}}\right) + \tau\right)\right)\,+\, \left(-\left(\left(-48.6654\, \texttt{Cos} \left[\texttt{0.057}\, \dot{\texttt{t}}\right] + 48.6654\, \texttt{Cos} \left[\texttt{0.057}\, \dot{\texttt{t}}\right]\right)\right)\,/\, \left(\left(\texttt{0.} - \texttt{0.1}\, \dot{\texttt{i}}\right) + \tau\right)\right)\,+\, \left(-\left(-48.6654\, \texttt{Cos} \left[\texttt{0.057}\, \dot{\texttt{t}}\right] + 48.6654\, \texttt{Cos} \left[\texttt{0.057}\, \dot{\texttt{t}}\right]\right)\right)
                                                                                        2.77393 \sin[0.057 t])^{2})^{3},
                                  (0. + 0. i) \left(\frac{1}{0.1 + i.\tau}\right)^{3/2} \left(0. - ((0. + 0.56941 i)) \cos[0.057 (t - \tau)]
                                                                                   (-((-48.6654 \cos[0.057 t] + 48.6654 \cos[0.057 (t - \tau)]) / ((0.-0.1 i) + \tau)) +
                                                                                                  2.77393 \sin[0.057 (t - \tau)]))
                                                                   \left(1. + \left(-\left(\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-\left(\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right)\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-\left(\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right)\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right)\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-6.654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-6.654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-6.654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-6.654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-6.654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-6.654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-6.654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) + \left(-6.654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0. - 0.1 i\right) + \tau\right)\right) / \left(-6.654 \cos \left[0.057 (t-\tau)\right]\right) / \left(-6.654 \cos 
                                                                                                                 2.77393 Sin[0.057 (t - \tau)])<sup>2</sup>)<sup>3</sup>),
                                 (0. + 0. i) \left(\frac{1}{0.1 + i \tau}\right)^{3/2} \left(0. - ((0. + 0.56941 i) \cos[0.057 (t - \tau)]\right)
                                                                                  (-((-48.6654 \cos[0.057 t] + 48.6654 \cos[0.057 (t-\tau)]) / ((0.-0.1 i) + \tau)) +
                                                                                                  2.77393 Sin[0.057 (t-\tau)]))/
                                                                   \left(1. + \left(-\left(\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right) / \left(\left(0.-0.1 i\right) + \tau\right)\right) + \left(1. + \left(-\left(\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right)\right) / \left(\left(0.-0.1 i\right) + \tau\right)\right) + \left(1. + \left(-\left(\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right)\right) / \left(\left(0.-0.1 i\right) + \tau\right)\right) + \left(1. + \left(-\left(\left(-48.6654 \cos \left[0.057 t\right] + 48.6654 \cos \left[0.057 (t-\tau)\right]\right)\right) / \left(\left(0.-0.1 i\right) + \tau\right)\right)\right)
                                                                                                                  2.77393 \sin[0.057(t-\tau)]^2)^3,
                          {\tau, 0, 165.347, 0.275578}], {\tau, 0, 110.231, 0.275578}]
```

and which can then be sprung into action using Activate:

```
AbsoluteTiming | postActivatedDipole = Activate |
      makeDipoleList[VectorPotential \rightarrow Function[t, \left\{\frac{F}{\omega} \sin[\omega t], 0, 0\right\}],
        \texttt{FieldParameters} \rightarrow \left\{\texttt{F} \rightarrow \sqrt{\texttt{10}} \ \texttt{0.05}, \ \omega \rightarrow \texttt{0.057}\right\}, \ \texttt{PointsPerCycle} \rightarrow \texttt{400},
        RunInParallel → {Inactive[ParallelTable], Inactive[Sum]}
     |;
spectrumPlotter[getSpectrum[postActivatedDipole[1;; -2]],
 Joined → False, PlotStyle → Darker [Blue, 0.15], ImageSize → 600]
{6.00778, Null}
-10
-15
-20
```

This looks like it shouldn't change anything, but it can help fix a noisy ParallelTable output. It can also, inexplicably, be rather faster than the in-package parallelization. (For a cleaner example of the latter, see this mathematica.stackexchange question.)

Multiple instances in parallel

Alternatively, one can also parallelize over each run by using ParallelTable and similar commands. In general, this requires some careful handling of contexts; in this package this has been resolved by calling

```
DistributeDefinitions["RBSFA'"];
```

at the end of the package, which should pre-load all the RB-SFA definitions into each subkernel as it is launched, even if a kernel dies or is re-spawned. If parallelization seems not to be working (calculations taking too long and using a single core), there is a chance that the parallel kernels are returning the RBSFA' functions unevaluated to the main kernel, which is then doing the work. This can be diagnosed by inserting an appropriate print statement of the \$Kernelld to force the calculating kernel to identify itself (0 for the main kernel, >0 for subkernels), and it can be fixed by suitable use of the DistributeDefinitions function and the \$DistributedContexts variable.

In addition to this, if a variable or function is used to store the results, this must be synchronized using SetShared.

Function or SetSharedVariable, as usual.

{Null, Null, Null, Null, Null, Null, Null, Null, Null}

```
SetSharedFunction[wavelengthScanDipole];
ParallelTable
Print AbsoluteTiming
   wavelengthScanDipole[\lambda] =
     \{F \rightarrow 0.05, \omega \rightarrow 45.6 / \lambda\}, CarrierFrequency \rightarrow 45.6 / \lambda, PointsPerCycle \rightarrow 400];
 , {λ, 800, 1600, 100}
{54.2716, Null}
{54.5384, Null}
{54.6478, Null}
{57.451, Null}
{53.0878, Null}
{53.9329, Null}
{55.5087, Null}
{54.6751, Null}
{51.4802, Null}
```

Show Table [$spectrumPlotter[getSpectrum[Most[wavelengthScanDipole[\lambda]]]]$ PlotStyle \rightarrow Blend[{Blue, Green, Red}, λ /800 - 1], CarrierFrequency \rightarrow 45.6 / λ , Joined → False, FrequencyAxis → "Frequency", PointsPerCycle → 400 , {λ, 800, 1600, 100}]] -15 -20 -25 10

Writing output to file

For very large calculations (many integration points per cycle, in particular), the limiting factor is available memory. In these situations, it can help to write the data directly to a file on disk. This is slower (by a factor of about 2) but it has a roughly constant RAM footprint, so it enables calculations of a bigger size than would be possible otherwise. (Of course, this can also be done from non-parallelized calls!) This is done via the ReportingFunction option:

? ReportingFunction

ReportingFunction is an option for makeDipole list which specifies a function used to report the results, either internally (by the default, Identity) or to an external file.

In essence, the integration loop consists of a Table construct, which goes over the time t at which the integral is performed, and an inner integration construct. Setting an option ReportingFunction→f interposes the function f between these two steps, as

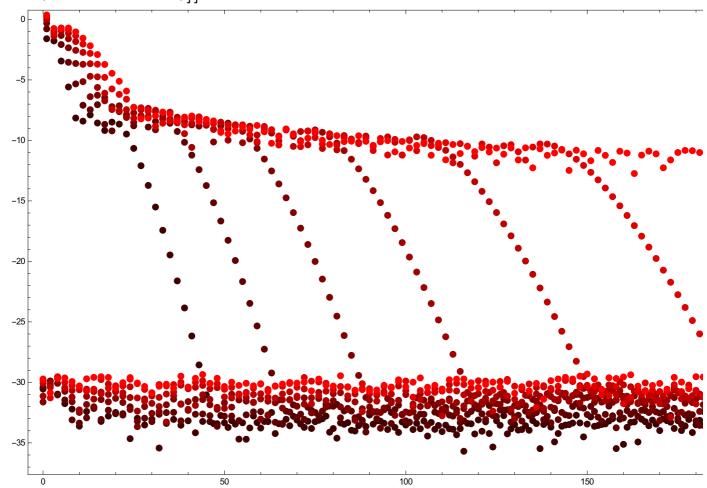
```
Table[ f[ integrator[t] ] , {t, tInitial, tFinal}]
```

The default is f=ldentity, which returns its input untouched, but it can also be replaced by a Write construct that can

shunt its input to the hard disk without telling the kernel what it is, so it is not kept in memory.

```
Ouit
DistributeDefinitions["RBSFA`"];
directory = NotebookDirectory[];
filename[F_] := FileNameJoin[{directory, "Field scan data at F=" <> ToString[F] <> ".txt"}];
ParallelTable
     Print | AbsoluteTiming |
              makeDipoleList[VectorPotential \rightarrow Function[t, \left\{\frac{\mathbf{F}}{\omega} \operatorname{Sin}[\omega t], 0, 0\right\}],
                         \texttt{FieldParameters} \rightarrow \{\omega \rightarrow \texttt{0.057}\}, \, \texttt{CarrierFrequency} \rightarrow \texttt{0.057}, \, \texttt{PointsPerCycle} \rightarrow \texttt{400}, \, \texttt{100}, \, \texttt
                         ReportingFunction → Function [Write [filename[F], #]]
      , {F, 0.05, 0.2, 0.025}
 {66.2765, Null}
 {68.2327, Null}
 {68.4573, Null}
 {69.0505, Null}
 {69.6457, Null}
 {69.8211, Null}
 {70.4778, Null}
 {Null, Null, Null, Null, Null, Null, Null}
The data in the files can then be pulled in quite simply using e.g.
Do[intensityScanDipole[F] = ReadList[filename[F]], {F, 0.05, 0.2, 0.025}]
This tends to litter the directories by creating lots of files for different parameters, so it is usually cleaner to Save
them into a single file, e.g. using
Save [FileNameJoin [{NotebookDirectory[], "Field scan collected data.txt"}],
     intensityScanDipole
which in turn can then be pulled in using
 << (FileNameJoin[{NotebookDirectory[], "Field scan collected data.txt"}]);</pre>
```

Show Table [${\tt spectrumPlotter[getSpectrum[Most[intensityScanDipole[F]]], CarrierFrequency} \rightarrow 0.057,$ Joined → False, PointsPerCycle → 400, PlotStyle → Blend[{Black, Red}, F / 0.2]] , {F, 0.05, 0.2, 0.025}]]



As written, though, this has the disadvantage that each subkernel must access the hard drive for every timestep of the computation, which obviously responsible for (at least most of) the slowdown. A middle ground is also possible by choosing an appropriate ReportingFunction: a function which will cache a specific number k of results on RAM, and then write them to file all in one go. This is on the development to do (wish) list, and will hopefully be implemented soon - if time allows.

Time and memory use

Benchmark evaluation

The benchmarks below were taken on a desktop machine with 8-thread, 4-core Intel i7-3770 CPU at 3.40GHz, 16GB RAM, running Mathematica 10.0.1 over Ubuntu 14.04. The time taken per computation depends most strongly on the PointsPerCycle used to sample and integrate, and the dependence is therefore quadratic.

