

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

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## Introduction

### Readme

RB-SFA is a compact and flexible *Mathematica* package for calculating High Harmonic Generation emission within the Strong Field Approximation. It combines *Mathematica*'s analytical integration capabilities with its numerical calculation capacities to offer a fast and user-friendly plug-and-play solver for calculating harmonic spectra and other properties. In addition, it can calculate first-order nondipole corrections to the SFA results to evaluate the effect of the driving laser's magnetic field on harmonic spectra.

The name RB-SFA comes from its first application (as Rotating Bicircular High Harmonic Generation in the Strong field Approximation) but the code is general so RB-SFA just stands for itself now. This first application was used to calculate the polarization properties of the harmonics produced by multi-colour circularly polarized fields, as reported in the paper

Spin conservation in high-order-harmonic generation using bicircular fields. E. Pisanty, S. Sukiasyan and M. Ivanov. *Phys. Rev. A* **90**, 043829 (2014), arXiv:1404.6242.

This code is dual-licensed under the GPL and CC-BY-SA licenses. If you use this code or its results in an academic publication, please cite the paper above or the GitHub repository where the latest version will always be available. An example citation is

E. Pisanty. RB-SFA: High Harmonic Generation in the Strong Field Approximation via *Mathematica*. <https://github.com/episanty/RB-SFA> (2014).

This software consists of this notebook, which contains the code and its documentation, a corresponding auto-generated package file. This notebook also contains a Usage and Examples section which explains how to use the code and documents the calculations used in the original publication.

### Specifications

This code calculates the harmonic dipole as per the original Lewenstein *et al.* paper,

M. Lewenstein, Ph. Balcou, M.Yu. Ivanov, A. L'Huillier and P.B. Corkum. Theory of high-harmonic generation by low-frequency laser fields. *Phys. Rev. A* **49** no. 3, 2117 (1994).

The time-dependent dipole is given by

$$\mathbf{D}(t) = i \int_0^t dt' \int d^3\mathbf{p} \, \mathbf{d}(\boldsymbol{\pi}(\mathbf{p}, t)) \times \mathbf{F}(t') \cdot \mathbf{d}(\boldsymbol{\pi}(\mathbf{p}, t')) \times \exp[-i S(\mathbf{p}, t, t')] + c.c.$$

Here  $\mathbf{F}(t)$  is the time-dependent applied electric field, with vector potential  $\mathbf{A}(t)$ ; the electron charge is taken to be  $-1$ . The integration time  $t'$  can be interpreted as the ionization time and the integration limit  $t$  represents the recollision time. (Upon applying the saddle-point approximation to the temporal integrals these notions apply exactly to the

corresponding quantum orbits.) The ionization and recollision events are governed by the corresponding dipole matrix elements, which are taken for a hydrogenic 1s-type orbital with characteristic momentum  $\kappa$  and ionization potential  $I_p = \frac{1}{2} \kappa^2$ :

$$\mathbf{d}(\mathbf{p}) = \langle \mathbf{p} | \hat{\mathbf{d}} | g \rangle = \frac{8i}{\pi} \frac{\sqrt{2\kappa^5} \mathbf{p}}{(\mathbf{p}^2 + \kappa^2)^3}.$$

(Taken from B. Podolsky & L. Pauling. *Phys. Rev.* **34** no. 1, 109 (1929).) The displaced momentum  $\boldsymbol{\pi}(\mathbf{p}, t) = \mathbf{p} + \mathbf{A}(t)$  is used to aid in the generalization to nondipole cases.

The action

$$S(\mathbf{p}, t, t') = \int_{t'}^t \left( \frac{1}{2} \kappa^2 + \frac{1}{2} \boldsymbol{\pi}(\mathbf{p}, \tau)^2 \right) d\tau$$

is the governing factor of the integral. It is highly oscillatory and must be dealt with carefully. The momentum integral is approximated using the saddle point method; this is valid and straightforward since there is always one unique saddle point,

$$\mathbf{p}_s(t, t') = - \frac{\int_{t'}^t \mathbf{A}(\tau) d\tau}{t - t'},$$

as long as the action's dependence on the momentum is quadratic. After the momentum has been integrated via the saddle point method, the time-dependent dipole is given by

$$\mathbf{D}(t) = i \int_0^t dt' \left( \frac{2\pi}{\epsilon + i(t-t')} \right)^{3/2} \mathbf{d}(\boldsymbol{\pi}(\mathbf{p}_s(t, t'), t)) \times \mathbf{F}(t') \cdot \mathbf{d}(\boldsymbol{\pi}(\mathbf{p}_s(t, t'), t')) \times \exp[-i S(\mathbf{p}_s(t, t'), t, t')] + c.c.$$

A regularization factor  $\epsilon$  has been introduced to prevent divergence of the prefactor as  $t'$  approaches  $t$ , representing the fact that at  $t = t'$  the  $\mathbf{p}$  integral no longer has a quadratic exponent.

The integral is performed with respect to the excursion time  $\tau = t - t'$  for simplicity. To reduce integration time, a gating function  $\text{gate}[\omega \tau]$  has been introduced, and the integration time has been cut short to a controllable length. This is physically reasonable as the wavepacket spreading (which scales as  $\tau^{-3/2}$ ) makes the contributions after the gate negligible.

