

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> (2016).

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.

■ Implementation

Supporting functions

Initialization

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

Version number

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 .";
$RBSFAtimestamp ::usage = "$RBSFAtimestamp prints the timestamp
                        of the current version of the RB-SFA package.";
Begin["`Private`"];
$RBSFAversion := "RB-SFA v2.1.3, "<>$RBSFAtimestamp ;
End[];

```

Old syntax (in functional form `RBSFAversion[]`), deprecated

```

RBSFAversion::usage = "RBSFAversion[] has been deprecated in favour of $RBSFAversion.";
RBSFAversion::dprc = "RBSFAversion[] has been deprecated in favour of $RBSFAversion.";
Begin["`Private`"];
RBSFAversion[] := (Message[RBSFAversion::dprc]; $RBSFAversion);
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-timestamp "] [[1]],
      Cell[
        BoxData[RowBox[{"Begin[\"`Private`\"]; \n$RBSFAtimestamp = \"<>
                        DateString[]<>\"; \nEnd[];"}]]
        , "Input", InitializationCell->True, CellTags->"version-timestamp "
      ], None, AutoScroll->False];
    NotebookSave[]
  }], PassEventsDown->True}
];

```

To reset this behaviour to normal, evaluate the cell below

```

SetOptions[EvaluationNotebook[],
  NotebookEventActions->{{"MenuCommand", "Save"}->{NotebookSave[]}, PassEventsDown->True}]

```

Timestamp

```

Begin["`Private`"];
$RBSFAtimestamp = "Wed 25 Jan 2017 14:30:27";
End[];

```

Directory

```

$RBSFAdirectory::usage = "$RBSFAdirectory is the directory
                        where the current RB-SFA package instance is located.";

```

```

Begin["`Private`"];
With[{softLinkTestString= StringSplit[StringJoin[ReadList[
    "! ls -la "<>StringReplace[$InputFileName, {" "→"\ "}], String]], " -> "]},
  If[Length[softLinkTestString]>1, (*Testing in case $InputFileName
    is a soft link to the actual directory.*)
    $RBSFAdirectory= StringReplace[DirectoryName [softLinkTestString[[2]]], {" "→"\ "}],
    $RBSFAdirectory= StringReplace[DirectoryName [$InputFileName ], {" "→"\ "}],
  ]];
End[];

```

Git commit hash and message

```

$RBSFAcommit ::usage= "$RBSFAcommit returns the git commit
    log at the location of the RB-SFA package if there is one.";
$RBSFAcommit ::OS= "$RBSFAcommit has only been tested on Linux.";

Begin["`Private`"];
$RBSFAcommit := (If[$OperatingSystem ≠ "Unix", Message[$RBSFAcommit ::OS];
  StringJoin[
    Riffle[ReadList["!cd "<>$RBSFAdirectory<>" && git log -1", String], {"\n"}]]];
End[];

```

Standard function (re)definitions

ConstantArray

This redefines ConstantArray to take the corner case of an empty dimensions list, which returns an error code (and an unevaluated ConstantArray) for Mathematica versions under 10.1.0 (cf. mma.se/q/133078).

```

Quiet[Check[
  ConstantArray[0, {}];,
  Unprotect[ConstantArray];
  ConstantArray[Private`x_, {}] := Private`x;
  Protect[ConstantArray];
]];

```

Similarly, this needs to be put inside an initialization code for any parallelized subkernels that may get launched later (cf. mma.se/q/131856).

```

Parallelize;
Parallel`Developer`$InitCode= Hold[
  Quiet[Check[
    ConstantArray[0, {}];,
    Unprotect[ConstantArray];
    ConstantArray[Private`x_, {}] := Private`x;
    Protect[ConstantArray];
  ]];
];

```

Relm

This adds the definition of Relm for those versions (<10.1) that don't have it.

```

If[
  Context[ReIm] != "System`",
  ReIm := usage =
    "\!\(\*RowBox[{\\"ReIm \", \\"[\", StyleBox[\"z\", \\"TI\"], \"}\"])\) gives the list
    \!\(\*RowBox[{\\"{\", RowBox[{\RowBox[{\\"Re\", \\"[\", StyleBox[\"z\",
    \\"TI\", \"}\"]}, \",\", RowBox[{\\"Im \", \\"[\", StyleBox[\"z\", \\"TI\",
    \"}\"]}], \"}\"])\) of the number \!\(\*StyleBox[\"z\", \\"TI\"]\).\";
  ReIm[Private`z_] := {Re[Private`z], Im[Private`z]};
  SetAttributes[ReIm, Listable];
  Protect[ReIm];
]

```

AssociationTranspose

```

AssociationTranspose := usage = "";
Begin["`Private`"];
AssociationTranspose[association] := GroupBy[
  Join@@Thread/@Normal // @association
  {First@*Last, First}
][[All, All, 1, 2, 2]]
End[];

```

The above function is taken from <http://mathematica.stackexchange.com/a/86526> by <http://mathematica.stackexchange.com/users/121/mr-wizard>. *Mathematica* 10.1 and higher, it can be replaced by a `Query[Transpose]` construct as below, but *Mathematica* 10.0, despite having most of the `Association` code, is unable to transpose ragged associations using that construct.

```

(*
AssociationTranspose[association] := DeleteMissing[
  Query[Transpose][
    association
  ]
  , 2]
*)

```

Dipole transition matrix elements

Default DTME, for a hydrogenic 1s state

```

hydrogenicDTME::usage =
  "hydrogenicDTME[p,κ] returns the dipole transitionmatrix element for
    a 1s hydrogenic state of ionizationpotential  $I_p = \frac{1}{2}\kappa^2$ .

hydrogenicDTME[p,κ,{n,l,m}] returns the dipole transitionmatrix element for an
  n,l,m hydrogenic state of ground-state ionizationpotential  $I_p = \frac{1}{2}\kappa^2$ .

hydrogenicDTME[p,κ,n,l,m] returns the dipole transitionmatrix element for an
  n,l,m hydrogenic state of ground-state ionizationpotential  $I_p = \frac{1}{2}\kappa^2$ .";
hydrogenicDTMERegularized::usage = "hydrogenicDTMERegularized[p,κ] returns the
  dipole transitionmatrix element for a 1s hydrogenic state of
  ionizationpotential  $I_p = \frac{1}{2}\kappa^2$ , regularized to remove the denominator
  of  $1/(p^2 + \kappa^2)^3$ , where the saddle-point solutions are singular.

hydrogenicDTMERegularized[p,κ,{n,l,m}] returns the dipole transitionmatrix element for
  an n,l,m hydrogenic state of ground-state ionizationpotential  $I_p = \frac{1}{2}\kappa^2$ ,
  regularized to remove factors of  $(p^2 + \kappa^2)$  from the denominator .