```
timingsList = Table
   n, AbsoluteTiming
       \text{MaxMemoryUsed} \Big[ \text{makeDipoleList} \Big[ \text{VectorPotential} \rightarrow \text{Function} \Big[ \text{t, } \Big\{ \frac{F}{\omega} \, \text{Sin} [\omega \, \text{t], 0, 0} \Big\} \Big] , 
         FieldParameters \rightarrow \left\{ F \rightarrow \sqrt{\frac{n}{100}} \ 0.053, \omega \rightarrow 0.057 \right\}, PointsPerCycle \rightarrow n]]]}
   {n,
    100,
    1000,
    100}
{{100, {2.36167, 4905296}}, {200, {9.40602, 19018888}},
 \{300, \{20.6878, 43497000\}\}, \{400, \{37.2461, 78976528\}\}, \{500, \{57.5847, 118770848\}\},
 {600, {82.7101, 173233496}}, {700, {112.082, 232621352}}, {800, {150.096, 301125912}},
 {900, {187.298, 387140808}}, {1000, {233.122, 473885368}}}
```

Timings

50

200

400

PointsPerCycle

```
 \texttt{timingsModel} = \texttt{LinearModelFit} \Big[ \Big( \texttt{Flatten} \, / @ \, \texttt{timingsList} \Big) \Big[ \Big[ \texttt{All}, \, \{1, \, 2\} \Big] , \, \Big\{ 1, \, n, \, n^2 \Big\}, \, \{n\} \Big] ; \\ 
   ListPlot[
      (Flatten /@ timingsList) [All, {1, 2}]
   Plot[timingsModel[n], {n, timingsList[1, 1], timingsList[-1, 1]]}]
 , Frame \rightarrow True, PlotLabel \rightarrow Row \left[\left\{\text{"time in seconds=", timingsModel}\left[100\text{"}\left(\frac{\text{PointsPerCycle}}{100}\right)\text{"}\right]\right\}\right],
 FrameLabel \rightarrow {"PointsPerCycle", "Time in seconds"}, ImageSize \rightarrow 600
   200
   150
   100
```

600

800

1000

Maximum memory used

```
 \label{eq:memoryModel} \\ \texttt{memoryModel} = \\ \texttt{LinearModelFit} \Big[ \Big( \texttt{Flatten} / \\ \texttt{@timingsList} \Big) \Big[ \\ \texttt{All}, \{1, 3\} \Big], \big\{ 1, n, n^2 \big\}, \{n\} \Big]; \\ \texttt{memoryModel} = \\ \texttt{LinearModelFit} \Big[ \Big( \texttt{Flatten} / \\ \texttt{@timingsList} \Big) \Big[ \\ \texttt{All}, \{1, 3\} \Big], \{1, n, n^2 \}, \{n\} \Big]; \\ \texttt{memoryModel} = \\ \texttt{LinearModelFit} \Big[ \Big( \texttt{Flatten} / \\ \texttt{@timingsList} \Big) \Big[ \texttt{All}, \{1, 3\} \Big], \{1, n, n^2 \}, \{n\} \Big]; \\ \texttt{memoryModel} = \\ \texttt{LinearModelFit} \Big[ \Big( \texttt{Flatten} / \\ \texttt{@timingsList} \Big) \Big[ \texttt{All}, \{1, 3\} \Big], \{1, n, n^2 \}, \{n\} \Big]; \\ \texttt{memoryModel} = \\ \texttt{LinearModelFit} \Big[ \Big( \texttt{Flatten} / \\ \texttt{@timingsList} \Big) \Big[ \texttt{All}, \{1, 3\} \Big], \{n, n, n^2 \}, \{n\} \Big]; \\ \texttt{memoryModel} = \\ \texttt{LinearModelFit} \Big[ \Big( \texttt{Flatten} / \\ \texttt{@timingsList} \Big) \Big[ \texttt{All}, \{1, 3\} \Big], \\ \texttt{MemoryModel} = \\ \texttt{MemoryModelFit} \Big[ \\ \texttt{MemoryModelFit} \Big] \Big[ \texttt{Mem
  Show {
                   ListPlot[
                                (Flatten /@ timingsList) [All, {1, 3}]
                    Plot[memoryModel[n], {n, timingsList[1, 1], timingsList[-1, 1]]}]
             , Frame → True,
           \label{thm:percycle} \texttt{FrameLabel} \rightarrow \big\{ \texttt{"PointsPerCycle", "Memory used"} \big\}, \; \texttt{ImageSize} \rightarrow 600
                   5 \times 10^{8}
                   4 \times 10^{8}
                   3 \times 10^{8}
  Memory used
                   2×108
                    1 × 108
                                                                                                                                                                                200
                                                                                                                                                                                                                                                                                                        400
                                                                                                                                                                                                                                                                                                                                                                                                                               600
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      800
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           1000
                                                                                                                                                                                                                                                                                                                                          PointsPerCycle
```

In parallel

Inside parallel environments the timings are somewhat slower, by a factor of about 1.8. The timings below were taken with 7 Mathematica kernels running in parallel.

```
DistributeDefinitions["RBSFA`"];
```

```
parallelTimingsList = ParallelTable
           n, AbsoluteTiming MaxMemoryUsed
                          makeDipoleList[VectorPotential \rightarrow Function[t, \left\{\frac{F}{\omega} \sin[\omega t], 0, 0\right\}], FieldParameters \rightarrow
                                    \left\{ F \rightarrow \sqrt{\frac{n}{100}} \ 0.053, \omega \rightarrow 45.6 / \lambda \right\}, CarrierFrequency \rightarrow 45.6 / \lambda, PointsPerCycle \rightarrow n \right] \right] \right\}
           , {λ, 770, 830, 10}, {n, 100, 1000, 100}
 \{\{\{100, \{4.71833, 7949312\}\}, \{200, \{18.2567, 19028920\}\},
           {300, {39.6818, 43507248}}, {400, {68.0825, 75529984}}, {500, {108.27, 118772272}},
           {600, {154.871, 173.234.856}}, {700, {211.182, 232.622.488}}, {800, {275.072, 301.126.208}},
           {900, {350.061, 387140984}}, {1000, {424.31, 473885664}}},
       \{\{100, \{3.7169, 7949264\}\}, \{200, \{17.4824, 19028912\}\}, \{300, \{40.1556, 43507248\}\},
           {400, {68.1348, 75529984}}, {500, {109.399, 118772272}},
           {600, {153.631, 173234976}}, {700, {211.956, 232622248}},
           {800, {279.29, 301126208}}, {900, {353.1, 387141104}}, {1000, {429.039, 473885664}}},
       \{\{100, \{4.70831, 7949264\}\}, \{200, \{17.3451, 19028912\}\}, \{300, \{40.1826, 43507248\}\},
           {400, {68.9951, 75.529.984}}, {500, {109.87, 118.772.272}}, {600, {156.143, 173.234.976}},
           {700, {209.361, 232622488}}, {800, {279.29, 301126208}},
           {900, {350.784, 387141104}}, {1000, {418.914, 473885664}}},
       \{\{100, \{4.27991, 7949264\}\}, \{200, \{18.6273, 19028912\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}, \{300, \{40.4553, 43507248\}\}
           {400, {67.5833, 75529984}}, {500, {107.493, 118772272}}, {600, {151.738, 173234976}},
           {700, {211.565, 232622368}}, {800, {276.237, 301126208}},
           {900, {352.376, 387141104}}, {1000, {429.842, 473885664}}},
       {{100, {4.80072, 7949264}}, {200, {17.9797, 19028912}}, {300, {38.2944, 43507248}},
           {400, {68.7844, 75529984}}, {500, {105.406, 118772272}}, {600, {151.986, 173234976}},
           {700, {216.018, 232622488}}, {800, {279.116, 301126208}},
           {900, {361.033, 387141104}}, {1000, {424.589, 473885664}}},
       \{\{100, \{4.24956, 7949264\}\}, \{200, \{17.1782, 19028912\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}, \{300, \{40.1991, 43507248\}\}
           {400, {67.2693, 75529864}}, {500, {108.852, 118772032}},
           {600, {156.147, 173.234.736}}, {700, {210.96, 232.622.008}}, {800, {279.971, 301.126.208}},
           {900, {352.399, 387141104}}, {1000, {423.345, 473885664}}},
       \{\{100, \{4.4809, 7949264\}\}, \{200, \{17.6272, 19028912\}\}, \{300, \{39.652, 43507248\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{300, \{4.4809, 7949264\}\}, \{400, \{4.4809, 7949264\}\}, \{400, \{4.4809, 7949264\}\}, \{400, \{4.4809, 7949264\}\}, \{400, \{4.4809, 7949264\}\}, \{400, \{4.4809, 7949264\}\}, \{400, \{4.4809, 7949264\}\}, \{400, \{4.4809, 7949264\}\}, \{400, \{4.4809, 7949264\}\}, \{400, \{4.4809, 7949264\}\}, \{400, \{4.480
           {400, {67.7538, 75529984}}, {500, {107.413, 118772272}}, {600, {156.833, 173234976}},
           {700, {213.902, 232622488}}, {800, {276.711, 301126208}},
           {900, {352.447, 387140984}}, {1000, {423.858, 473885544}}}}
parallelTimingsListAveraged =
     Table [\{parallelTimingsList^{\mathsf{T}}[k, 1, 1], Mean[parallelTimingsList^{\mathsf{T}}[k, All, 2]]\},
           {k, Length[parallelTimingsList<sup>T</sup>]}]
\left\{\left\{100, \left\{4.42209, \frac{55644896}{7}\right\}\right\}, \left\{200, \left\{17.7852, \frac{133202392}{7}\right\}\right\}\right\}
      \{300, \, \{39.803, \, 43\,507\,248\}\}, \, \Big\{400, \, \Big\{68.0862, \, \frac{528\,709\,768}{7}\Big\}\Big\}, \, \Big\{500, \, \Big\{108.101, \, \frac{831\,405\,664}{7}\Big\}\Big\}, \, \Big\{600, \, \Big\{108.101, \, \frac{831\,405\,664}{7}\Big\}\Big\}, \, \Big\{1000, \, \Big\{1000, \, \frac{1}{1}, \,
     \left\{600, \left\{154.479, \frac{1212644472}{7}\right\}\right\}, \left\{700, \left\{212.135, 232622368\right\}\right\}, \left\{800, \left\{277.955, 301126208\right\}\right\}, \left\{800, \left\{277.955, 301126208\right\}\right\}
     \left\{900, \left\{353.171, \frac{2709987488}{7}\right\}\right\}, \left\{1000, \left\{424.842, \frac{3317199528}{7}\right\}\right\}\right\}
```

Timings

1000