More physically, suppressing the contributions from large excursion times represents the fact that the extra-long trajectories they represent produce harmonics which are much harder to phase match (as their harmonic phase is very sensitively dependent on many factors) which means that they are rarely present in experimental spectra unless a concerted effort is performed to observe them.

## First-order nondipole calculations

This code can also be used to calculate the first-order effect of nondipole terms, which become relevant at high intensities or long wavelengths, when the electron's speed from the laser-driven oscillations (which scales as  $F/\omega$ ) becomes comparable to the speed of light (equal to  $c = 1/\alpha \approx 137$  in atomic units). (More specifically, the nondipole effects on the harmonic generation become relevant when the magnetic pushing per cycle, which offsets the returning wavepacket by  $F^2/c\omega^3$ , becomes comparable with the wavepacket spread upon recollision.)

This code implements a generalization of the theory presented in various forms in the papers N.J. Kylstra et al. *J. Phys B: At. Mol. Opt. Phys.* **34** no. 3, L55 (2001); N.J. Kylstra et al. *Laser Phys.* **12** no. 2, 409 (2002); M.W. Walser et al. *Phys. Rev. Lett.* **85** no. 24, 5082 (2000); V. Averbukh et al. *Phys Rev. A* **65**, 063402 (2002); and C.C. Chirilă et al. *Phys. Rev. A* **66**, 063411 (2002).

The nondipole-HHG code calculates the harmonic dipole of exactly the same form as the standard SFA,

$$\mathbf{D}(t) = i \int_0^t dt' \int d^3 \mathbf{p} \, \mathbf{d}(\boldsymbol{\pi}(\mathbf{p}, t, t')) \times \mathbf{F}(t') \cdot \mathbf{d}(\boldsymbol{\pi}(\mathbf{p}, t', t')) \times \exp[-i S(\mathbf{p}, t, t')] + c.c.$$

with  $S(\mathbf{p}, t, t') = \int_{t'}^t dt'' \left( \frac{1}{2} \kappa^2 + \frac{1}{2} \boldsymbol{\pi}(\mathbf{p}, t'', t')^2 \right)$  as before, but with a nondipole term in the displaced momentum, which now reads

$$\boldsymbol{\pi}(\mathbf{p}, t, t') = \mathbf{p} + \mathbf{A}(t) - \int_{t'}^t \nabla \mathbf{A}(\tau) \cdot (\mathbf{p} + \mathbf{A}(\tau)) d\tau,$$

or in component notation

$$\pi_j(\mathbf{p}, t, t') = p_j + A_j(t) - \int_{t'}^t \partial_j A_k(\tau) (p_k + A_k(\tau)) d\tau.$$

## Implementation: supporting functions

### Initialization

```
BeginPackage["RBSFA`"];
```

### Version number and timestamp

The command `RBSFAversion` prints the version of the RB-SFA package currently loaded and its timestamp

```
RBSFAversion::usage = "RBSFAversion[] prints the current
    version of the RB-SFA package in use and its timestamp .";
Begin["`Private`"];
RBSFAversion[] = "RB-SFA v2.0.1, Thu 4 Feb 2016 22:51:14";
End[];
```

The timestamp is updated every time the notebook is saved via an appropriate notebook option, which is set by the code below.

```

SetOptions[
  EvaluationNotebook[],
  NotebookEventActions->{{"MenuCommand  ", "Save"}-> (
    NotebookWrite[
      Cells[CellTags->"version-definition"][[1]],
      Cell[BoxData[RowBox[{
        "RBSFAversion::usage=\"RBSFAversion[] prints the current version of the
          RB-SFA package in use and its timestamp .\";
        Begin[\"`Private`\"];
        RBSFAversion[]=\"\"<>First[StringSplit[
          Select[
            Flatten[
              NotebookRead[Cells[CellTags->"version-definition"][[1]]
                /. {Cell->List, BoxData->List, RowBox->List}
            ],
            Quiet[StringContainsQ#, "RB-SFA v"]]&
          ][[1], {"\"\", \"\", \"\"}]]<>\", \"<>DateString[]<>\";
        End[];\"
      }]], "Input", InitializationCell->True, CellTags->"version-definition"
    ], None
  ]];
  NotebookSave[]
], PassEventsDown->True}
];

```

## Dipole transition matrix elements

Default DTME is for a hydrogenic 1s state.

```

hydrogenicDTME::usage =
  "hydrogenicDTME[p,κ] returns the dipole transition matrix element for
    a 1s hydrogenic state of ionization potential  $I_p = \frac{1}{2}\kappa^2$ .";
Begin["`Private`"];
hydrogenicDTME[p_, κ_] :=  $\frac{8i}{\pi} \frac{\sqrt{2}\kappa^5 p}{(\text{Norm}[p]^2 + \kappa^2)^3}$ 
End[];

```

Another possibility is for a gaussian orbital

```

gaussianDTME::usage = "gaussianDTME[p,κ] returns the dipole transition
  matrix element for a gaussian state of characteristic size 1/κ."
Begin["`Private`"];
gaussianDTME[p_, κ_] :=  $-i(4\pi)^{3/4}\kappa^{-7/2}p\text{Exp}\left[-\frac{\text{Norm}[p]^2}{2\kappa^2}\right]$ 
End[]
gaussianDTME[p,κ] returns the dipole transition
  matrix element for a gaussian state of characteristic size 1/κ.
RBSFA`Private`