hydrogenicDTMERegularized[p,κ,n,l,m] returns the dipole transitionmatrix element for an
  n,l,m hydrogenic state of ground-state ionizationpotential  $I_p = \frac{1}{2}\kappa^2$ ,
  regularized to remove factors of  $(p^2 + \kappa^2)$  from the denominator .";
Begin["`Private`"];

hydrogenicDTME[p_List, κ_] :=  $\frac{8 \, i}{\pi} \frac{\sqrt{2 \, \kappa^5} \, p}{(Total[p^2] + \kappa^2)^3}$ 

hydrogenicDTME[p_?NumberQ, κ_] :=  $\frac{8 \, i}{\pi} \frac{\sqrt{2 \, \kappa^5} \, p}{(p^2 + \kappa^2)^3}$ 

hydrogenicDTMERegularized[p_List, κ_] :=  $\frac{8 \, i}{\pi} \frac{\sqrt{2 \, \kappa^5} \, p}{1}$ 

hydrogenicDTMERegularized[p_?NumberQ, κ_] :=  $\frac{8 \, i}{\pi} \frac{\sqrt{2 \, \kappa^5} \, p}{1}$ 

End[];

```

For a gaussian orbital

```

gaussianDTME::usage =
  "gaussianDTME[p,κ] returns the dipole transitionmatrix element for a gaussian
    state of characteristic size 1/κ.";
Begin["`Private`"];

gaussianDTME[p_List, κ_] := -i (4 π)3/4 κ-7/2 p Exp[- $\frac{\text{Total}[p^2]}{2 \kappa^2}$ ]

gaussianDTME[p_?NumberQ, κ_] := -i (4 π)3/4 κ-7/2 p Exp[- $\frac{p^2}{2 \kappa^2}$ ]

End[];

```

SolidHarmonicS

This function implements the solid harmonic $S_{l,m}(r) = r^l Y_{l,m}(\theta, \phi)$, which is a homogeneous polynomial of degree l , and lends itself much better to symbolic differentiation than explicit spherical harmonics.

Code provided by J.M. at <http://mathematica.stackexchange.com/a/124336/1000> under the WTFPL.

```

SolidHarmonicS::usage =
  "SolidHarmonicS[l,m,x,y,z] calculates the solid harmonic  $S_{lm}(x,y,z) = r^l Y_{lm}(x,y,z)$ ."

SolidHarmonicS[l,m,{x,y,z}] does the same.";
Begin["`Private`"];
SolidHarmonicS[λ_Integer, μ_Integer, x_, y_, z_] /; λ ≥ Abs[μ] :=
  Sqrt[ $\frac{2 \lambda + 1}{4 \pi}$ ] Sqrt[ $\frac{\Gamma[\lambda - \text{Abs}[\mu] + 1]}{\Gamma[\lambda + \text{Abs}[\mu] + 1]}$ ] 2-λ (-1)(μ - Abs[μ])/2 ×
  If[Rationalize[μ] == 0, 1, (x + Sign[μ] i y)Abs[μ]] ×
  Sum [
    (-1)μ+k Binomial[λ, k] Binomial[2 λ - 2 k, λ] Pochhammer[λ - Abs[μ] - 2 k + 1, Abs[μ]] ×
    If[Rationalize[k] == 0, 1, (x2 + y2 + z2)k] ×
    If[Rationalize[λ - Abs[μ] - 2 k] == 0, 1, zλ - Abs[μ] - 2 k]
    , {k, 0, Quotient[λ, 2]}]
SolidHarmonicS[λ_Integer, μ_Integer, {x_, y_, z_}] /; λ ≥ Abs[μ] :=
  SolidHarmonicS[λ, μ, x, y, z]
End[];

```

hydrogenicΨ and hydrogenicY (momentum-space wavefunctions)

This implements the dipole transition matrix element from an arbitrary hydrogenic orbital n, l, m , where the ground-state ionization potential is given by $I_p = \frac{1}{2} \kappa^2$, as described in Luke Chipperfield's PhD thesis (Imperial College London, 2008, p. 52). This code uses partial memoization as in mm.se/q/21782.

hydrogenicΨ:usage =
 "hydrogenicΨ[n,l,m ,κ,px,py,pz] calculates the momentum -space wavefunction
 $\Psi(p)=\langle p|nlm \rangle$ for a hydrogenic atom with ionizationpotential $\kappa^2/2$.

hydrogenicΨ[n,l,m ,κ,{px,py,pz}] calculates the momentum -space wavefunction
 $\Psi(p)=\langle p|nlm \rangle$ for a hydrogenic atom with ionizationpotential $\kappa^2/2$."

Begin["`Private`"];

hydrogenicΨ[n_, l_, m_ , κκ_, ppκ_, ppy_, ppz_] := Block[{κ, px, py, pz},
 hydrogenicΨ[n, l, m , κ_, px_, py_, pz_] = Simplify [

$$-\text{SolidHarmonicsS}[1, m , px, py, pz] \frac{(-i)^1 \pi 2^{21+4} 1!}{(2 \pi \kappa)^{3/2}} \sqrt{\frac{n (n-1-1)!}{(n+1)!}}$$

$$\frac{\kappa^{1+4}}{(px^2+py^2+pz^2+\kappa^2)^{1+2}} \text{GegenbauerC}[n-1-1, 1+1, \frac{px^2+py^2+pz^2-\kappa^2}{px^2+py^2+pz^2+\kappa^2}]$$

];
 hydrogenicΨ[n, l, m , κκ, ppκ, ppy, ppz]
];

hydrogenicΨ[n_, l_, m_ , κ_, {px_, py_, pz_}] := hydrogenicΨ[n, l, m , κ, px, py, pz];
 End[];

Regularized version, removing the powers of $p^2 + \kappa^2$ in the denominator, to eliminate poles at the saddle-point momentum $p = i \kappa$.

hydrogenicΨRegularized:usage =
 "hydrogenicΨRegularized[n,l,m ,κ,px,py,pz] calculates the momentum -space
 wavefunction $\Psi(p)=\langle p|nlm \rangle$ for a hydrogenic atom with
 ionizationpotential $\kappa^2/2$, multiplied by $(p^2+\kappa^2)^{n+1}$
 to remove any factors of $p^2+\kappa^2$ in the denominator .

hydrogenicΨRegularized[n,l,m ,κ,{px,py,pz}] calculates the momentum -space wavefunction
 $\Psi(p)=\langle p|nlm \rangle$ for a hydrogenic atom with ionizationpotential $\kappa^2/2$, multiplied
 by $(p^2+\kappa^2)^{n+1}$ to remove any factors of $p^2+\kappa^2$ in the denominator ."

Begin["`Private`"];

hydrogenicΨRegularized[n_, l_, m_ , κκ_, ppκ_, ppy_, ppz_] := Block[{κ, px, py, pz},
 hydrogenicΨRegularized[n, l, m , κ_, px_, py_, pz_] = Simplify [Cancel [

$$-\text{SolidHarmonicsS}[1, m , px, py, pz] \frac{(-i)^1 \pi 2^{21+4} 1!}{(2 \pi \kappa)^{3/2}} \sqrt{\frac{n (n-1-1)!}{(n+1)!}}$$

$$\kappa^{1+4} (px^2+py^2+pz^2+\kappa^2)^{n-1-1} \text{GegenbauerC}[n-1-1, 1+1, \frac{px^2+py^2+pz^2-\kappa^2}{px^2+py^2+pz^2+\kappa^2}]$$

]]
 hydrogenicΨRegularized[n, l, m , κκ, ppκ, ppy, ppz]
];

hydrogenicΨRegularized[n_, l_, m_ , κ_, {px_, py_, pz_}] :=
 hydrogenicΨRegularized[n, l, m , κ, px, py, pz];
 End[];

Upsilon function, given by $Y(\mathbf{p}) = \left(\frac{1}{2} \mathbf{p}^2 + l_p\right) \Psi(\mathbf{p}) = \frac{1}{2} (\mathbf{p}^2 + \kappa^2) \langle \mathbf{p} | n, l, m \rangle$, which can be used in the form

$Y(\mathbf{p} + \mathbf{A}(t'))$ as a replacement for the ionization dipole $\mathbf{d}(\mathbf{p} + \mathbf{A}(t')) \cdot \mathbf{F}(t')$, particularly for cases where the latter is singular but the former is not. (For details cf. arXiv:1304.2413, appendix A.)

hydrogenicY::usage =

"hydrogenicY[n,l,m ,κ,px,py,pz] calculates the Upsilon function $Y(p) = (\frac{1}{2}p^2 + I_p) \langle p | nlm \rangle$ for a hydrogenic atom with ionization potential $\kappa^2/2$.

hydrogenicY[n,l,m ,κ,{px,py,pz}] calculates the Upsilon function $Y(p) = (\frac{1}{2}p^2 + I_p) \langle p | nlm \rangle$ for a hydrogenic atom with ionization potential $\kappa^2/2$."

Begin["`Private`"];

hydrogenicY[n_, l_, m_ , κ_, px_, py_, pz_] :=

$\frac{1}{2} (px^2 + py^2 + pz^2 + \kappa^2)$ hydrogenicY[n, l, m , κ, px, py, pz];

hydrogenicY[n_, l_, m_ , κ_, {px_, py_, pz_}] := hydrogenicY[n, l, m , κ, px, py, pz];

End[];

hydrogenicDTME for arbitrary states

Begin["`Private`"];

hydrogenicDTME[{ppx_, ppy_, ppz_}, κκ_, n_, l_, m_] := Block[{κ, px, py, pz},

hydrogenicDTME[{px_, py_, pz_}, κ_, n, l, m] =

Simplify [Grad[hydrogenicY[n, l, m , κ, px, py, pz], {px, py, pz}]];

hydrogenicDTME[{ppx, ppy, ppz}, κκ, n, l, m]

];

hydrogenicDTME[{px_, py_, pz_}, κ_, {n_, l_, m_ }] := hydrogenicDTME[{px, py, pz}, κ, n, l, m];

End[];

Regularized version, removing the powers of $p^2 + \kappa^2$ in the denominator, to eliminate poles at the saddle-point momentum $p = i\kappa$.

Begin["`Private`"];

hydrogenicDTMERegularized[{px_, py_, pz_}, κ_, n_, l_, m_] :=

$(px^2 + py^2 + pz^2 + \kappa^2)^{n+1}$ hydrogenicDTME[{px, py, pz}, κ, n, l, m];

hydrogenicDTMERegularized[{px_, py_, pz_}, κ_, {n_, l_, m_ }] :=

hydrogenicDTMERegularized[{px, py, pz}, κ, n, l, m];

End[];

Various field envelopes

flatTopEnvelope

flatTopEnvelope::usage =

"flatTopEnvelope[ω,num ,nRamp] returns a Function object representing a flat-top envelope at carrier frequency ω lasting a total of num cycles and with linear ramps nRamp cycles long."

Begin["`Private`"];

flatTopEnvelope[ω_, 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  $1 - \cos(\omega t/2 \text{ num})^{\text{power}}$ ";
Begin["`Private`"];
cosPowerFlatTop[ $\omega_{\_}$ , num_ , power_] := Function[t, 1 - Cos[ $\frac{\omega t}{2 \text{ num}}$ ]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, IntegrationPointsPerCycle → Automatic };
```