```
parallelTimingsModel =
   Show {
   ListPlot[
      ( \verb|Flatten /@parallelTimingsListAveraged ) [ [All, \{1, 2\}] ] 
   Plot[parallelTimingsModel[n],
     [n, parallelTimingsListAveraged[1, 1]], parallelTimingsListAveraged[-1, 1]]
  , Frame → True,
 \texttt{PlotLabel} \rightarrow \texttt{Row} \Big[ \Big\{ \texttt{"time in seconds=", parallelTimingsModel} \Big[ 100 \, \texttt{"} \, \big( \frac{\texttt{PointsPerCycle}}{100} \big) \, \texttt{"} \Big] \Big\} \Big] \, ,
 FrameLabel \rightarrow {"PointsPerCycle", "Time in seconds"}, ImageSize \rightarrow 600
                    time in seconds=4.19986 (\frac{\text{PointsPerCycle}}{100})<sup>2</sup> + 1.07899 (\frac{\text{PointsPerCycle}}{100}) – 1.55094
   400
   300
ime in seconds
   200
   100
```

PointsPerCycle

Memory

```
parallelMemoryModel =
   Show {
   ListPlot[
     (Flatten /@parallelTimingsListAveraged) [All, {1, 3}]
   1,
   Plot[parallelMemoryModel[n],
     \{n, parallelTimingsListAveraged[1, 1], parallelTimingsListAveraged[-1, 1]]\}
  , Frame \rightarrow True, PlotLabel \rightarrow
    \text{Row}\Big[\Big\{\text{"Memory used=", Simplify}\Big[\text{parallelMemoryModel}\Big[100."(\frac{\text{PointsPerCycle}}{100})"\Big]\ 10^{-6}\ \text{"MB"}\Big]\Big\}\Big], 
  FrameLabel → {"PointsPerCycle", "Memory used"}, ImageSize → 600
                  Memory used=4.79633 \left(1.\left(\frac{\text{PointsPerCycle}}{100}\right)^2 - 0.153257\left(\frac{\text{PointsPerCycle}}{100}\right) + 0.555441\right) MB
   5 \times 10^{8}
   4 \times 10^{8}
   3 \times 10^{8}
Memory used
   1 × 10<sup>8</sup>
                                               400
                                                                   600
                                                                                      800
                                                                                                         1000
```

Decoupling integration and sampling

If the quadratic scaling with respect to PointsPerCycle becomes too onerous, the sampling rate for the evaluation and for the numerical integration can be decoupled by providing an explicit option for IntegrationPointsPerCycle, which will set how many points are used per cycle in the numerical integration.

PointsPerCycle

? IntegrationPointsPerCycle

IntegrationPointsPerCycle is an option for makeDipoleList which controls the number of points per cycle to use for the integration. Set to Automatic, to follow PointsPerCycle, or to an integer.

Obviously, if this option is taken, then the outcome should be checked for numerical convergence with respect to IntegrationPointsPerCycle.

```
DateString[]
decoupledTimingsList = Table
   nSampling, nIntegration, AbsoluteTiming
     \texttt{MaxMemoryUsed} \Big[ \texttt{makeDipoleList} \Big[ \texttt{VectorPotential} \rightarrow \texttt{Function} \Big[ \texttt{t,} \Big\{ \frac{\texttt{F}}{\omega} \texttt{Sin}[\omega \, \texttt{t}], \, \texttt{0,} \, \texttt{0} \Big\} \Big] \Big]
        , FieldParameters \rightarrow \left\{ F \rightarrow \sqrt{\frac{\text{nSampling}}{100}} \ 0.053, \omega \rightarrow 0.057 \right\}
         , PointsPerCycle \rightarrow nSampling, IntegrationPointsPerCycle \rightarrow nIntegration
   , \{nSampling, 100, 500, 100\}, \{nIntegration, 100, 500, 100\}
DateString[]
Fri 5 Feb 2016 17:08:36
\{\{\{100, 100, \{2.39139, 4789112\}\}\},\
   {100, 200, {4.76862, 9473168}}, {100, 300, {7.07336, 14241584}},
   {100, 400, {9.39992, 19138656}}, {100, 500, {11.7964, 24035936}}},
 \{\{200, 100, \{4.72937, 9447040\}\}, \{200, 200, \{9.3758, 19017072\}\},
   {200, 300, {14.1647, 28478336}}, {200, 400, {18.8825, 38195832}},
   {200, 500, {23.4484, 47916856}}}, {{300, 100, {7.02226, 14177120}}},
   {300, 200, {14.067, 28434560}}, {300, 300, {21.5271, 43233320}},
   {300, 400, {28.4153, 56993480}}, {300, 500, {35.2399, 70747672}}},
  \{\{400, 100, \{9.41508, 19027632\}\}, \{400, 200, \{18.6957, 38108104\}\},
   {400, 300, {28.159, 56949288}}, {400, 400, {37.5268, 75259432}},
   {400, 500, {46.83, 95676600}}}, {{500, 100, {11.6672, 23882240}},
   {500, 200, {23.5225, 47786456}}, {500, 300, {35.0966, 70660928}},
   {500, 400, {46.7308, 95634048}}, {500, 500, {58.5078, 118501720}}}}
Fri 5 Feb 2016 17:17:24
```

```
decoupledTimingsModel = LinearModelFit[
       \left( \texttt{Flatten} / \texttt{@Flatten} \Big[ \texttt{decoupledTimingsList}, \left\{ \left\{ 1, \, 2 \right\} \right\} \Big] \right) \left[ \texttt{All}, \left\{ 1, \, 2, \, 3 \right\} \right] 
      , {1, nSampling, nIntegration, nSampling x nIntegration}, {nSampling, nIntegration}];
Show
   Plot3D
     decoupledTimingsModel[nSampling, nIntegration]
      , {nSampling, 0, 500}, {nIntegration, 0, 500}
      , AxesLabel \rightarrow \{"npps=PointsPerCycle", "nppi=IntegrationPointsPerCycle", "Timing (s)"\}
      \texttt{PlotLabel} \rightarrow \texttt{Row} \Big[ \Big\{ \texttt{"time in seconds=", decoupledTimingsModel} \Big[ 100 \, \texttt{"} \, (\frac{\texttt{npps}}{100}) \, \texttt{", } 100 \, \texttt{"} \, (\frac{\texttt{nppi}}{100}) \, \texttt{"} \Big] \Big\} \Big] 
      , ImageSize \rightarrow 650
   ListPointPlot3D[
      (Flatten / @ Flatten [decoupled Timings List, {{1, 2}}])[[All, {1, 2, 3}]]
      , PlotStyle \rightarrow \{\{Black, PointSize[Large]\}\}
                 time in seconds = 2.33613 (\frac{\text{nppi}}{100})(\frac{\text{npps}}{100}) + 0.0260245 (\frac{\text{nppi}}{100}) - 0.00404974 (\frac{\text{npps}}{100}) + 0.0470921
                                                                                                                                      40
                                                                                                                                         Timing(s)
npps=PointsPerCycle
                                                                                                                  400
                                400
                                                                                          npp⊨IntegrationPointsPerCycl
```

```
decoupledMemoryModel = LinearModelFit[
     (Flatten / @ Flatten [decoupled Timings List, {{1, 2}}]) [All, {1, 2, 4}]
     , {1, nSampling, nIntegration, nSampling x nIntegration}, {nSampling, nIntegration}];
Show | {
  Plot3D
    decoupledMemoryModel[nSampling, nIntegration]
     , {nSampling, 0, 500}, {nIntegration, 0, 500}
     , AxesLabel \rightarrow \{"npps=PointsPerCycle", "nppi=IntegrationPointsPerCycle", "Memory (B)"\}
    , PlotLabel → Row \left[\left\{\text{"Memory used (B)=", decoupledMemoryModel}\left[100"(\frac{\text{npps}}{100})", 100"(\frac{\text{nppi}}{100})"\right]\right\}\right]
     , ImageSize \rightarrow 650
   ListPointPlot3D
     (Flatten/@Flatten[decoupledTimingsList, {{1, 2}}])[[All, {1, 2, 4}]]
     , PlotStyle → {{Black, PointSize[Large]}}
                  Memory used (B)=4.72186 \times 10^6 \left(\frac{\text{nppi}}{100}\right) \left(\frac{\text{npps}}{100}\right) + 104696. \left(\frac{\text{nppi}}{100}\right) + 65224.7 \left(\frac{\text{npps}}{100}\right) - 214229.
Memory(B)
        5×107
                                                                                                     nppi⊨IntegrationPointsPerCyc
                                                                                             200
                          npps=PointsPerCycle
```

Cutting off the long trajectories

This section shows, as an example of the use of the package, the use of the integration gate to eliminate the contribution from long trajectories. This can be tested by the reduced presence of quantum path interference patterns in the spectrum, and more practically by examining the dependence of the quantum phase on the field intensity.

The gating cutoff time

Given the classical trajectory,

```
trajectory[\omegat_, \omegat0_] := (x[\omegat] /. First@DSolve[
        \{x''[\omega t] = Cos[\omega t], x'[\omega t0] = 0, x[\omega t0] = 0\}
        , x, \omega t
      1)
```

the recollision kinetic energy and excursion time can be found as

```
recollisionKE[\omegat0_?NumericQ] := (D[trajectory[\omegatt, \omegat0], \omegatt]<sup>2</sup> /. \omegatt \rightarrow \omegat) /.
      First \Big[ Quiet \Big[ NSolve \Big[ \Big\{ trajectory[\omega t, \omega t0] = 0, \frac{\pi}{2} \le \omega t < 2 \pi \Big\}, \omega t \Big] \Big] \Big] 
recollisionExcursionTime[\omegat0_?NumericQ] :=
   (\omega \texttt{t} - \omega \texttt{t0}) \text{ /. First} \Big[ \texttt{Quiet} \Big[ \texttt{NSolve} \Big[ \Big\{ \texttt{trajectory}[\omega \texttt{t, } \omega \texttt{t0}] == 0 \text{, } \frac{\pi}{2} \leq \omega \texttt{t} < 2 \text{ } \pi \Big\} \text{, } \omega \texttt{t} \Big] \Big] \Big]
```

and the excursion time at the cutoff can be found by maximizing the kinetic energy.