```

## Various field envelopes

### flatTopEnvelope

```
flatTopEnvelope::usage =
  "flatTopEnvelope[ $\omega$ , num , nRamp ] returns a Function object representing
  a flat-top envelope at carrier frequency  $\omega$  lasting a total
  of num cycles and with linear ramps nRamp cycles long.";
Begin["`Private`"];
flatTopEnvelope[ $\omega$ _ , num_ , nRamp_ ] := Function[t,
  Piecewise[{{0, t < 0}, {Sin[ $\frac{\omega t}{4 nRamp}$ ]2, 0 ≤ t <  $\frac{2\pi}{\omega}$  nRamp }, {1,  $\frac{2\pi}{\omega}$  nRamp ≤ t <  $\frac{2\pi}{\omega}$  (num - nRamp ) },
    {Sin[ $\frac{\omega (\frac{2\pi}{\omega} num - t)}{4 nRamp}$ ]2,  $\frac{2\pi}{\omega}$  (num - nRamp ) ≤ t <  $\frac{2\pi}{\omega}$  num }, {0,  $\frac{2\pi}{\omega}$  num ≤ t}}]]
End[];
```

### cosPowerFlatTop

```
cosPowerFlatTop::usage =
  "cosPowerFlatTop[ $\omega$ , num , power] returns a Function object representing
  a smooth flat-top envelope of the form 1-Cos( $\omega t/2$  num )power";
Begin["`Private`"];
cosPowerFlatTop[ $\omega$ _ , num_ , power_] := Function[t, 1-Cos[ $\frac{\omega t}{2 num}$ ]power]
End[];
```

## Field duration standard options

The standard options for the duration of the pulse and the resolution are

```
PointsPerCycle::usage =
  "PointsPerCycle is a sampling option which specifies the number of sampling
  points per cycle to be used in integrations";
TotalCycles::usage = "TotalCycles is a sampling option which specifies
  the total number of periods to be integrated over.";
CarrierFrequency::usage = "CarrierFrequency is a sampling option which
  specifies the carrier frequency to be used.";
Protect[PointsPerCycle, TotalCycles, CarrierFrequency];

standardOptions = {PointsPerCycle → 90, TotalCycles → 1, CarrierFrequency → 0.057};
```

PointsPerCycle dictates how many sampling points are used per laser cycle (at frequency CarrierFrequency, of the infrared laser), and it should be at least twice the highest harmonic of interest. The total duration is TotalCycles cycles. CarrierFrequency is the frequency of the fundamental laser, in atomic units.

### harmonicOrderAxis

harmonicOrderAxis produces a list that can be used as a harmonic order axis for the given pulse parameters.

The length can be fine-tuned (to match exactly a spectrum, for instance, and get a matrix of the correct shape) using the correction option, or a TargetLength can be directly specified.

```

harmonicOrderAxis::usage =
  "harmonicOrderAxis[opt→value] returns a list of frequencies which can be used as
    a frequency axis for Fourier transforms , scaled in units of harmonic
    order, for the provided field duration and sampling options.";
TargetLength::usage = "TargetLength is an option for harmonicOrderAxis which
    specifies the total length required of the resulting list.";
LengthCorrection::usage = "LengthCorrection is an option for harmonicOrderAxis which
    allows for manual correction of the length of the resulting list.";
Protect[LengthCorrection, TargetLength];
Begin["`Private`"];
Options[harmonicOrderAxis] =
  standardOptions~Join~{TargetLength→Automatic , LengthCorrection→1};
harmonicOrderAxis::target =
  "Invalid TargetLength option `1`. This must be a positive integer or Automatic .";
harmonicOrderAxis[OptionsPattern[]] :=
  Module[{num = OptionValue[TotalCycles], npp = OptionValue[PointsPerCycle]},
    Piecewise[{
      { $\frac{1}{\text{num}}$  Range[0., Round[ $\frac{\text{npp num} + 1}{2.}$ ] - 1 + OptionValue[LengthCorrection]],
        OptionValue[TargetLength] === Automatic },
      { $\frac{\text{Round}[\frac{\text{npp num} + 1}{2.}]}{\text{num}}$  Range[0, OptionValue[TargetLength] - 1],
        IntegerQ[OptionValue[TargetLength]] && OptionValue[TargetLength] ≥ 0 }
    },
    Message[harmonicOrderAxis::target, OptionValue["TargetLength"]];
    Abort[]
  ]
End[];

```

## frequencyAxis

frequencyAxis produces a list that can be used as a harmonic order axis for the given pulse parameters. Identical to harmonicOrderAxis but produces a frequency axis (in atomic units) instead.

```

frequencyAxis::usage =
  "frequencyAxis[opt→value] returns a list of frequencies which can be used
    as a frequency axis for Fourier transforms , in atomic units of
    frequency, for the provided field duration and sampling options.";
Begin["`Private`"];
Options[frequencyAxis] = Options[harmonicOrderAxis];
frequencyAxis[options:OptionsPattern[]] :=
  OptionValue[CarrierFrequency] harmonicOrderAxis[options]
End[];