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 ω , TotalCycles and PointsPerCycle,
- a polarization parameter ϵ , which gives an unpolarized spectrum when given False, or polarizes along an ellipticity vector ϵ (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 ω , ω Power, 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 Abs[##]² & are reasonable choices).

If no option is passed to ω Power and DifferentiationOrder, the pulse parameters do not really affect the output, except by a global factor of 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="ComplexPart 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.";
ωPower::usage="ωPower 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, ComplexPart, ωPower, DifferentiationOrder];

Begin["`Private`"];
Options[getSpectrum] = {Polarization→False, ComplexPart → (#&),
ωPower → 0, DifferentiationOrder→0}~Join~standardOptions;

getSpectrum::diffOrd="Invalid differentiationorder `1`.";
getSpectrum::ωPow="Invalid ω power `1`.";

getSpectrum [dipoleList_, OptionsPattern[]] := Block[
{polarizationVector, differentiatedList, depth, dimensions,
num = OptionValue[TotalCycles],
npp = OptionValue[PointsPerCycle], ω = OptionValue[CarrierFrequency], δt =  $\frac{2\pi/\omega}{npp}$ 
},
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[ωPower]], Null;, Message[getSpectrum::ωPow, OptionValue[ωPower]];
Abort[]];

num Table[
( $\frac{\omega}{\text{num}}$ )2OptionValue[ωPower], {k, 1, Round[ $\frac{\text{Length}[differentiatedList]}{2}$ ]}
] × 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 ]
    }^r
, 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, +i},
      Sequence@@FilterRules[{options}, Options[getSpectrum]]],
    PlotStyle→Red, Sequence@@FilterRules[{options}, Options[spectrumPlotter]]],
  spectrumPlotter [
    getSpectrum [dipoleList, Polarization→{1, -i},
      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[ $\frac{2\pi n\text{Gate} - \omega\tau}{4n\text{GateRamp}}$ ]2, 2π(nGate - nGateRamp) < ωτ ≤ 2πnGate},
  {0, nGate < ωτ}}]
LinearRampGate [nGateRamp_][ωτ_, nGate_] := Piecewise[{
  {1, ωτ ≤ 2π(nGate - nGateRamp)},
  {- $\frac{\omega\tau - 2\pi(n\text{Gate} + n\text{GateRamp})}{2\pi n\text{GateRamp}}$ , 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.