```
FindMaximum[recollisionKE[\omegat0], {\omegat0, 0.3}]
recollisionExcursionTime[ωt0] /. Last[%]
\{1.58657, \{\omega t0 \rightarrow 0.313408\}\}
0.650239
```

In other words, the cutoff trajectories occur at excursion times of $\omega \tau = 0.65 \times 2 \,\pi$, i.e. at a gate number of 0.65 cycles.

Calculation

This calculation runs a standard linearly-polarized field with intensity between 0.8 and 2×10¹⁴ W/cm², with a fine intensity resolution. We compare the standard, non-gated calculation against a calculation with nGate set to 0.65, as per the above, and a sharp sin² cutoff of 0.05 cycles.

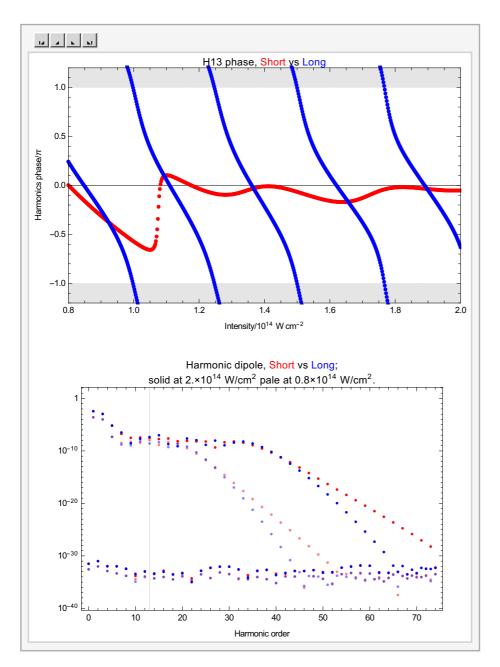
```
intRange = Range[0.8, 2., 0.002];
npps1 = 150;
SetSharedFunction[quantumPhaseScan, fourierDipole];
LaunchKernels[];
DistributeDefinitions["RBSFA`"];
nFlat = 0.65;
nGateRamp = 0.05;
```

The actual calculation,

```
DateString[]
AbsoluteTiming
 ParallelTable
    quantumPhaseScan[trajectories, int] = makeDipoleList[
         VectorPotential \rightarrow Function \left[t, \left\{\frac{F}{\omega} \sin[\omega t], 0, 0\right\}\right],
         FieldParameters \rightarrow \left\{ F \rightarrow \sqrt{\text{int}} \ 0.053, \omega \rightarrow 0.057 \right\}
         PointsPerCycle \rightarrow nppsl,
         If[trajectories === "Short", Sequence@@
            \left\{ \texttt{Gate} \rightarrow \texttt{SineSquaredGate[nGateRamp], nGate} \rightarrow \left( \texttt{nFlat+nGateRamp} \right) \right\}, \; \texttt{### \&[], \# \&[]} 
    , {int, intRange}, {trajectories, {"Short", "Long"}}];
DateString[]
Wed 2 Dec 2015 19:28:50
{1216.8, Null}
Wed 2 Dec 2015 19:49:07
and the energy-domain dipole.
AbsoluteTiming[
 Table[
    fourierDipole[trajectories, int] = Fourier[
         Re[quantumPhaseScan[trajectories, int][1;; -2, 1]]
         , FourierParameters \rightarrow \{-1, 1\}];
     , {int, intRange}, {trajectories, {"Short", "Long"}}];
{0.093762, Null}
```

Analysis

```
Block [ {background},
 background = ListLogPlot |
    Flatten Table
        {\text{Range}[0, \text{nppsl}/2-1], \text{Abs}[\text{fourierDipole}[\text{trajectories}, \text{m}[\text{intRange}]][1;; \text{nppsl}/2]]^2}^{\intercal}
        , {m, {Min, Max}}, {trajectories, {"Short", "Long"}}], 1]
     , ImageSize \rightarrow 420
     , PlotStyle \rightarrow \{\{Red, Opacity[0.5]\}, \{Blue, Opacity[0.5]\}, \{Red\}, \{Blue\}\}\}
     , PlotLabel → "Harmonic dipole, Short vs Long;\nsolid at " <> ToString[Max[intRange]] <>
        "\times 10^{14} W/cm<sup>2</sup> pale at "<> ToString[Min[intRange]] <> "\times 10^{14} W/cm<sup>2</sup>."
     , FrameLabel → {"Harmonic order", ""}
     , Frame → True
 SlideView Table
    Row
        Show | {
           \texttt{RegionPlot}\big[\texttt{Abs}[\phi] > 1, \big\{\texttt{int}, \texttt{Min}\big[\texttt{intRange}\big], \texttt{Max}\big[\texttt{intRange}\big]\big\}, \big\{\phi, -1.2, 1.2\big\}, 
            PlotStyle \rightarrow GrayLevel[0.9], Method \rightarrow {"AxesInFront" \rightarrow False}, BoundaryStyle \rightarrow None],
           ListPlot
            Table
              Flatten Table
                   \{ \#, \; \{ \# \llbracket 1 \rrbracket, \; \# \llbracket 2 \rrbracket + 2 \}, \; \{ \# \llbracket 1 \rrbracket, \; \# \llbracket 2 \rrbracket - 2 \} \} \; \& @
                   {int, \frac{1}{\tau} \text{ Arg[fourierDipole[trajectories, int][HO + 1]]}}
                  , {int, intRange[1;; -1]}], 1]
               , {trajectories, {"Short", "Long"}}
             , PlotStyle → {{PointSize[0.01], Red}, {PointSize[0.01], Blue}}
             , Joined → False
         , PlotRange \rightarrow 1.2 {-1, 1}, AspectRatio \rightarrow 0.6
          , PlotRangePadding → {None, Automatic}
          , Axes → True
          , ImageSize \rightarrow 450
          , PlotLabel \rightarrow "H" <> ToString[HO] <> " phase, Short vs Long"
          , FrameLabel → \{"Intensity/10^{14} W cm<sup>-2</sup>", "Harmonics phase/\pi"\}
        Show[\{background\}, GridLines \rightarrow \{\{HO\}, None\}]
    , {HO, 1, npps1/2, 2}], 7]
```



The short- and long-trajectory calculations are in red and blue respectively. It is clear that, in the plateau regions, the gated calculation has a much smoother dependence of the harmonic phase on the field intensity. On the other hand, the cutoff is perfectly preserved. These are the hallmarks that the contributions from long trajectories have been mostly eliminated.

Nondipole contributions

Nondipole contributions can be specified by setting a nonzero vector potential gradient:

? VectorPotentialGradient

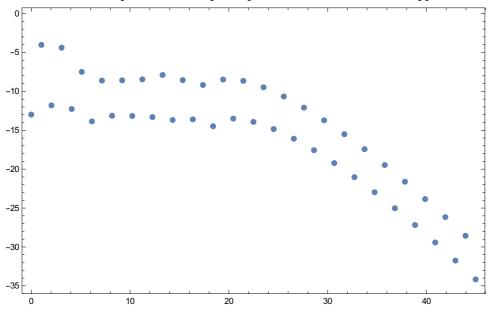
"VectorPotentialGradient is an option for makeDipole list which specifies the gradient of the field's vector potential. Usage should be VectorPotentialGradient→GA, where GA[t]//.pars must yield a square matrix of the same dimension as the vector potential for numeric t and parameters indicated by FieldParameters \rightarrow pars. The indices must be such that GA[t][i,j] returns $\partial_i A_i[t]$."

If, for example, the travelling-wave form of the vector potential is of the form $\mathbf{A}(\mathbf{r}, t) = \frac{F}{\omega} \hat{\mathbf{x}} \cos(kz - \omega t)$, then at the

origin the vector potential is $\mathbf{A}(\mathbf{0}, t) = \frac{F}{\omega} \hat{\mathbf{x}} \cos(\omega t)$ and it has a single nonzero entry in its gradient matrix $\nabla \mathbf{A}$, i.e. $\partial_z A_x = -\frac{kF}{\omega} \sin(\omega t)$. This is entered into the VectorPotentialGradient option as

nonDipoleContributions = makeDipoleList VectorPotential \rightarrow Function[t, $\left\{\frac{F}{\omega} \cos[\omega t], 0, 0\right\}$], $\text{VectorPotentialGradient} \rightarrow \text{Function} \left[\text{t, } \left\{ \{0, 0, 0\}, \{0, 0, 0\}, \left\{ -\frac{\text{k F}}{C} \text{Sin}[\omega \, \text{t}], 0, 0 \right\} \right\} \right],$ FieldParameters $\rightarrow \{F \rightarrow 0.05, \omega \rightarrow 0.057, k \rightarrow \omega / c, c \rightarrow 137\}$

 $\verb|spectrumPlotter[getSpectrum[Most[nonDipoleContributions]]|, \verb|Joined| \rightarrow False, \verb|ImageSize| \rightarrow 500|$



At low wavelengths, the first obvious effect is the appearance of even harmonics. This is the expected behaviour, with the harmonics along the laser propagation direction. (Informally, the magnetic pushing on the wavepacket acts on the propagation direction on both halves of each laser period. This off-axis recollision causes the dipole to oscillate in the propagation direction with an even symmetry. More formally, the dynamical symmetries of the problem permit even (but not odd) harmonics along this direction.) This is indeed what is observed:

```
Show[{
  spectrumPlotter[getSpectrum[nonDipoleContributions[1;; -2, {1, 2}]]],
   Joined → False, PlotStyle → Black],
  spectrumPlotter[getSpectrum[nonDipoleContributions[1;; -2, {3}]]],
    Joined \rightarrow False, PlotStyle \rightarrow Red
   PlotRange \rightarrow All, ImageSize \rightarrow 500
-15
-20
-25
-30
```

Benchmarking the nondipole contributions

Nondipole contributions in a crossed-beam setup

This section explores the harmonic emission by a crossed-beam setup, with nondipole contributions, as a benchmarking step for the latter. The crossed-beam setup was proposed by X.-M. Tong and S.-I. Chu in Phys. Rev. A 58 no .4, R2656 (1998), and it was explored in a nondipole setting by V. Averbukh et al. in Phys Rev. A 65, 063402 (2002). The results below reproduce those of Averbukh et al.

In short, we consider the harmonic emission by a circularly polarized pulse propagating along the z direction, at frequency ω , and a linearly polarized pulse of frequency $r \omega$ propagating along the x direction and polarized along the z direction.