```

## timeAxis

timeAxis produces a list that can be used as a time axis for the given pulse parameters.

```

Quit

timeAxis::usage =
  "timeAxis[opt→value] returns a list of times which can be used as a time axis ";
TimeScale::usage = "TimeScale is an option for timeAxis which specifies the units the
  list should use: AtomicUnits by default, or LaserPeriods if required.";
AtomicUnits::usage = "AtomicUnits is a value for the option TimeScale of timeAxis
  which specifies that the times should be in atomic units of time .";
LaserPeriods::usage = "LaserPeriods is a value for the option TimeScale of timeAxis which
  specifies that the times should be in multiples of the carrier laser period.";
Protect[TimeScale, AtomicUnits, LaserPeriods];
Begin["`Private`"];
Options[timeAxis] =
  standardOptions~Join~{TimeScale → AtomicUnits, PointNumberCorrection → 0};
timeAxis::scale =
  "Invalid TimeScale option `1`. Available values are AtomicUnits and LaserPeriods";
timeAxis[OptionsPattern[]] := Block[{T = 2 π / ω, ω = OptionValue[CarrierFrequency],
  num = OptionValue[TotalCycles], npp = OptionValue[PointsPerCycle]},
  Piecewise[{
    {1, OptionValue[TimeScale] === AtomicUnits},
    {1/T, OptionValue[TimeScale] === LaserPeriods}
  },
  Message[timeAxis::scale, OptionValue[TimeScale]]; Abort[]
] × Table[t
  , {t, 0, num  $\frac{2\pi}{\omega}$ ,  $\frac{\text{num}}{\text{num} \times \text{npp} + \text{OptionValue[PointNumberCorrection]}} \frac{2\pi}{\omega}$ }
]
]
End[];

tInit = 0;
tFinal =  $\frac{2\pi}{\omega} \text{num}$  ;
δt =  $\frac{\text{tFinal} - \text{tInit}}{\text{num} \times \text{npp} + \text{OptionValue[PointNumberCorrection]}}$ ; (*integration and looping timestep *)

```

## getSpectrum

getSpectrum takes a time-dependent dipole list and returns its Fourier transform in absolute-value-squared. It takes as options

- pulse parameters  $\omega$ , TotalCycles and PointsPerCycle,
- a polarization parameter  $\epsilon$ , which gives an unpolarized spectrum when given False, or polarizes along an ellipticity vector  $\epsilon$  (this is meant primarily to select right- and left-circularly polarized spectra using  $\epsilon = \{1, i\}$  and  $\epsilon = \{1, -i\}$  respectively),
- a DifferentiationOrder, which can return the dipole value (default, = 0), velocity (= 1), or acceleration (= 2),
- a power of  $\omega$ , ωPower, with which to multiply the spectrum before returning it (which should be equivalent to DifferentiationOrder except for pathological cases), and
- a ComplexPart function to apply immediately after differentiation (default is the identity function, but Re, Im, or

$\text{Abs}[\#]^2$  & are reasonable choices).

If no option is passed to  $\omega\text{Power}$  and  $\text{DifferentiationOrder}$ , the pulse parameters do not really affect the output, except by a global factor of  $\text{TotalCycles}$ .

```

getSpectrum ::usage= "getSpectrum [DipoleList] returns the power spectrum of DipoleList";
Polarization::usage=
  "Polarization is an option for getSpectrum which specifies a polarization
  vector along which to polarize the dipole list. The default,
  Polarization->False, specifies an unpolarized spectrum .";
ComplexPart ::usage= "part is an option for getSpectrum which specifies a
  function (like Re, Im , or by default #&) which should be
  applied to the dipole list before the spectrum is taken.";
 $\omega\text{Power}::\text{usage}= \omega\text{Power}$  is an option for getSpectrum which specifies a
  power of frequency which should multiply the spectrum .";
DifferentiationOrder::usage= "DifferentiationOrder is an option for
  getSpectrum which specifies the order to which the dipole
  list should be differentiated before the spectrum is taken.";
Protect[Polarization, part,  $\omega\text{Power}$ , DifferentiationOrder];

Begin["`Private`"];
Options[getSpectrum] = {Polarization->False, ComplexPart -> (#&),
   $\omega\text{Power}$ ->0, DifferentiationOrder->0}~Join~standardOptions;

getSpectrum ::diffOrd= "Invalid differentiationorder `1`.";
getSpectrum :: $\omega\text{Pow}$ = "Invalid  $\omega$  power `1`.";

getSpectrum [dipoleList_, OptionsPattern[]] := Block[
  {polarizationVector, differentiatedList, depth, dimensions ,
    num = OptionValue[TotalCycles],
    npp = OptionValue[PointsPerCycle],  $\omega$  = OptionValue[CarrierFrequency],  $\delta t = \frac{2\pi/\omega}{\text{npp}}$ 
  },
  polarizationVector=  $\frac{\text{OptionValue[Polarization]}}{\text{Norm} [\text{OptionValue[Polarization]}]}$ ;

  differentiatedList= OptionValue[ComplexPart] [Piecewise[{
    {dipoleList, OptionValue[DifferentiationOrder]==0},
    { $\frac{1}{2\delta t}$  (Most[Most[dipoleList]] - Rest[Rest[dipoleList]]),
      OptionValue[DifferentiationOrder]==1},
    { $\frac{1}{\delta t^2}$  (Most[Most[dipoleList]] - 2Most[Rest[dipoleList]] + Rest[Rest[dipoleList]]),
      OptionValue[DifferentiationOrder]==2}}],
    Message[getSpectrum ::diffOrd, OptionValue[DifferentiationOrder]];
    Abort[]
  ]];

If[NumberQ [OptionValue[ $\omega\text{Power}$ ]], Null;;, Message[getSpectrum :: $\omega\text{Pow}$ , OptionValue[ $\omega\text{Power}$ ]];
  Abort[]];