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"])]
getIonizationPotential[{Target_, Charge_: 0}] := getIonizationPotential[Target, Charge]
End[];

```

makeDipoleList: main numerical integrator

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  $\partial_i A_j[t]$ .";
ElectricField::usage = "ElectricField is an option for makeDipole list which specifies
    an electric field to use in the ionizationmatrix element, in case the
    time derivative of the vector potential is not desired. Usage should
    be ElectricField→F, where F[t]//.pars must yield a list of numbers
    for numeric t and parameters indicated by FieldParameters→pars.";
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 ionization potential  $I_p$  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  $f$  to
    use as the dipole transition matrix element, or a pair of
    functions  $\{f_{\text{ion}}, f_{\text{rec}}\}$  to be used separately for the ionization and
    recombination dipoles, to be used in the form  $f[p, \kappa] = f[p, \sqrt{2 I_p}]$ .";
eCorrection::usage = "eCorrection is an option for makeDipoleList which specifies the
    regularization correction  $\epsilon$ , i.e. as used in the factor  $\frac{1}{(t - t_t + i\epsilon)^{3/2}}$ .";
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.";
IntegrationPointsPerCycle::usage = "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.";
RunInParallel::usage = "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]}.";
Simplifier::usage = "Simplifier is an option for makeDipoleList which specifies a
    function to use to simplify the intermediate and final analytical results.";
CheckNumericFields::usage = "CheckNumericFields is an option for
    makeDipoleList which specifies whether to check for
    numeric values of A[t] and GA[t] for numeric t.";
QuadraticActionTerms::usage = "QuadraticActionTerms is an option for makeDipoleList
    which specifies whether to use quadratic terms in  $\nabla A^2$  in the action.";

Protect[VectorPotential, VectorPotentialGradient, ElectricField, FieldParameters,
    Preintegrals, ReportingFunction, Gate, nGate, IonizationPotential, Target, eCorrection,
    PointNumberCorrection, DipoleTransitionMatrixElement, IntegrationPointsPerCycle,
    RunInParallel, Simplifier, CheckNumericFields, QuadraticActionTerms];

Begin["`Private`"];
Options[makeDipoleList] = standardOptions ~ Join ~ {
    VectorPotential → Automatic, FieldParameters → {},
    VectorPotentialGradient → None, ElectricField → Automatic,
    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, CheckNumericFields → True,
    RunInParallel → Automatic,
    Simplifier → Identity, QuadraticActionTerms → True
};
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::efield = "The electric field f provided as ElectricField → `1` is incorrect
    or is missing FieldParameters. Its usage as F[`2`] returns `3` and should

```

```

        return a list of numbers . Alternatively, use ElectricFieldAutomatic .";
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 VectorPotentialGradientNone.";
makeDipoleList::preint="Wrong Preintegrals option `1`. Valid
options are \"Analytic\" and \"Numeric \".";
makeDipoleList::runpar="Wrong RunInParallel option `1`. ";
makeDipoleList::carrfreq="Non-numeric option CarrierFrequency `1`. ";

```

```

makeDipoleList [OptionsPattern[]] := Block[
{
    num = OptionValue[TotalCycles], npp = OptionValue[PointsPerCycle],  $\omega$ ,
    dipoleRec, dipoleIon,  $\kappa$ ,
    A, F, GA, pi, ps, S,
    gate, tGate, setPreintegral,
    tInit, tFinal,  $\delta t$ ,  $\delta tint$ ,  $\epsilon$  = OptionValue[eCorrection],
    AInt, A2Int, GAInt, GAdotAInt, AdotGAInt, GAIntInt,
    PSCorrectionInt, constCorrectionInt, GAIntdotGAIntInt, QuadMatrix, q,
    simplifier, prefactor, integrand, dipoleList,
    TableCommand , SumCommand
},

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

 $\omega$  = OptionValue[CarrierFrequency];
If[!NumberQ [ $\omega$ ] && TrueQ[OptionValue[CheckNumericFields ]],
    Message[makeDipoleList::carrfreq,  $\omega$ ];
    Abort[]];
tInit = 0;
tFinal =  $\frac{2\pi}{\omega}$  num ;
(*looping timestep *)
 $\delta t$  =  $\frac{tFinal - tInit}{num \times npp + OptionValue[PointNumberCorrection]}$ ;
(*integration timestep *)
 $\delta tint$  = If[OptionValue[IntegrationPointsPerCycle] === Automatic ,
     $\delta t$ , (tFinal - tInit) / (num  $\times$  OptionValue[IntegrationPointsPerCycle] +
    OptionValue[PointNumberCorrection])];
tGate = OptionValue[nGate]  $\frac{2\pi}{\omega}$ ;
(*Check potential and potential gradient for correctness.*)
(*To do: change logic conditions to constructions on VectorQ[# , NumberQ ] &
and MatrixQ.*)
If[TrueQ[OptionValue[CheckNumericFields ]],

```

```

With[{wtRandom = RandomReal[{wtInit, wtFinal}]},
  If[!And@@(NumberQ /@A[wtRandom /  $\omega$ ]), Message[makeDipoleList::pot,
    OptionValue[VectorPotential], wtRandom, A[wtRandom]];
  Abort[]];
  If[!And@@(NumberQ /@Flatten[GA[wtRandom /  $\omega$ ]]), Message[makeDipoleList::gradpot,
    OptionValue[VectorPotentialGradient], wtRandom, GA[wtRandom]];
  Abort[]];
  If[!And@@(NumberQ /@F[wtRandom /  $\omega$ ]), Message[makeDipoleList::efield,
    OptionValue[ElectricField], wtRandom, F[wtRandom]];
  Abort[]];
];

gate[wt_] := OptionValue[Gate][wt, OptionValue[nGate]];
With[{wtRandom = RandomReal[{wtInit, wtFinal}]},
  If[!TrueQ[NumberQ[gate[wtRandom]]],
    Message[makeDipoleList::gate,
      OptionValue[Gate], wtRandom, OptionValue[nGate], gate[wtRandom]];
    Abort[]];
];

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

With[{dim = Length[A[RandomReal[{wtInit, wtFinal}]]]},
  (*Explicit conjugation of the
    recombination matrix element to keep the integrand analytic.*)
  Which[
    Head[OptionValue[DipoleTransitionMatrixElement]] === List,
    dipoleIon[{p1_, p2_, p3_}][1 ;; dim],  $\kappa$  =
      First[OptionValue[DipoleTransitionMatrixElement]][{p1, p2, p3}][1 ;; dim],  $\kappa$ ;
    dipoleRec[{p1_, p2_, p3_}][1 ;; dim],  $\kappa$  =
      Assuming[{p1, p2, p3,  $\kappa$ }  $\in$  Reals], Simplify[
        Conjugate[Last[OptionValue[DipoleTransitionMatrixElement]][
          {p1, p2, p3}][1 ;; dim],  $\kappa$ ]]
      ];
    , True,
    dipoleIon[{p1_, p2_, p3_}][1 ;; dim],  $\kappa$  =
      OptionValue[DipoleTransitionMatrixElement][{p1, p2, p3}][1 ;; dim],  $\kappa$ ;
    dipoleRec[{p1_, p2_, p3_}][1 ;; dim],  $\kappa$  =
      Assuming[{p1, p2, p3,  $\kappa$ }  $\in$  Reals], Simplify[
        Conjugate[OptionValue[DipoleTransitionMatrixElement][
          {p1, p2, p3}][1 ;; dim],  $\kappa$ ]]
      ];
  ];
];

simplifier = OptionValue[Simplifier];
q = Boole[TrueQ[OptionValue[QuadraticActionTerms]]];

setPreintegral[integralVariable_, 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_] = simplifier[
    ((# /. {τ → t}) - (# /. {τ → tt})) & [Integrate[preintegrand[τ, tt], τ]]];

  , OptionValue[Preintegrals] == "Numeric ",
  Which[
    TrueQ[Not[parametric]],
    Block[{innerVariable},
      integralVariable[t_, tt_] = (innerVariable[t] - innerVariable[tt] /. First[
        NDSolve[{innerVariable'[τ] == preintegrand[τ],
          innerVariable[tInit] == ConstantArray[0, dimensions]},
          innerVariable[τ, tInit, tFinal], MaxStepSize → 0.25/ω]
      ]
    );
    , True,
    Block[{matrixpreintegrand, innerVariable τpre},
      matrixpreintegrand[indices_, t_?NumericQ, tt_?NumericQ] :=
        preintegrand[t, tt][[## & @@ indices]];
      integralVariable[t_, tt_] = Array[(
        innerVariable[##][t - tt, tt] /. First@NDSolve[{
          D[innerVariable[##][τpre, tt], τpre] ==
            Piecewise[{{matrixpreintegrand[##, tt + τpre, tt],
              tt + τpre ≤ tFinal}}, 0],
          innerVariable[##][0, tt] == 0
        }, innerVariable[##]
        , {τpre, 0, tFinal - tInit}, {tt, tInit, tFinal}
        , MaxStepSize → 0.25/ω
      ) &, 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          A[#1] &
  A2Int         A[#1].A[#1] &
  GAIInt        GA[#1] &
  GAdotAInt     GA[#1].A[#1] &
  AdotGAInt     A[#1].GA[#1] &
  GAIIntInt     GAIInt[#1, #2] &
  PScorrectionInt GAdotAInt[#1, #2] + A[#1].GAIInt[#1, #2] - q GAIInt[#1, #2]^T.GAdotAInt[#1, #2] &
  GAIntdotGAIntInt q GAIInt[#1, #2]^T.GAIInt[#1, #2] &
  constCorrectionInt (A[#1] -  $\frac{q}{2}$  GAdotAInt[#1, #2]).GAdotAInt[#1, #2] &