```
\left( crossedBeamsA[x_, z_] = Function[t,
       \left\{ \frac{\text{F1}}{\omega} \cos \left[ k z - \omega t \right], \frac{\text{F1}}{\omega} \sin \left[ k z - \omega t \right], \frac{\text{F2}}{r \omega} \sin \left[ r k x - r \omega t + \theta 0 \right] \right\}
      ])[t] // MatrixForm
(crossedBeamsGA[x_] = Function[t, Evaluate[{
           D[crossedBeamsA[x, z][t], x] /. \{z \rightarrow 0\},
           D[crossedBeamsA[x, z][t], y] /. \{z \rightarrow 0\},
           D[crossedBeamsA[x, z][t], z] /. \{z \rightarrow 0\}
   )[t] // MatrixForm
     F1 \cos [kz-t\omega]
     F1 Sin[k z-tω]
The dipole selection rules allow harmonic orders of the form 2 r/± 1, with /= 0, 1, 2, 3, ..., with polarization in the
x, y plane, and harmonics of order r(2/+1), with r=0, 1, 2, 3, ..., polarized along the z direction.
allowedHarmonics[r_, {1, 2}] := Select [Union[2 r Range[0, 100] + 1, 2 r Range[0, 100] - 1], # > 0 &]
allowedHarmonics[r_{,} {3}] := r (2 Range[0, 100] + 1)
For the calculation, then, some preliminaries,
\alphaRange = {0, 1 / 137};
nppcb = 240;
crossedBeamsParameters[rr] := \{F1 \rightarrow 0.1, F2 \rightarrow 0.2, \omega \rightarrow 0.057, \theta0 \rightarrow 0, r \rightarrow rr, k \rightarrow \alpha\omega\};
DistributeDefinitions["RBSFA`"];
SetSharedFunction[crossedBeamsResults];
and the calculation itself for r = 2 and r = 5.
Print[DateString[]]
ParallelTable AbsoluteTiming
   crossedBeamsResults[r, α] = makeDipoleList[
       VectorPotential → crossedBeamsA[0, 0], VectorPotentialGradient → crossedBeamsGA[0],
       FieldParameters → crossedBeamsParameters[r]
       , DipoleTransitionMatrixElement \rightarrow Function [\{p, \kappa\}, gaussianDTME[p, 1/1.3]]
       , CarrierFrequency \rightarrow 0.057, PointsPerCycle \rightarrow nppcb
      ];
 ], \{r, \{2, 5\}\}, \{\alpha, \alpha \text{Range}\}]
Print[DateString[]]
```

Results for r = 2, comparable to Fig. 1 in Averbukh et al. Dashed lines mark the dipole-allowed harmonics. The lefthand column has nondipole contributions turned off ($\alpha = 0$), and the right-hand column includes the nondipole contributions and observes a massive increase in the amplitude of the dipole-forbidden harmonics.

{{{29.6518, Null}, {34.7323, Null}}, {{28.9947, Null}, {34.9678, Null}}}

Thu 1 Oct 2015 15:42:15

Thu 1 Oct 2015 15:43:20

```
Grid[Table[
   ListLogPlot[
      \texttt{getSpectrum} \Big[ \texttt{crossedBeamsResults} [2, \alpha] \, [\![ 1 \ ; ; -2 , \, \texttt{part} ]\!], \, \omega \texttt{Power} \rightarrow 2 \Big] \, [\![ 2 \ ; ; ]\!]
      , Joined \rightarrow False, ImageSize \rightarrow 600, PlotTheme \rightarrow "Detailed", PlotRange \rightarrow Full
      , GridLines \rightarrow \{allowedHarmonics[2, part], None\}
      , PlotLabel \rightarrow Row[{"\alpha=", \alpha, ", part ", {"x", "y", "z"}[[part]]}]
    ], {part, {{1, 2}, {3}}}, {\alpha, \alphaRange}]]
                                                                \alpha=0, part {x, y}
10-11
                                                                                                                                             10-10
                                                                                                                                             10-15
10-21
                                                                                                                                             10-20
                                                                                                                                             10^{-25}
                                                                                                                  100
                            20
                                                                 \alpha=0, part {z}
                                                                                                                                              10
10-12
                                                                                                                                              10<sup>-9</sup>
                                                                                                                                             10-14
10^{-22}
                                                                                                                                             10-19
                                                                                                                                             10-24
10-32
                                                                                                                  100
```

Results for r = 5, comparable to Fig. 2 in Averbukh et al.

```
Grid[Table[
    ListLogPlot[
      \texttt{getSpectrum} \big[ \texttt{crossedBeamsResults} [5, \alpha] \, [\![ 1 \ ; ; -2 , \, \texttt{part} ]\!], \, \omega \texttt{Power} \rightarrow 2 \big] \, [\![ 2 \ ; ; ]\!]
       , Joined \rightarrow False, ImageSize \rightarrow 600, PlotTheme \rightarrow "Detailed", PlotRange \rightarrow Full
      , GridLines \rightarrow \{allowedHarmonics[5, part], None\}
      , PlotLabel \rightarrow Row[{"$\alpha=$", $\alpha$, ", part ", {"$x", "$y", "$z"}[part]}}]
    ], {part, {{1, 2}, {3}}}, {\alpha, \alphaRange}]]
                                                                     \alpha=0, part {x, y}
  100
                                                                                                                                                         10-4
 10<sup>-8</sup>
10-18
                                                                                                                                                        10-14
                                                                                                                                                        10<sup>-19</sup>
10^{-28}
                                                                                                                                                        10-24
                                                                                                                           100
                                                                                                                                                  120
                                                                      \alpha=0, part {z}
   10
 10<sup>-9</sup>
                                                                                                                                                         10<sup>-9</sup>
10<sup>-19</sup>
                                                                                                                                                        10-19
10<sup>-29</sup>
                                                                                                                                                        10-29
                               20
                                                      40
                                                                                                    80
                                                                                                                           100
```

Multiple plateaus in HHG in ions

This section benchmarks this code against the results of N.J. Kylstra et al. reported in J. Phys B: At. Mol. Opt. Phys. 34 no. 3, L55 (2001); In particular, we study HHG in the He⁺ ion at high intensity ($I = 5.6 \times 10^{15} \,\mathrm{W} \,\mathrm{cm}^{-2}$) and reasonable (800nm) wavelength.

```
\left( \text{kylstraA[z]} = \text{Function} \left[ \text{t, } \left\{ \frac{\text{F}}{\omega} \, \text{Sin} \left[ \frac{\omega \, \text{t-kz}}{4} \right]^2 \, \text{Sin} \left[ \omega \, \text{t-kz} \right], \, 0, \, 0 \right\} \right] \right) \left[ \text{t]} \, \text{// MatrixForm} \right] = \text{MatrixForm} \left[ \frac{\omega \, \text{t-kz}}{4} \right] = \text{MatrixForm} \left[ \frac{\omega \, \text{t-kz}}{4}
   (kylstraGA = Function[t, Evaluate[{
                                                       D[kylstraA[z][t], x] /. \{z \rightarrow 0\},
                                                        D[kylstraA[z][t], y] /. \{z \rightarrow 0\},
                                                        D[kylstraA[z][t], z] /. \{z \rightarrow 0\}
                )[t] // MatrixForm
nppk = 1500;
DateString[]
AbsoluteTiming
       kylstraTest = makeDipoleList
                               \label{eq:VectorPotential} VectorPotential Gradient \rightarrow kylstraGA,
                               FieldParameters \rightarrow \left\{ F \rightarrow \sqrt{5.6 \times 10^{15} / 10^{14}} \right. 0.053, \omega \rightarrow 0.057, k \rightarrow \alpha \omega, \alpha \rightarrow 1 / 137 \right\}
                                IonizationPotential \rightarrow 2,
                                 PointsPerCycle \rightarrow nppk, TotalCycles \rightarrow 2
DateString[]
Thu 1 Oct 2015 18:25:47
 {1619.16, Null}
Thu 1 Oct 2015 18:52:46
```

Plotting the results. The x component (along the laser polarization) is in black, the z component (along the laser propagation) is in red.