```



```

num Table[
  ( $\frac{\omega}{\text{num}}$ k)2OptionValue[ωPower], {k, 1, Round[ $\frac{\text{Length}[\text{differentiatedList}]}{2}$ ]}
]×If[
  OptionValue[Polarization]===False, (*unpolarized spectrum *)
  (*funky depth thing so this can take lists of numbers and lists of vectors,
  of arbitrary length. Makes for easier benchmarking .*)
  depth=Length[Dimensions[dipoleList]];
  dimensions = If[Length[#]>1, #[[2]], 1(*#[[1]]*)] &[Dimensions[dipoleList]];
  Sum[Abs[
    Fourier[
      If[depth>1, Re[differentiatedList[[All, i]]], Re[differentiatedList[[All]]]]
      , FourierParameters→{-1, 1}
    ][[1;;Round[ $\frac{\text{Length}[\text{differentiatedList}]}{2}$ ]]]]
  ]2, {i, 1, dimensions}]
, (*polarized spectrum *)
Abs[
  Transpose[Table[
    Fourier[
      Re[differentiatedList[[All, i]]]
      , FourierParameters→{-1, 1}
    ]
    , {i, 1, 2}]]][
  1;;Round[Length[differentiatedList]/2]].polarizationVector
]2
]
End[];

```

## spectrumPlotter

spectrumPlotter takes a spectrum and a list of options and returns a plot of the spectrum. The available options are

- a FrequencyAxis option, which will give the harmonic order as a horizontal axis by default, and an arbitrary scale with any other option,

- all the options of harmonicOrderAxis, which will be passed to the call that makes the horizontal axis, and
- all the options of ListLinePlot, which will be used to format the plot.

```

spectrumPlotter ::usage = "spectrumPlotter [spectrum ] plots
    the given spectrum  with an appropriate axis in a log10 scale.";
FrequencyAxis::usage = "FrequencyAxis is an option for spectrumPlotter
    which specifies the axis to use.";
Protect[FrequencyAxis];
Begin["`Private`"];
Options[spectrumPlotter ] = Join[{FrequencyAxis→"HarmonicOrder "},
    Options[harmonicOrderAxis ], Options[ListLinePlot]];
spectrumPlotter [spectrum_ , options:OptionsPattern[]] := ListPlot[
    {Which[
        OptionValue[FrequencyAxis] === "HarmonicOrder ",
        harmonicOrderAxis ["TargetLength"→Length[spectrum ], Sequence@@FilterRules[
            {options}~Join~Options[spectrumPlotter ], Options[harmonicOrderAxis ]]],
        OptionValue[FrequencyAxis] === "Frequency",
        frequencyAxis["TargetLength"→Length[spectrum ], Sequence@@FilterRules[
            {options}~Join~Options[spectrumPlotter ], Options[harmonicOrderAxis ]]],
        True, Range[Length[spectrum ]]
    ],
    Log[10, spectrum ]
    ]^
, Sequence@@FilterRules[{options}, Options[ListLinePlot]]
, Joined→True
, PlotRange→Full
, PlotStyle→Thick
, Frame →True
, Axes→False
, ImageSize →800
]
End[];

```

## biColorSpectrum

biColorSpectrum takes a time-dependent dipole list and produces overlaid plots of the right- and left-circular components of the spectrum, in red and blue respectively. It takes all the options of getSpectrum and spectrumPlotter, which are passed directly to the corresponding calls, as well as the options of Show, which can be used to modify the plot appearance.

Quit

```

biColorSpectrum ::usage =
  "biColorSpectrum [DipoleList] produces a two-colour spectrum of DipoleList
    separating the two circular polarizations";
Begin["`Private`"];
Options[biColorSpectrum] = Join[{PlotRange → All}, Options[Show],
  Options[spectrumPlotter], DeleteCases[Options[getSpectrum], Polarization → False]];
biColorSpectrum [dipoleList_, options:OptionsPattern[]] := Show[{
  spectrumPlotter [
    getSpectrum [dipoleList, Polarization → {1, +1},
      Sequence@@FilterRules[{options}, Options[getSpectrum]]],
    PlotStyle → Red, Sequence@@FilterRules[{options}, Options[spectrumPlotter]]],
  spectrumPlotter [
    getSpectrum [dipoleList, Polarization → {1, -1},
      Sequence@@FilterRules[{options}, Options[getSpectrum]]],
    PlotStyle → Blue, Sequence@@FilterRules[{options}, Options[spectrumPlotter]]]
  }, PlotRange → OptionValue[PlotRange],
  Sequence@@FilterRules[{options}, Options[Show]]
]
End[];