```

```

)
, {1}];

(*{
  ∫t0t A(τ) dτ, ∫t0t A(τ)2 dτ, ∫t0t ∇A(τ) dτ, ∫t0t ∇A(τ) · A(τ) dτ, ∫t0t A(τ) · ∇A(τ) dτ, ∫tt ∫tτ ∇A(τ') dτ' dτ,
  ∫tt ∫tτ ∂jAk(τ') Ak(τ') dτ' + Ak(τ) ∫tt ∂kAj(τ') dτ' - ∫tt ∂iAj(τ') dτ' ∫tt ∂iAk(τ') Ak(τ') dτ' dτ,
  ∫tt ∫tτ ∂iAj(τ') Aj(τ') dτ' ∫tt ∂iAk(τ') Ak(τ') dτ' dτ,
  ∫tt (Ak(τ) - 1/2 ∫tτ ∂kAi(τ') Ai(τ') dτ') · ∫tτ ∂kAj(τ') Aj(τ') dτ' dτ}; *)

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

(*Quadratic coefficient in nondipole action*)
QuadMatrix[t_, tt_] := (GAIntInt[t, tt] + GAIntInt[t, tt]T)/2 - 1/2 GAIntdotGAIntInt[t, tt];

(*Stationary momentum and action*)
ps[t_, tt_] := ps[t, tt] =
  -1/(t - tt - iε) Inverse[IdentityMatrix[Length[A[tInit]]] - 1/(t - tt - iε) 2 QuadMatrix[t, tt]].
  (AInt[t, tt] - PSCorrectionInt[t, tt]);
S[t_, tt_] := simplifier[
  1/2 (Total[ps[t, tt]2] + κ2) (t - tt) + ps[t, tt].AInt[t, tt] + 1/2 A2Int[t, tt] - (
    ps[t, tt].QuadMatrix[t, tt].ps[t, tt] +
    ps[t, tt].PSCorrectionInt[t, tt] + constCorrectionInt[t, tt]
  )
];

prefactor[t_, τ_] := i (2π / (ε + iτ))3/2 dipoleRec[pi[ps[t, t - τ], t, t - τ], κ] ×
  dipoleIon[pi[ps[t, t - τ], t - τ, t - τ], κ].F[t - τ];
integrand[t_, τ_] := prefactor[t, τ] Exp[-i S[t, t - τ]] gate[ωτ];

(*Debugging constructs. Verbose→
  1 prints information about the internal functions. Verbose→
  2 returns all the relevant internal functions and stops. Verbose→
  3 for quantum -orbit constructs.*)
Which[
  OptionValue[Verbose] == 1, Information /@ {A, GA, ps, pi, S, AInt, A2Int, GAInt, GAdotAInt,
    AdotGAInt, GAIntInt, PSCorrectionInt, constCorrectionInt, GAIntdotGAIntInt},
  OptionValue[Verbose] == 2, Return[With[{t = Symbol["t"],
    tt = Symbol["tt"], τ = Symbol["τ"],
    p = {Symbol["p1"], Symbol["p2"], Symbol["p3"]}], Length[A[ωtInit]]]],
  {A[t], GA[t], ps[t, tt], pi[p, t, tt], S[t, tt], AInt[t, tt],
    A2Int[t, tt], GAInt[t, tt], GAdotAInt[t, tt], AdotGAInt[t, tt],

```

```

        GAIntInt[t, tt], PScorrectionInt[t, tt], constCorrectionInt[t, tt],
        GAIntdotGAIntInt[t, tt], QuadMatrix[t, tt], integrand[t,  $\tau$ ]]],
    OptionValue[Verbose] == 3,
    Return[{
        Function[Evaluate[prefactor[#1, #1 - #2]]], Function[Evaluate[S[#1, #2]]]
    }]
];

(*Single-run parallelization*)
Which[
    OptionValue[RunInParallel] == Automatic ||
        OptionValue[RunInParallel] == False, TableCommand = Table;
    SumCommand = Sum ;,
    OptionValue[RunInParallel] == True, TableCommand = ParallelTable;
    SumCommand = Sum ;,
    True, TableCommand = OptionValue[RunInParallel][[1]];
    SumCommand = OptionValue[RunInParallel][[2]];
];

(*Numerical integration loop*)
dipoleList= Table[
    OptionValue[ReportingFunction][
         $\delta$ tintSum [(
            integrand[t,  $\tau$ ]
        ), { $\tau$ , 0,
            If[OptionValue[Preintegrals] == "Analytic", tGate, Min[t - tInit, tGate]],  $\delta$ tint}]
    ]
    , {t, tInit, tFinal,  $\delta$ t}
];
dipoleList

]
End[];