```
Show
 Table
   spectrumPlotter[getSpectrum[kylstraTest[1;;-2,part]], \omega Power \rightarrow 2], Joined \rightarrow True,
    PointsPerCycle \rightarrow nppk, TotalCycles \rightarrow 2, PlotStyle \rightarrow (part /. \{\{1, 2\} \rightarrow Black, \{3\} \rightarrow Red\})
   , {part, {{1}, {3}}}]
   PlotRange → All
-15
-20
-25
```

The results are a good qualitative match to the dipoles reported by Kylstra et al., with the notable exception of the low-order harmonics below n≤50.

On the other hand, taken naively this code cannot be applied to the harder targets described in that paper (Li2+ and Be³⁺, at intensities between 0.9 and 3.6×10¹⁷ W cm⁻²), which have cutoffs of order as high as 35 000, which requires several days to several months of calculation using the naive scaling. (That said, using a smarter choice of ReportingFunction, judicious use of parallelization and lots of waiting, those targets are probably within reach of this code.)

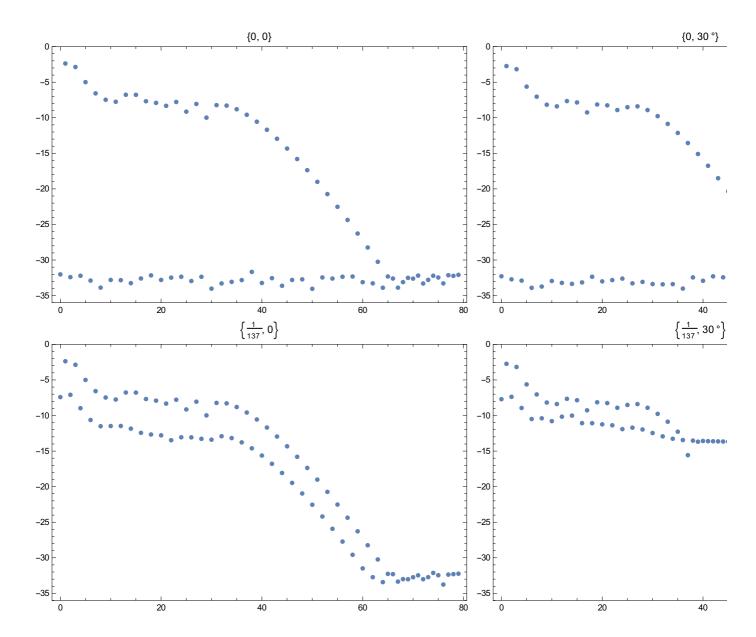
Perodicity of nondipole contributions

Quit

```
crossedBeamsA[t_] = First /@ Sum[
        \frac{F}{\omega} \begin{pmatrix} \cos[\theta] \\ 0 \\ -s\sin[\theta] \end{pmatrix} \cos[k \{ s\sin[\theta], 0, \cos[\theta] \}. \{x, y, z\} - \omega t - s \phi]
         , {s, {-1, 1}}] // MatrixForm;
(crossedBeamsGA[t_] = Evaluate[{
         D[crossedBeamsA[t], x],
         D[crossedBeamsA[t], y],
         D[crossedBeamsA[t], z]
        }]) // MatrixForm;
crossedBeamsParameters = \{x \rightarrow 0, y \rightarrow 0, z \rightarrow 0, F \rightarrow \sqrt{0.5} \ 0.053, \omega \rightarrow 0.057, \theta \rightarrow 10.^{\circ}, k \rightarrow \alpha \omega\};
DateString[]
Table[
 First AbsoluteTiming
    symmetryTestDipole[\alpha, \phi] = makeDipoleList[
         VectorPotential → crossedBeamsA,
         VectorPotentialGradient → crossedBeamsGA, FieldParameters → crossedBeamsParameters,
         PointsPerCycle → 160
 , \{\alpha, \{0, 1/137\}\}, \{\phi, \{0, 30^\circ\}\}
DateString[]
Fri 16 Oct 2015 12:09:53
\{\{5.97834, 6.65576\}, \{8.31512, 11.9895\}\}
Fri 16 Oct 2015 12:10:26
```

```
Grid[Table[
    spectrumPlotter[
      getSpectrum[symmetryTestDipole[\alpha, \phi][1;; -2, {1, 2, 3}]]
      , Joined \rightarrow False, PointsPerCycle \rightarrow 160,
      {\tt ImageSize} \rightarrow 450, \, {\tt PlotLabel} \rightarrow \{\alpha, \, \phi\}, \, {\tt PlotRange} \rightarrow \{-36, \, 0\}
    , \{\alpha, \{0, 1/137\}\}, \{\phi, \{0, 30^\circ\}\}]]
                                                                                                                                                                    \{0, 30 ^{\circ}\}
-10
                                                                                                                -10
-15
                                                                                                                -15
-20
                                                                                                                -20
-25
                                                                                                                -30
                                                                                                           80
                               20
                                                        40
                                                                                  60
                                                                                                                                               20
                                                    \left\{\frac{1}{137}, 0\right\}
                                                                                                                                                                  \left\{\frac{1}{137}, 30^{\circ}\right\}
-15
                                                                                                                -15
-20
                                                                                                                -20
-25
                                                                                                                -25
-30
                                                                                                                -30
                               20
                                                        40
                                                                                  60
                                                                                                            80
                                                                                                                                               20
                                                                                                                                                                        40
```

Compare this with the unacceptably high noise floor from the previous version for the case $\alpha = 1/137$, $\phi = 30$ °.



Debugging and benchmarking tools

If something goes funny with your calls, then before you start taking makeDipoleList apart you can try using its Verbose option to diagnose the internal functions it is using. In particular:

■ Setting Verbose→1 makes makeDipoleList print the Information of the key internal functions it is using, before it goes on to the integration loop.

$$\begin{split} \text{makeDipoleList} \Big[\text{VectorPotential} &\rightarrow \text{Function} \Big[\text{t}, \, \Big\{ \frac{\text{F}}{\omega} \, \text{Sin} [\omega \, \text{t}] \,, \, 0 \,, \, 0 \Big\} \Big] \,, \\ \text{FieldParameters} &\rightarrow \{ \text{F} \rightarrow 0.05, \, \omega \rightarrow 0.057 \} \,, \, \text{Verbose} \rightarrow 1 \Big] \, [\![1 \,\, ; ; \, 10]\!] \end{split}$$

```
RBSFA`Private`A
```

RBSFA`Private`A[RBSFA`Private`t\$_] = {0.877193 Sin[0.057 RBSFA`Private`t\$], 0, 0}

RBSFA`Private`GA

RBSFA'Private'GA[RBSFA'Private't\$_] = {{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}

```
RBSFA`Private`ps
RBSFA`Private`ps[RBSFA`Private`t_?RBSFA`Private`gridPointQ,
    RBSFA`Private`tt_?RBSFA`Private`gridPointQ] :=
  RBSFA`Private`ps[RBSFA`Private`t, RBSFA`Private`tt] =
    - (Inverse[IdentityMatrix[Length[RBSFA`Private`A[RBSFA`Private`tInit]]] -
                 (RBSFA`Private`GAIntInt[RBSFA`Private`t, RBSFA`Private`tt] +
                       Transpose[RBSFA`Private`GAIntInt[RBSFA`Private`t, RBSFA`Private`tt]]) /
                   (RBSFA`Private`t - RBSFA`Private`tt - i RBSFA`Private`\epsilon)].
             (RBSFA`Private`AInt[RBSFA`Private`t, RBSFA`Private`tt] -
                RBSFA`Private`bigPScorrectionInt[RBSFA`Private`t, RBSFA`Private`tt]) /
           (RBSFA`Private`t - RBSFA`Private`tt - i RBSFA`Private`∈))
  RBSFA`Private`pi
RBSFA`Private`pi[RBSFA`Private`p_, RBSFA`Private`t_] :=
  RBSFA`Private`p + RBSFA`Private`A[RBSFA`Private`t] -
    RBSFA`Private`GAInt[RBSFA`Private`t].RBSFA`Private`p - RBSFA`Private`GAdotAInt[RBSFA`Private`t]
  RBSFA'Private'S
RBSFA`Private`S[RBSFA`Private`t_?RBSFA`Private`gridPointQ,
    RBSFA`Private`tt_?RBSFA`Private`gridPointQ] :=
   \frac{1}{2} \left(\text{Norm}[RBSFA\cappa\cdot Private\cdot ps[RBSFA\cappa\cdot Private\cdot t, RBSFA\cappa\cdot Private\cdot \cdot t]]^2 + RBSFA\cappa\cdot Private\cdot \cdot \chi^2\right)
      (RBSFA`Private`t - RBSFA`Private`tt) + RBSFA`Private`ps[RBSFA`Private`t, RBSFA`Private`tt].
      RBSFA`Private`AInt[RBSFA`Private`t, RBSFA`Private`tt] +
     1/2 RBSFA`Private`A2Int[RBSFA`Private`t, RBSFA`Private`tt] -
     (RBSFA`Private`ps[RBSFA`Private`t, RBSFA`Private`tt].RBSFA`Private`GAIntInt[
            RBSFA`Private`t, RBSFA`Private`tt].RBSFA`Private`tp] + RBSFA`Private`t, RBSFA`Private`tt] + RBSFA`Private`
        RBSFA`Private`ps[RBSFA`Private`t, RBSFA`Private`tt].
          RBSFA`Private`bigPScorrectionInt[RBSFA`Private`t, RBSFA`Private`tt] +
        RBSFA`Private`AdotGAdotAInt[RBSFA`Private`t, RBSFA`Private`tt])
  RBSFA`Private`AInt
RBSFA`Private`AInt[RBSFA`Private`t$_] = {-15.3894 Cos[0.057 RBSFA`Private`t$], 0, 0}
RBSFA`Private`AInt[RBSFA`Private`t$_, RBSFA`Private`tt$_] =
  {15.3894 Cos[0.057 RBSFA`Private`tt$] - 15.3894 Cos[0.057 RBSFA`Private`t$], 0, 0}
  RBSFA`Private`A2Int
RBSFA`Private`A2Int[RBSFA`Private`t$_] =
 0.769468 (0.5 RBSFA`Private`t$ - 4.38596 Sin[0.114 RBSFA`Private`t$])
RBSFA`Private`A2Int[RBSFA`Private`t$_, RBSFA`Private`tt$_] =
  -0.769468 (0.5 RBSFA`Private`tt$ -4.38596 Sin[0.114 RBSFA`Private`tt$]) +
    0.769468 (0.5 RBSFA`Private`t$ - 4.38596 Sin[0.114 RBSFA`Private`t$])
  RBSFA`Private`GAInt
RBSFA`Private`GAInt[RBSFA`Private`t\$_] = {{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}
RBSFAPrivate GAInt[RBSFA Private t$_, RBSFA Private t$_] = {{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}
(abridged.)
```

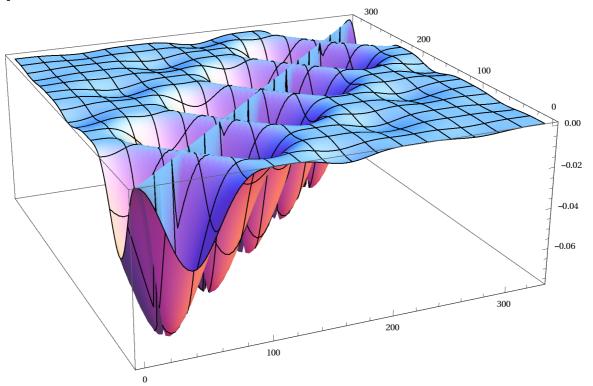
```
\{\{-0.0198736+0.00113629 i, 0.+0.i, 0.+0.i\}, \{-0.0166186-1.44349 i, 0.+0.i, 0.+0.i\},
   \{-0.0132498 - 5.34015 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}, \{-0.00957477 - 10.5721 \text{ i}, 0. + 0. \text{ i}, 0. + 0. \text{ i}\}\}
   \{-0.00563402 - 15.8027 \, i, \, 0. + 0. \, i, \, 0. + 0. \, i\}, \, \{-0.00185819 - 19.9418 \, i, \, 0. + 0. \, i, \, 0. + 0. \, i\}, \, \{-0.00185819 - 19.9418 \, i, \, 0. + 0. \, i, \, 0. + 0. \, i\}
    \{0.0053967 - 22.4 \, \text{i}, \, 0.+0. \, \text{i}, \, 0.+0. \, \text{i}\}, \, \{0.00707192 - 20.6646 \, \text{i}, \, 0.+0. \, \text{i}, \, 0.+0. \, \text{i}\}\}
```

■ Setting Verbose→2 makes makeDipoleList output its key internal functions and shut down before the integration takes place. Its results can be caught as follows:

```
{A[t_], GA[t_], ps[t_, tt_], pi[p_, t_], S[t_, tt_], AInt[t_], AInt[t_, tt_], A2Int[t_],
    A2Int[t_, tt_], GAInt[t_], GAInt[t_, tt_], GAdotAInt[t_], GAdotAInt[t_, tt_], AdotGAInt[t_],
    AdotGAInt[t_, tt_], GAIntInt[t_], GAIntInt[t_, tt_], bigPScorrectionInt[t_],
    \label{eq:bigPScorrectionInt[t_, tt_], AdotGAdotAInt[t_], AdotGAdotAInt[t_, tt_], integrand[t_, \tau_]} \\
   \Big\} = \texttt{makeDipoleList}\Big[ \texttt{VectorPotential} \rightarrow \texttt{Function}\Big[\texttt{t,} \Big\{ \frac{\texttt{F}}{\omega} \, \texttt{Sin}[\omega \, \texttt{t}] \,, \, 0 \,, \, 0 \Big\} \Big] \,,
    FieldParameters \rightarrow {F \rightarrow 0.05, \omega \rightarrow 0.057}, Verbose \rightarrow 2];
```

This then enables examination of e.g. the action:

```
Block \left[ \{ \omega = 0.057 \} \right],
  Plot3D
    Im[S[t, tt]]
     , \left\{ \text{t, 0, 3} \, \frac{2\,\pi}{\omega} \right\}, \left\{ \text{tt, 0, 3} \, \frac{2\,\pi}{\omega} \right\}
     , PlotRange \rightarrow Full, ImageSize \rightarrow 600, PlotTheme \rightarrow "Classic", PlotPoints \rightarrow 100
```



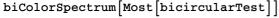
See the implementation notes in the code for makeDipoleList for further definitions of what each term entails.

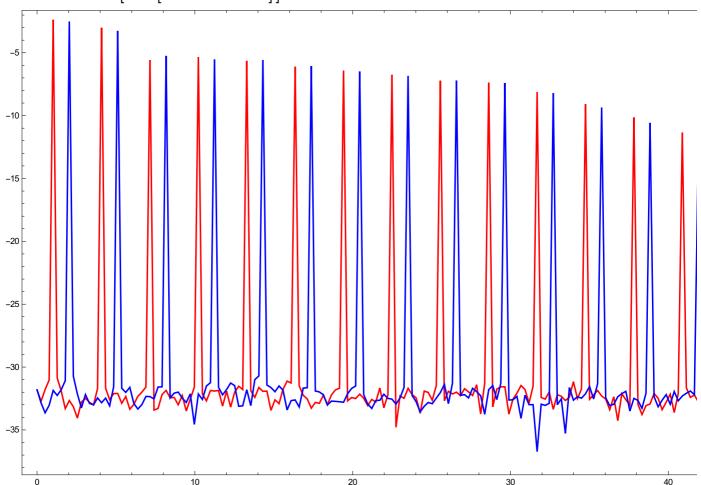
Bicircular fields

As a slightly less trivial example, consider a bicircular field: two counter-rotating, circularly polarized fields of different frequencies. The 'standard' case - as first demonstrated experimentally - has one field as the second harmonic of the fundamental, with both at equal intensities. The resultant harmonics appear at all integer orders except those divisible by three, with the 3n+1 harmonics polarized as the fundamental, and the 3n-1 harmonics polarized as the second-harmonic driver.

```
bicircularA[t_]:=
    \left(\frac{\text{F1}}{\omega 1} \left\{ \, \text{Cos}[\text{t} \, \omega 1] \, \text{Sin}[\alpha] \, , \, - \, \text{Cos}[\alpha] \, \text{Sin}[\text{t} \, \omega 1] \, \right\} + \frac{\text{F2}}{\omega 2} \left\{ \text{Cos}[\beta] \, \text{Cos}[\omega 2 \, \text{t}] \, , \, \text{Sin}[\beta] \, \text{Sin}[\omega 2 \, \text{t}] \right\} \right)
\texttt{bicircularParameters} = \left\{\texttt{F1} \rightarrow \texttt{0.075}, \ \texttt{F2} \rightarrow \texttt{0.075}, \ \alpha \rightarrow \texttt{45} \ ^{\circ}, \ \beta \rightarrow \texttt{45} \ ^{\circ}, \ \omega \texttt{1} \rightarrow \texttt{45.6} \ / \ \texttt{800}, \ \omega \texttt{2} \rightarrow \texttt{45.6} \ / \ \texttt{400} \right\};
AbsoluteTiming[bicircularTest = makeDipoleList[VectorPotential → bicircularA,
            FieldParameters → bicircularParameters, TotalCycles → 4];]
 {8.45739, Null}
```

The function biColorSpectrum takes the spectrum and plots it, separating the two circular polarizations into different colours.



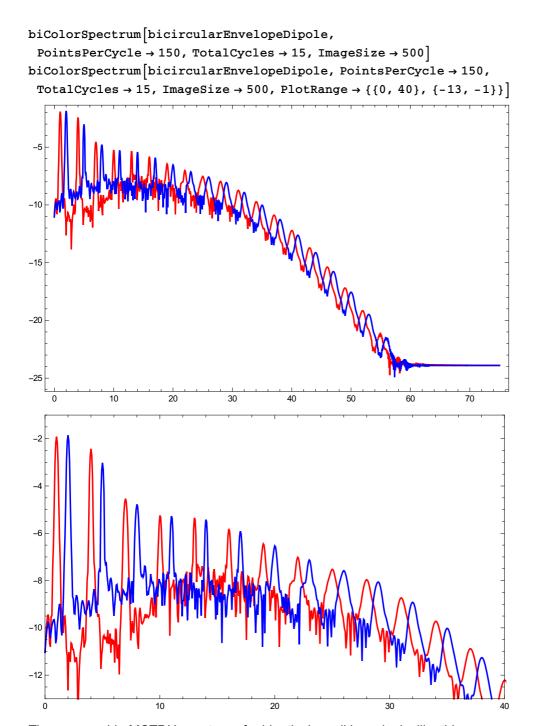


Bicircular fields with a sine-squared envelope

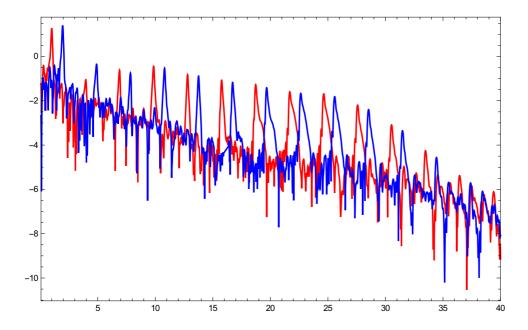
To benchmark the original calculations, we compared them with the output of full MCTDH calculations. Here we used a sin² envelope as the TDSE numerics require a finite pulse; the calculations take correspondingly longer but they are still very manageable (two/three minutes per calculation for a fifteen-cycle pulse, resolving up to ~70 harmonics). One distinctive feature is that the harmonics near the cutoff are broader, because less cycles contribute to those energies.