```

## Various gate functions

Gate functions are used to suppress the contributions of extra-long trajectories with long excursion times, partly to reflect the effect of phase matching but mostly to keep integration times reasonable. They are provided to the main numerical integrator `makeDipoleList` via its `Gate` option.

```

SineSquaredGate::usage =
  "SineSquaredGate[nGateRamp] specifies an integration gate with a sine-squared
    ramp, such that SineSquaredGate[nGateRamp][ωt, nGate]
    has nGate flat periods and nGateRamp ramp periods.";
LinearRampGate ::usage = "LinearRampGate [nGateRamp] specifies an integration gate
  with a linear ramp, such that SineSquaredGate[nGateRamp][ωt, nGate]
  has nGate flat periods and nGateRamp ramp periods.";
Begin["`Private`"];
SineSquaredGate[nGateRamp_][ωτ_, nGate_] := Piecewise[{
  {1, ωτ ≤ 2π(nGate - nGateRamp)},
  {Sin[ $\frac{2\pi nGate - \omega\tau}{4nGateRamp}$ ]2, 2π(nGate - nGateRamp) < ωτ ≤ 2πnGate},
  {0, nGate < ωτ}}];
LinearRampGate [nGateRamp_][ωτ_, nGate_] := Piecewise[{
  {1, ωτ ≤ 2π(nGate - nGateRamp)},
  {- $\frac{\omega\tau - 2\pi(nGate + nGateRamp)}{2\pi nGateRamp}$ , 2π(nGate - nGateRamp) < ωτ ≤ 2πnGate},
  {0, nGate < ωτ}}];
End[];

```

## getIonizationPotential

```
getIonizationPotential::usage =
  "getIonizationPotential[Target] returns the ionizationpotential
    of an atomic target, e.g. \"Hydrogen\", in atomic units.

getIonizationPotential[Target,q] returns the ionizationpotential
  of the q-th ion of the specifiedTarget, in atomic units.";
Begin["`Private`"];
getIonizationPotential[Target_, Charge_: 0] :=
  UnitConvert[ElementData [Target, "IonizationEnergies"][[Charge+1]]/
    (Quantity[1, "AvogadroConstant"] Quantity[1, "Hartrees"])]
End[];
```

## Implementation: main integrator function

The main integration function is `makeDipoleList`, and its basic syntax is of the form `makeDipoleList[VectorPotential→A]`. Here the vector potential `A` must be a function object, such that for numeric `t` the construct `A[t]` returns a list of numbers after the appropriate field parameters have been introduced: thus the criterion is that, for a call of the form `makeDipoleList[VectorPotential→A, FieldParameters→pars]`, a call of the form `A[t]//.pars` returns a list of numbers for numeric `t`. To see the available options use `Options[makeDipoleList]`, and to get information on each option use the `?VectorPotential` construct.

```
makeDipoleList::usage = "makeDipoleList [VectorPotential→A]
  calculates the dipole response to the vector potential A.";

VectorPotential::usage =
  "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.";
VectorPotentialGradient::usage = "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 →pars.
  The indices must be such that GA[t][[i,j]] returns  $\partial_i A_j[t]$ .";
FieldParameters::usage = "FieldParameters is an option for makeDipole list which ";
Preintegrals::usage =
  "Preintegrals is an option for makeDipole list which specifies whether the preintegrals
    of the vector potential should be \"Analytic\" or \"Numeric \".";
ReportingFunction::usage = "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.";
Gate::usage = "Gate is an option for makeDipole list which specifies the integration
  gate to use. Usage as Gate→g, nGate→n will gate the integral at
  time  $\omega t/\omega$  by  $g[\omega t, n]$ . The default is Gate→SineSquaredGate[1/2].";
nGate::usage = "nGate is an option for makeDipole list which specifies
  the total number of cycles in the integration gate.";
IonizationPotential::usage = "IonizationPotential is an option for makeDipoleList
  which specifies the ionizationpotential  $I_p$  of the target.";
```

```

Target::usage="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.";
DipoleTransitionMatrixElement::usage="DipoleTransitionMatrixElement is an option
for makeDipoleList which specifies a function f, of the form
 $f[p,\kappa]=f[p,\sqrt{2 I_p}]$ , to use as the dipole transitionmatrix element .";
eCorrection::usage="eCorrection is an option for makeDipoleList which specifies the
regularization correction  $\epsilon$ , i.e. as used in the factor  $\frac{1}{(t-tt+i\epsilon)^{3/2}}$ .";
PointNumberCorrection::usage="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.";

Protect[VectorPotential, VectorPotentialGradient, FieldParameters , Preintegrals,
ReportingFunction, Gate, IonizationPotential, Target, nGate, eCorrection];

Begin["`Private`"];
Options[makeDipoleList ] = standardOptions~Join~{
  VectorPotential→Automatic , FieldParameters → {}, VectorPotentialGradient→None,
  Preintegrals→"Analytic", ReportingFunction→Identity,
  Gate→SineSquaredGate[1/2], nGate→3/2, eCorrection→0.1,
  IonizationPotential→0.5,
  Target→Automatic , DipoleTransitionMatrixElement→hydrogenicDTME,
  PointNumberCorrection → 0, Verbose → 0
};
makeDipoleList::gate =
  "The integration gate g provided as Gate→`1` is incorrect. Its usage as
  g[`2`,`3`] returns `4` and should return a number .";
makeDipoleList::pot = "The vector potential A provided as VectorPotential→`1`
  is incorrect or is missing FieldParameters . Its usage as
  A[`2`] returns `3` and should return a list of numbers .";
makeDipoleList::gradpot = "The vector potential GA provided as VectorPotentialGradient→`1`
  is incorrect or is missing FieldParameters . Its usage as
  GA[`2`] returns `3` and should return a square matrix of
  numbers . Alternatively, use VectorPotentialGradient→None.";
makeDipoleList::preint = "Wrong Preintegrals option `1`. Valid
  options are \"Analytic\" and \"Numeric \".";

makeDipoleList::numnondip =
  "The option Preintegrals→\"Numeric \" is currently unreliable when
  a vector potential is specified";

makeDipoleList [OptionsPattern[]] := Block[
  {
    num = OptionValue[TotalCycles],
    npp = OptionValue[PointsPerCycle],  $\omega$  = OptionValue[CarrierFrequency],
  }