```

Quantum orbit functions suite

Complex root finder

This section implements a routine for solving contains subroutines for the numerical solution of multiple simultaneous complex-valued transcendental equations, essentially by using the Newton's-method solver implemented in FindRoot, and seeding it multiple times with a random (or quasi-random) seed from a box. This code has been taken from the EPTtoolbox package, which is located and better documented at <https://github.com/episanty/EPTtoolbox>, and it is also documented in <http://mathematica.stackexchange.com/a/57821/1000>.

```

FindComplexRoots ::usage =
  "FindComplexRoots [e1==e2, {z, zmin, zmax}] attempts to find complex roots of the
    equation e1==e2 in the complex rectangle with corners zmin and zmax .

FindComplexRoots [{e1==e2, e3==e4, ...}, {z1, z1min, z1max },
  {z2, z2min, z2max }, ...] attempts to find complex roots of
  the given system of equations in the multidimensional complex
  rectangle with corners z1min, z1max, z2min, z2max, ....";
Seeds::usage = "Seeds is an option for FindComplexRoots which determines how many
  initialseeds are used to attempt to find roots of the given equation.";
SeedGenerator::usage = "SeedGenerator is an option for FindComplexRoots which determines
  the function used to generate the seeds for the internal FindRoot
  call. Its value can be RandomComplex, RandomNiederreiterComplexes,
  RandomSobolComplexes, DeterministicComplexGrid, or any
  function f such that f[{zmin, zmax}, n] returns n complex
  numbers in the rectangle with corners zmin and zmax .";

Options[FindComplexRoots] = Join[Options[FindRoot], {Seeds -> 50,
  SeedGenerator -> RandomComplex, Tolerance -> Automatic, Verbose -> False}];
SyntaxInformation[FindComplexRoots] = {"ArgumentsPattern" ->
  {_, {_, _, _}, OptionsPattern[]}, "LocalVariables" -> {"Table", {2, ∞}}};
FindComplexRoots ::seeds = "Value of option Seeds -> `1` is not a positive integer.";
FindComplexRoots ::tol =
  "Value of option Tolerance -> `1` is not Automatic or a number in [0,∞).";
$MessageGroups = Join[$MessageGroups, {"FindComplexRoots" -> {FindRoot::1stol}}]

Protect[Seeds];
Protect[SeedGenerator];

Begin["`Private`"];
FindComplexRoots [equations_List, domainSpecifiers__, ops : OptionsPattern[]] :=
  Block[{seeds, tolerances},
    If[! IntegerQ[Rationalize[OptionValue[Seeds]]] || OptionValue[Seeds] ≤ 0,
      Message[FindComplexRoots ::seeds, OptionValue[Seeds]]];
    If[! (OptionValue[Tolerance] === Automatic || OptionValue[Tolerance] ≥ 0),
      Message[FindComplexRoots ::tol, OptionValue[Seeds]]];

    seeds = OptionValue[SeedGenerator][{domainSpecifiers}][[All, {2, 3}], OptionValue[Seeds]];
    tolerances = Which[
      ListQ[OptionValue[Tolerance]], OptionValue[Tolerance],
      True, ConstantArray[
        Which[
          NumberQ [OptionValue[Tolerance]], OptionValue[Tolerance],
          True, 10^If[NumberQ [OptionValue[WorkingPrecision]],
            2-OptionValue[WorkingPrecision], 2-$MachinePrecision]
        ],
        Length[{domainSpecifiers}]]
    ];

    If[OptionValue[Verbose], Hold[], Hold[FindRoot::1stol]] /. {
      Hold[messageSequence___] :> Quiet[
        DeleteDuplicates[
          Select[
            Check[
              FindRoot[
                equations
              , Evaluate[Sequence@@Table[{domainSpecifiers}][[j, 1],
                #][j]], {j, Length[{domainSpecifiers}]]}]]]
    ]
  ];

```

```

        , Evaluate[Sequence @@ FilterRules[{ops}, Options[FindRoot]]]
    ],
    ## &[]
  ] &/@seeds,
Function[
  repList,
  ReplaceAll[
    Evaluate[And@@Table[
      And[
        Re[{domainSpecifiers}[[j, 2]]] ≤ Re[
          {domainSpecifiers}[[j, 1]] ≤ Re[{domainSpecifiers}[[j, 3]],
        Im[{domainSpecifiers}[[j, 2]]] ≤ Im[{domainSpecifiers}[[
          j, 1]]] ≤ Im[{domainSpecifiers}[[j, 3]]
        ]
      ], {j, Length[{domainSpecifiers}]]]]
    , repList]
  ],
Function[{repList1, repList2},
  And@@Table[
    Abs[( {domainSpecifiers}[[j, 1]] /. repList1) -
      ( {domainSpecifiers}[[j, 1]] /. repList2)] < tolerances[[j]]
    , {j, Length[{domainSpecifiers}]]]
  ]
], {messageSequence }]]}

FindComplexRoots [e1_ == e2_, {z_, zmin_, zmax_}, ops:OptionsPattern[]] :=
  FindComplexRoots [{e1 == e2}, {z, zmin, zmax}, ops]
End[];

```

Quasirandom number generators

This section implements quasirandom number generators for use with FindComplexRoots. As above, this code has been taken from the EPToolbox package, which is located and better documented at <https://github.com/episanty/EP-Toolbox>, and it is also documented in <http://mathematica.stackexchange.com/a/57821/1000>.

RandomSobolComplexes

```

RandomSobolComplexes ::usage =
  "RandomSobolComplexes [{zmin, zmax}, n] generates a low-discrepancy
  Sobol sequence of n quasirandom complex numbers
  in the rectangle with corners zmin and zmax .

RandomSobolComplexes [{z1min, z1max}, {z2min, z2max}, ..., n] generates a low-discrepancy
  Sobol sequence of n quasirandom complex numbers in the multi -dimensional
  rectangle with corners {z1min, z1max}, {z2min, z2max}, ....";

```



```

Begin["`Private`"];
RandomSobolComplexes [pairsList_, number_] := Map[
  Function[randsList ,
    pairsList[[All, 1]] + Complex @@@Times [
      ReIm [pairsList[[All, 2]] - pairsList[[All, 1]],
      randsList
    ]
  ],
  BlockRandom [
    SeedRandom [Method → {"MKL", Method → {"Sobol", "Dimension" → 2 Length[pairsList]}]];
    SeedRandom [];
    RandomReal [{0, 1}, {number, Length[pairsList], 2}]
  ]
]
RandomSobolComplexes [{zmin_ ?NumericQ, zmax_ ?NumericQ}, number_] :=
  RandomSobolComplexes [{zmin, zmax}, number][[All, 1]]
End[];