```
bicircular Envelope A[t_] := cosPowerFlatTop[\omega1, TotalCycles, 2][t]
      \left(\frac{\text{F1}}{\omega 1}\left\{\text{Cos}[\text{t}\,\omega 1]\,\text{Sin}[\alpha]\,,\,-\text{Cos}[\alpha]\,\text{Sin}[\text{t}\,\omega 1]\right\}+\frac{\text{F2}}{\omega 2}\left\{\text{Cos}[\beta]\,\text{Cos}[\omega 2\,\text{t}]\,,\,\text{Sin}[\beta]\,\text{Sin}[\omega 2\,\text{t}]\right\}\right);
bicircular Parameters = \{F1 \rightarrow 0.075, F2 \rightarrow 0.075, \alpha \rightarrow 45 ^{\circ}, \beta \rightarrow 45 ^{\circ}, \omega 1 \rightarrow 45.6 / 800, \omega 2 \rightarrow 45.6 / 400\};
If (as in this case) the field depends on a number-of-cycles parameter, care must be taken that it matches the num
option of the main call.
AbsoluteTiming[
 bicircularEnvelopeDipole =
     makeDipoleList [VectorPotential → bicircularEnvelopeA, FieldParameters →
         Join[bicircularParameters, {TotalCycles → 15}], PointsPerCycle → 150, TotalCycles → 15];
{141.302, Null}
```

Plotting the spectrum, and a zoom at the plateau:



The comparable MCTDH spectrum, for identical conditions, looks like this:



Original RB-SFA: 'rotating' bicircular fields

Calculation

Here the fundamental laser driver has been set at an elliptical polarization (as in the original experiment, A. Fleischer et al., Nature Photon. 8, 543 (2014)), which helps investigate the spin-angular-momentum conservation properties of HHG. In the model proposed in the original paper (Phys. Rev. A 90, 043829 (2014)), the photon model is validated by splitting the elliptical field itself into two circular components, which can then be tuned independently:

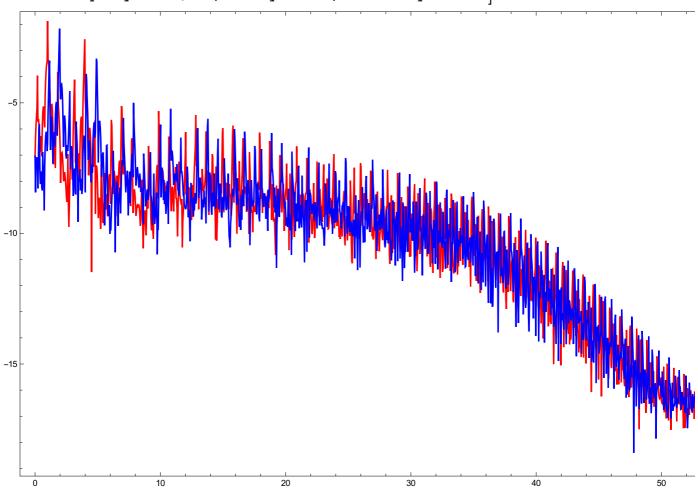
```
\texttt{rotatingBicircularA[t\_]} := \texttt{envelope[t]} \left( \frac{\texttt{F2}}{\omega 2} \left\{ \texttt{Cos[\beta]} \ \texttt{Cos[} \omega \texttt{2} \ \texttt{t} - \phi \texttt{1} \texttt{]} \,, \ \texttt{Sin[\beta]} \ \texttt{Sin[} \omega \texttt{2} \ \texttt{t} - \phi \texttt{1} \texttt{]} \right\} + \texttt{Invelope[t]} \left( \frac{\texttt{F2}}{\omega 2} \left\{ \texttt{Cos[\beta]} \ \texttt{Cos[} \omega \texttt{2} \ \texttt{t} - \phi \texttt{1} \texttt{]} \,, \ \texttt{Sin[\beta]} \ \texttt{Sin[} \omega \texttt{2} \ \texttt{t} - \phi \texttt{1} \texttt{]} \right\} + \texttt{Invelope[t]} \right) \right)
                 \frac{\text{F1}}{\sqrt{2}} \left( \frac{1}{\omega 1} \cos \left[ \alpha - \frac{\pi}{4} \right] \left\{ \cos \left[ \omega 1 \, t + \phi 1 \right], \, -\sin \left[ \omega 1 \, t + \phi 1 \right] \right\} +
                            \frac{1}{(1+\delta) \omega 1} \operatorname{Sin} \left[ \alpha - \frac{\pi}{4} \right] \left\{ \operatorname{Cos} \left[ (1+\delta) \omega 1 \, t - \phi 1 + \phi 2 \right], + \operatorname{Sin} \left[ (1+\delta) \omega 1 \, t - \phi 1 + \phi 2 \right] \right\} \right) \right\};
DistributeDefinitions["RBSFA`"];
directory = FileNameJoin[{NotebookDirectory[], "Temp Data"}];
filename [\delta_{-}] :=
       FileNameJoin[{directory, "data 25.09 detuning scan at \delta=" <> ToString[\delta] <> ".txt"}];
Length[\deltaRange = Range[0, 0.25, 0.001]]
251
```

To test the validity of the photon model, we ran a scan over the detuning δ , using the calculation below.

```
DateString[]
Print["Total = ", Length[\deltaRange], " points at ~230s/point will be done at approximately ",
 DateString[AbsoluteTime[] + Length[δRange] * 230. /7], "."]
ParallelTable[
   Print AbsoluteTiming
     makeDipoleList[
        VectorPotential → rotatingBicircularA,
        FieldParameters \rightarrow {\alpha \rightarrow 35°, \beta \rightarrow 45°, F1 \rightarrow 0.075, F2 \rightarrow 0.075, \omega1 \rightarrow 0.057,
           \omega 2 \rightarrow 1.95 \times 0.057, \phi 1 \rightarrow 0, \phi 2 \rightarrow 0, envelope \rightarrow flatTopEnvelope[\omega 1, 26, 3],
        CarrierFrequency → 0.057, TotalCycles → 26, PointsPerCycle → 115,
        nGate → 1.8, PointNumberCorrection → 1, Preintegrals → "Numeric",
        ReportingFunction \rightarrow Function [Write [filename [\delta], #]]
       ];]];
   Print[DateString[]];
   , \{\delta, \delta \text{Range}\};
DateString[]
NotebookSave[]
Total time 2h 32min. (Desktop machine with 8-thread, 4-core Intel i7-3770 CPU at 3.40GHz, 16GB RAB, running 7
Mathematica kernels in parallel.)
Expand this cell to see the calculation log.
The results can be pulled in from the files using this:
Do[detunedDipole[\delta] = ReadList[filename[\delta]], {\delta, \deltaRange}]
Or saved into a single location using this:
Save [FileNameJoin [{NotebookDirectory[], "Detuning scan collected data.txt"}], detunedDipole]
DumpSave[
   FileNameJoin[{NotebookDirectory[], "Detuning scan collected data.mx"}], detunedDipole];
and pulled in from the single location using this:
<< (FileNameJoin[{NotebookDirectory[], "Detuning scan collected data.txt"}]);
```

A sample spectrum looks like this:

biColorSpectrum[detunedDipole[0.001 RandomInteger[{0, 1000}]], CarrierFrequency → 45.6 / 800, TotalCycles → 3, PointsPerCycle → 115



Plots from the original paper

The plots from the original paper were produced using the code below. For simplicity we pre-define an interpolation function.

conditions := Sequence [CarrierFrequency → 45.6 / 800, TotalCycles → 26, PointsPerCycle → 115]

```
Remove [detuningInterpolation]
With [\{length = Length | getSpectrum | detunedDipole[0.], Polarization <math>\rightarrow \{1, i\}]]\},
   AbsoluteTiming[
       Table[
              detuningInterpolation[\epsilon] = Interpolation[
                     Flatten Table
                            {{
                                         harmonicOrderAxis[TargetLength → length, conditions],
                                          Table [\delta, \{length\}]
                                  \texttt{Log} \left[\texttt{10, getSpectrum} \left[ \texttt{detunedDipole} \left[ \delta \right], \, \texttt{Polarization} \rightarrow \{\texttt{1, e i}\} \right] \right]
                            , \{\delta, \delta \text{Range}\}, 1]
              , \{ \epsilon, \{1, -1\} \} ];
{2.99829, Null}
Some plotting admin:
CMRwithMin[minIn_, minOut_: 1. / 9] :=
   \texttt{Function}\Big[\texttt{x, CMRmap}\Big[\texttt{If}\Big[\texttt{x < minIn}, \, \frac{\texttt{minOut}}{\texttt{minIn}}\,\texttt{x, minOut} + \big(1 - \texttt{minOut}\big) \, \frac{\texttt{x - minIn}}{1 - \texttt{minIn}}\Big]\Big]\Big]
min = 6. \times 10^{-9};
\max = 5. \times 10^{-7};
colorfunction = CMRwithMin[min/max];
HOTicks[\epsilon_{-}] :=
    \left(\left\{\#,\ \text{If}\left[\varepsilon=1,\ \text{Style}\left[\#,\ \text{Black}\right],\ ""\right],\ \left\{0.02,\ 0\right\},\ \left\{\text{Thickness}\left[0.005\right],\ \text{Gray}\right\}\right\} \&\ /@\ \text{Range}\left[12,\ 18,\ 1\right]\right) \sim 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 + 1.5 +
      Join~ \left\{ \#, \#, \#, \{0.01, 0\}, \left\{ \text{Thickness}[0.004], \text{Gray} \right\} \right\} \& / @ \text{Range} \left[ 11 + \frac{1}{2}, 18 + \frac{1}{4}, 1/4 \right] \right\}
({#, Style[#, Black], {0.015, 0}, {Thickness[0.005], Gray}} &/@Range[0.05, 0.20, 0.05])~
           Join~({#, "", {0.01, 0}, {Thickness[0.004], Gray}} & /@Range[0.01, 0.24, 0.01]);
upTicks = (\{\#, "", \{0.015, 0\}, \{Thickness[0.005], Gray\}\} \& /@Range[0.05, 0.20, 0.05]) \sim (\{\#, "", \{0.015, 0\}, \{Thickness[0.005], Gray\}\})
           Join~({#, "", {0.01, 0}, {Thickness[0.004], Gray}} &/@Range[0.01, 0.24, 0.01]);
```

The plot itself:

```
RowTable
    splittingsScan[e] = RegionPlot
         , \{\delta, 0, 0.25\}, \{HO, 11.25, 18.5\}
         , AspectRatio \rightarrow 1.2
         , PlotRangePadding \rightarrow None
         , ImagePadding \rightarrow 1 {{35 + 15 \epsilon, 20}, {70, 6}}
         , ImageSize \rightarrow {Automatic, 550}
         , PlotPoints \rightarrow 600
         , FrameStyle \rightarrow Automatic
        FrameLabel \rightarrow \left\{ \text{Style} \left[ \frac{\omega'}{\alpha'} - 1^{"}, \text{ Black, 12} \right], \text{ If } \left[ \epsilon = 1, \text{ Style} \left[ \text{"Harmonic Order", Black, 16} \right], \text{""} \right] \right\}
         , ColorFunctionScaling \rightarrow False
        , FrameTicks \rightarrow {{HOTicks[1], HOTicks[-1]}, {downTicks, upTicks}}
         , ColorFunction \rightarrow Function \left[\{\delta,\, \text{HO}\}\,,\, \text{colorfunction}\left[\frac{10\,^{\circ}\text{detuningInterpolation}[\varepsilon]\,[\text{HO},\,\delta]}{\text{max}}\right]\right]
         , PlotLabel \rightarrow
          Style \Big[ \texttt{StringJoin} \Big[ \texttt{\epsilon /.} \Big\{ \texttt{1} \rightarrow \texttt{"Right", -1} \rightarrow \texttt{"Left"} \Big\}, \, \texttt{"-circular harmonics"} \Big], \, \texttt{Black, 16} \Big] \\
    , {e, {1, -1}}
(Removed to keep file size low.)
```