```

```

dipole= OptionValue[DipoleTransitionMatrixElement],  $\kappa$ ,
A, F, GA, pi, ps, S,
gate, tGate, setPreintegral,
tInit, tFinal,  $\delta t$ ,  $\epsilon$  = OptionValue[eCorrection],
AInt, A2Int, GAInt, GAdotAInt, AdotGAInt, GAIntInt, bigPSCorrectionInt, AdotGAdotAInt,
AIntList, A2IntList, GAIntList, GAdotAIntList,
AdotGAIntList, GAIntIntList, bigPSCorrectionIntList, AdotGAdotAIntList,
dipoleList
},

A[t_] = OptionValue[VectorPotential][t] /. OptionValue[FieldParameters];
F[t_] = -D[A[t], t];
GA[t_] = If[
  TrueQ[OptionValue[VectorPotentialGradient] == None],
  Table[0, {Length[A[tInit]]}, {Length[A[tInit]]}],
  OptionValue[VectorPotentialGradient][t] /. OptionValue[FieldParameters]
];

Which[
  OptionValue[Target] == Automatic,  $\kappa = \sqrt{2 \text{OptionValue[IonizationPotential]}}$ ,
  True,  $\kappa = \sqrt{2 \text{getIonizationPotential[OptionValue[Target]}}$ 
];

tInit= 0;
tFinal=  $\frac{2\pi}{\omega} \text{num}$ ;
 $\delta t = \frac{tFinal - tInit}{\text{num} \times \text{npp} + \text{OptionValue[PointNumberCorrection]}}$ ;
(*integration and looping timestep *)
tGate = OptionValue[nGate]  $\frac{2\pi}{\omega}$ ;
(*Check potential and potential gradient for correctness.*)
With[{ $\omega tRandom$  = RandomReal[{ $\omega tInit$ ,  $\omega tFinal$ ]}},
  If[!And@@(NumberQ /@A[ $\omega tRandom$  /  $\omega$ ]),
    Message[makeDipoleList::pot, OptionValue[VectorPotential],  $\omega tRandom$ , A[ $\omega tRandom$ ]];
    Abort[]];
  If[!And@@(NumberQ /@Flatten[GA[ $\omega tRandom$  /  $\omega$ ]]), Message[makeDipoleList::gradpot,
    OptionValue[VectorPotentialGradient],  $\omega tRandom$ , GA[ $\omega tRandom$ ]];
    Abort[]];
];

gate[ $\omega \tau$ ] := OptionValue[Gate][ $\omega \tau$ , OptionValue[nGate]];
With[{ $\omega tRandom$  = RandomReal[{ $\omega tInit$ ,  $\omega tFinal$ ]}},
  If[!TrueQ[NumberQ [gate[ $\omega tRandom$ ]]],
    Message[makeDipoleList::gate,
      OptionValue[Gate],  $\omega tRandom$ , OptionValue[nGate], gate[ $\omega tRandom$ ]];
    Abort[]];
];

```

```

setPreintegral[integralVariable_, listVariable_, preintegrand_,
  dimensions_, integrateWithoutGradient_, parametric_] := Which[
  OptionValue[VectorPotentialGradient] != None || TrueQ[integrateWithoutGradient],
  (*Vector potential gradient specified
  or integral variable does not depend on it, so integrate*)
  Which[
    OptionValue[Preintegrals] == "Analytic",
    integralVariable[t_, tt_] =
      ((# /. {τ → t}) - (# /. {τ → tt})) & [Integrate[preintegrand[τ, tt], τ]];

    , OptionValue[Preintegrals] == "Numeric ",
    Which[
      TrueQ[Not[parametric]],
      integralVariable[t_, tt_] = (innerVariable[t] - innerVariable[tt] /. First[
        NDSolve[{innerVariable'[τ] == preintegrand[τ],
          innerVariable[tInit] == ConstantArray[0, dimensions]},
          innerVariable[τ, tInit, tFinal]]
      ]);
      , True, (*change τ to protected tpre before you're done*)
      Message[makeDipoleList::numnondip];
      Block[{matrixpreintegrand, innerVariable},
        matrixpreintegrand[indices_, t_?NumericQ, tt_?NumericQ] :=
          preintegrand[t, tt][[## & @@ indices]];
        integralVariable[t_, tt_] = Array[
          innerVariable[##][t - tt, tt] /. First@NDSolve[{
            D[innerVariable[##][τ, tt], τ] == matrixpreintegrand[{##},
              tt + τ, tt] +  $\frac{0.00001}{\omega} \nabla_{\{\tau, tt\}}^2$  innerVariable[##][τ, tt],
            innerVariable[##][0, tt] == 0
          }, innerVariable[##],
            {τ, 0, tFinal - tInit}, {tt, tInit, tFinal}
          (*, {τ, tt} ∈ Triangle[
            {{tInit, tInit}, {tInit, tFinal}, {tFinal, tInit}}] *)
          (*Restricted triangular domain currently not
            working until mm .se/q/105687 is resolved - this
            causes the makeDipoleList::numnondip error here.*)
        ], dimensions];
      ];
    ];
  ];
  , OptionValue[VectorPotentialGradient] === None,
  (*Vector potential gradient has not been specified
  and integral variable depends on it, so return appropriate zero matrix *)