```

RandomNiederreiterComplexes

```

RandomNiederreiterComplexes ::usage =
  "RandomNiederreiterComplexes [{zmin, zmax}, n] generates
  a low-discrepancy Niederreiter sequence of n quasirandom
  complex numbers in the rectangle with corners zmin and zmax .

RandomNiederreiterComplexes [{z1min, z1max }, {z2min, z2max }, ..., n]
  generates a low-discrepancy Niederreiter sequence of n
  quasirandom complex numbers in the multi-dimensional
  rectangle with corners {z1min, z1max }, {z2min, z2max }, ....";

Begin["`Private`"];
RandomNiederreiterComplexes [pairsList_, number_] := Map[
  Function[randsList ,
    pairsList[[All, 1]] + Complex @@@Times [
      ReIm [pairsList[[All, 2]] - pairsList[[All, 1]],
      randsList
    ]
  ],
  BlockRandom [
    SeedRandom [
      Method → {"MKL", Method → {"Niederreiter", "Dimension" → 2 Length[pairsList]}]];
    SeedRandom [];
    RandomReal [{0, 1}, {number, Length[pairsList], 2}]
  ]
]
RandomNiederreiterComplexes [{zmin_ ?NumericQ, zmax_ ?NumericQ}, number_] :=
  RandomNiederreiterComplexes [{zmin, zmax}, number][[All, 1]]
End[];

```

DeterministicComplexGrid

```

DeterministicComplexGrid::usage =
  "DeterministicComplexGrid [{zmin , zmax } , n] generates a grid of about n equally
    spaced complex numbers in the rectangle with corners zmin and zmax .

DeterministicComplexGrid [{z1min , z1max } , {z2min , z2max } , ... , n] generates a regular grid
  of about n equally spaced complex numbers in the multi -dimensional
  rectangle with corners {z1min , z1max } , {z2min , z2max } , ... .";

Begin["`Private`"];
DeterministicComplexGrid [pairsList_ , number_ ] :=
  Block[{sep , separationsList , gridPointBasis k},
    sep = NestWhile[0.99 # & , Min[Flatten[ReIm [pairsList[[All, 2]] - pairsList[[All, 1]]]],
      Times @@  $\frac{1}{0.99 \#}$  Floor[Flatten[ReIm [pairsList[[All, 2]] - pairsList[[All, 1]]], 0.99 #] <
        number &];
    separationsList = Round[ $\frac{1}{sep}$  Floor[Flatten[ReIm [pairsList[[All, 2]] - pairsList[[All, 1]]]],
      sep]];
    gridPointBasis = MapThread[
      Function[{1 , n}, Range[1[[1]], 1[[2]],  $\frac{1[[2]] - 1[[1]]}{n + 1}$ ] [2 ;; -2]],
      {Flatten[Transpose[ReIm [pairsList], {1, 3, 2}], 1], separationsList}
    ];
    Flatten[Table[
      Table[k[2 j - 1] + i k[2 j], {j, 1, Length[pairsList]}],
      Evaluate[Sequence@@Table[{k[j], gridPointBasis[[j]]}, {j, 1, 2 Length[pairsList]}]]
    ], Evaluate[Range[1, 2 Length[pairsList]]]]
  ]
DeterministicComplexGrid [{zmin_ ?NumericQ , zmax_ ?NumericQ } , number_ ] :=
  DeterministicComplexGrid [{zmin , zmax } , number ] [[All, 1]]
End[];

```

RandomComplex

Updating RandomComplex to handle input of the form RandomComplex[{{0, 1+i}, {2, 3+i}}, n].

```

Begin["`Private`"];
Unprotect[RandomComplex ];
RandomComplex [{range1_List , moreRanges___ } , number_ ] :=
  Transpose[RandomComplex [# , number ] & /@ {range1 , moreRanges } ]
Protect[RandomComplex ];
End[];

```

The following code places this redefinition as an initialization code for any parallelized subkernels that may get launched later (cf. mm.se/q/131856). This version, in addition, checks whether there is already any code in \$InitCode and, if there is, it appends its own code there.

```

Parallelize;
If[Head[Parallel`Developer`$InitCode] != Hold,
  Parallel`Developer`$InitCode = Hold[]
];
Parallel`Developer`$InitCode = Join[
  Parallel`Developer`$InitCode,
  Hold[
    Unprotect[RandomComplex ];
    RandomComplex [
      {Private`range1_List, Private`moreRanges___ }, Private`number_ ] := Transpose[
        RandomComplex [# , Private`number ] & /@ {Private`range1, Private`moreRanges }];
    Protect[RandomComplex ];
  ]
];

```

GetSaddlePoints

```

GetSaddlePoints::usage =
  "GetSaddlePoints[Ω,S,{tmin ,tmax },{τmin ,τmax }] finds a list of solutions {t,τ}
  of the HHG temporal saddle-point equations at harmonic energy Ω
  for action S, in the range {tmin , tmax } of recombination time and
  {τmin , τmax } of excursion time , where both ranges should be the
  lower-left and upper-right corners of rectangles in the complex plane.

GetSaddlePoints[ΩRange,S,{tmin ,tmax },{τmin ,τmax }] finds solutions of
  the HHG temporal saddle-point equations for a range of harmonic
  energies ΩRange, and returns an Association with each harmonic
  energy Ω indexing a list of saddle-point solution pairs {t,τ}.

GetSaddlePoints[Ωspec,S,{{tmin _1,tmax _1},{τmin _1,τmax _1}},{{tmin _2,tmax _2},{τmin _2,τmax _2}},
  ...] uses multiple time domains and combines the solutions.

GetSaddlePoints[Ωspec,S,{{urange,vrange},...},IndependentVariables→{u,v}] uses the explicit
  independent variables u and v to solve the equations and over the given ranges,
  where u and v can be any of \"RecombinationTime \", \"IonizationTime\"
  and \"ExcursionTime\", or their shorthands \"t\", \"tt\" and \"τ\" resp.";
SortingFunction::usage = "SortingFunction is an option of GetSaddlePoints
  which sets a function f, to be used as f[t,τ,S,Ω], to be
  used to sort the solutions, or a list of such functions.";
SelectionFunction::usage = "SelectionFunction is an option of GetSaddlePoints
  that sets a function f, to be used as f[t,τ,S,Ω],
  such that roots are only kept if f returns True.";
IndependentVariables::usage = "IndependentVariables is an option for GetSaddlePoints
  that specifies the two independent variables, out of \"RecombinationTime \",
  \"IonizationTime\" and \"ExcursionTime\" (or their shorthands
  \"t\", \"tt\" and \"τ\", respectively), to be used in solving the
  saddle-point equations, and which range over the given regions.";

FiniteDifference::usage =
  "FiniteDifference is a value for the option Jacobian of FindRoot, FindComplexRoots ,
  GetSaddlePoints, and related functions, which specifies that the Jacobian at
  each step should be evaluated using numerical finite difference procedures.";

GetSaddlePoints::error = "Errors encountered for harmonic energy Ω=`1`.";

Begin["`Private`"];
Options[GetSaddlePoints] =
  Join[{SortingFunction→(#2 &), SelectionFunction→(True &), IndependentVariables→
    {"RecombinationTime ", "ExcursionTime "}}, Options[FindComplexRoots ]];