```

```

    integralVariable[t_] = ConstantArray[0, dimensions];
    integralVariable[t_, tt_] = ConstantArray[0, dimensions];
];
Apply[setPreintegral,

{AInt          AIntList          A[#1] &          {Lengt
A2Int          A2IntList         A[#1].A[#1] &       {}
GAInt          GAIntList         GA[#1] &          {Lengt
GAdotAInt      GAdotAIntList     GA[#1].A[#1] &      {Lengt
AdotGAInt      AdotGAIntList     A[#1].GA[#1] &      {Lengt
GAIntInt       GAIntIntList      GAInt[#1, #2] &  {Lengt
AdotGAdotAInt AdotGAdotAIntList A[#1].GAdotAInt[#1, #2] & {}
bigPSCorrectionInt bigPSCorrectionIntList GAdotAInt[#1, #2] + A[#1].GAInt[#1, #2] & {Lengt

}, {1}];

(*{

$$\int_{t_0}^t A(\tau) d\tau, \int_{t_0}^t A(\tau)^2 d\tau, \int_{t_0}^t \nabla A(\tau) d\tau, \int_{t_0}^t \nabla A(\tau) \cdot A(\tau) d\tau, \int_{t_0}^t A(\tau) \cdot \nabla A(\tau) d\tau, \int_{t'}^t \int_{t'}^t \nabla A(\tau') d\tau' d\tau,$$


$$\int_{t'}^t A_k(\tau) \cdot \int_{t'}^t \partial_k A_j(\tau') A_j(\tau') d\tau' d\tau, \int_{t'}^t \int_{t'}^t (A_k(\tau') \partial_j A_k(\tau') + A_k(\tau) \partial_k A_j(\tau')) d\tau' d\tau \}; *)$$


(*Displaced momentum *)
pi[p_, t_, tt_] := p + A[t] - GAInt[t, tt].p - GAdotAInt[t, tt];

(*Stationary momentum and action*)
ps[t_, tt_] := ps[t, tt] = - $\frac{1}{t - tt - i\epsilon}$  Inverse[
    IdentityMatrix[Length[A[tInit]]] -  $\frac{1}{t - tt - i\epsilon}$  (GAIntInt[t, tt] + GAIntInt[t, tt]')].
    (AInt[t, tt] - bigPSCorrectionInt[t, tt]);

S[t_, tt_] :=  $\frac{1}{2}$  (Norm[ps[t, tt]]2 +  $\kappa^2$ ) (t - tt) + ps[t, tt].AInt[t, tt] +  $\frac{1}{2}$  A2Int[t, tt] - (
    ps[t, tt].GAIntInt[t, tt].ps[t, tt] +
    ps[t, tt].bigPSCorrectionInt[t, tt] + AdotGAdotAInt[t, tt]
);

(*Debugging constructs. Verbose→
1 prints information about the internal functions. Verbose→
2 returns all the relevant internal functions and stops.*)
Which[

```



```

OptionValue[Verbose] = 1, Information /@ {A, GA, ps, pi, S, AInt, A2Int, GAInt,
    GAdotAInt, AdotGAInt, GAIntInt, bigPSCorrectionInt, AdotGAdotAInt},
OptionValue[Verbose] = 2, Return[With[{t = Global`t,
    tt = Global`tt, p = Global`t,  $\tau$  = Global` $\tau$ },
    {A[t], GA[t], ps[t, tt], pi[p, t, tt], 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], bigPSCorrectionInt[t, tt], AdotGAdotAInt[t],
    AdotGAdotAInt[t, tt],  $i \left( \frac{2\pi}{\epsilon + i\tau} \right)^{3/2}$  dipole[pi[ps[t, t- $\tau$ ], t, t- $\tau$ ],  $\kappa$ ]*x
    dipole[pi[ps[t, t- $\tau$ ], t- $\tau$ , t- $\tau$ ],  $\kappa$ ].F[t- $\tau$ ] Exp[-iS[t, t- $\tau$ ]] gate[ $\omega\tau$ ]}]}]
];

(*Numerical integration loop*)
(dipoleList = Table[
    OptionValue[ReportingFunction][
         $\delta t$  Sum [ (
             $i \left( \frac{2\pi}{\epsilon + i\tau} \right)^{3/2}$  dipole[pi[ps[t, t- $\tau$ ], t, t- $\tau$ ],  $\kappa$ ]*x
            dipole[pi[ps[t, t- $\tau$ ], t- $\tau$ , t- $\tau$ ],  $\kappa$ ].F[t- $\tau$ ] Exp[-iS[t, t- $\tau$ ]] gate[ $\omega\tau$ ]
        ), { $\tau$ , 0, If[OptionValue[Preintegrals] == "Analytic",
            tGate, Min[t-tInit, tGate]]},  $\delta t$ ]
    ], {t, tInit, tFinal,  $\delta t$ }]
];
dipoleList
]
End[];
EndPackage[]

```