```

```

Protect[SortingFunction, SelectionFunction, IndependentVariables, FiniteDifference];

GetSaddlePoints[Ωspec_, S_, {tmin_, tmax_}, {τmin_, τmax_}, options:OptionsPattern[]] :=
  GetSaddlePoints[Ωspec, S, {{tmin, tmax}, {τmin, τmax}}, options]

GetSaddlePoints[Ω_, S_, timeRanges_, options:OptionsPattern[]] :=
  Block[{equations, roots, t = Symbol["t"], tt = Symbol["tt"],
    τ = Symbol["τ"], indVars, depVar, depVarRule, tolerances},
    indVars = OptionValue[IndependentVariables] /.
      {"RecombinationTime" → "t", "ExcursionTime" → "τ", "IonizationTime" → "tt"};
    depVar = First[DeleteCases[{t, τ, tt}, Alternatives@@indVars]];
    depVarRule = depVar /. {"tt" → {tt → t - τ}, "t" → {t → tt + τ}, "τ" → {τ → t - tt}};
    equations = {D[S[t, tt], t] == Ω, D[S[t, tt], tt] == 0} /. depVarRule;
    tolerances = Which[
      ListQ[OptionValue[Tolerance]], OptionValue[Tolerance],
      True, ConstantArray[
        Which[
          NumberQ[OptionValue[Tolerance]], OptionValue[Tolerance],
          True, 10^If[NumberQ[OptionValue[WorkingPrecision]],
            2 - OptionValue[WorkingPrecision], 2 - $MachinePrecision]
        ],
        2]];

SortBy[
  DeleteDuplicates[
    Flatten[Table[
      Select[
        Check[
          roots = ({t, τ} /. depVarRule) /. (FindComplexRoots [
            equations
            , Evaluate[Sequence[{Symbol[indVars[[1]]], range[[1, 1]], range[[1,
              2]]}, {Symbol[indVars[[2]]], range[[2, 1]], range[[2, 2]]}]]
            , Evaluate[Sequence@@FilterRules[{options},
              Options[FindComplexRoots]]]
            , SeedGenerator → RandomSobolComplexes
            , Seeds → 50
          ] /. {{}} → ({t, τ} /. depVarRule) → {}))
          (*to deal with empty results*)
        , Message[GetSaddlePoints::error, Ω]; roots
      ]
    , Function[timesPair,
      OptionValue[SelectionFunction][timesPair[[1]], timesPair[[2]], S, Ω]
    ]
    , {range, timeRanges}], 1]
  , Function[{timesPair1, timesPair2},
    And@@Thread[Abs[timesPair1 - timesPair2] < tolerances] ]
]
, If[
  ListQ[OptionValue[SortingFunction]],
  Table[Function[timesPair, f[timesPair[[1]], timesPair[[2]], S, Ω]],
    {f, OptionValue[SortingFunction]}],
  Function[timesPair, OptionValue[SortingFunction][timesPair[[1]], timesPair[[2]], S, Ω]
]
]
]

GetSaddlePoints[ΩRange_List, S_, timeRanges_, options:OptionsPattern[]] :=

```

```
Association[ParallelTable[
   $\Omega \rightarrow$  GetSaddlePoints[ $\Omega$ , S, timeRanges, options]
  , { $\Omega$ , Sort[ $\Omega$ Range]}]]
```

```
End[];
```

GetSaddlesFromSeeds

GetSaddlesFromSeeds ::usage =

"GetSaddlesFromSeeds [{ $\{t_1, \tau_1\}, \{t_2, \tau_2\}, \dots\}$, Ω , S] finds a list of solutions { t, τ } of the HHG temporal saddle-point equations at harmonic energy Ω for action S, using the given { t_i, τ_i } as seeds for the process.

GetSaddlesFromSeeds [<| $\Omega_1 \rightarrow \{\{t_{11}, \tau_{11}\}, \{t_{12}, \tau_{12}\}, \dots\}$, $\Omega_2 \rightarrow \{\{t_{21}, \tau_{21}\}, \{t_{22}, \tau_{22}\}, \dots\}, \dots$ |>, Ω , S] finds solutions of the HHG temporal saddle-point equations, using the seeds list from the Ω_i that's closest to Ω , or as specified by the value of KeyChooserFunction.

GetSaddlesFromSeeds [seeds, { $\Omega_1, \Omega_2, \dots$ }, S] iterates over the given set of harmonic energies."

SeedsChooserFunction::usage =

"SeedsChooserFunction is an option for GetSaddlesFromSeeds that specifies a function f (set by default to Nearest) that, when used as f[{ $\Omega_1, \Omega_2, \dots$ }, Ω], should return the indices { $\Omega_i, \Omega_j, \dots$ } corresponding to the seed sets {{ $\{t_{i1}, \tau_{i1}\}, \dots\}$, {{ $\{t_{j1}, \tau_{j1}\}, \dots\}$ } to be used to solve the HHG saddle-point equations."

RecalculateRoots::usage = "RecalculateRoots is an option for GetSaddlesFromSeeds that specifies whether to re-solve the saddle-point equations if the given harmonic energy Ω is among the set of keys of the given seeds association. The default is False, which is appropriate for S being the same action used to find the seeds, in which case setting RecalculateRoots→True will produce multiple FindRoot errors. If using a different action than used to find the seeds, set to True."

GetSaddlesFromSeeds ::error = "Errors encountered for harmonic energy $\Omega = \text{'1'}$."

GetSaddlesFromSeeds ::norecalc =

"Skipping re-calculation of roots at harmonic energy '1' since it is already in the key set of the given seeds association. To run the calculation for this case set RecalculateRoots to True."

```
Begin["`Private`"];
```

```
Options[GetSaddlesFromSeeds] =
```

```
Join[{RecalculateRoots→False, SeedsChooserFunction→Nearest}, Options[GetSaddlePoints]];
```

```
Protect[SeedsChooserFunction, RecalculateRoots];
```

```
GetSaddlesFromSeeds [seedsSpec_,  $\Omega$ Range_List, S_, options:OptionsPattern[]] :=
```

```
Association[ParallelTable[
   $\Omega \rightarrow$  GetSaddlesFromSeeds [seedsSpec,  $\Omega$ , S, options]
  , { $\Omega$ , Sort[ $\Omega$ Range]}]]
```

```
GetSaddlesFromSeeds [seedsAssociation_Association $\Omega$ _, S_, options:OptionsPattern[]] :=
```

```
With[{keys = OptionValue[SeedsChooserFunction][Keys[seedsAssociation],  $\Omega$ ]},
```

```
If[MemberQ[keys,  $\Omega$ ] && TrueQ[!OptionValue[RecalculateRoots]],
```

```
Message[GetSaddlesFromSeeds ::norecalc,  $\Omega$ ];
```

```
Return[seedsAssociation[ $\Omega$ ]]];
```

```
GetSaddlesFromSeeds [Flatten[Values[seedsAssociation[[Key/@keys]]], 1],  $\Omega$ , S, options]
```

```
]
```

```

GetSaddlesFromSeeds [seedsList_List,  $\Omega$ ?NumberQ, S_, options:OptionsPattern[]] := Block[
  {equations, roots, t = Symbol["t"], tt = Symbol["tt"],
    $\tau$  = Symbol[" $\tau$ "], indVars, depVar, depVarRule, fullSeedVars, tolerances},
  indVars = OptionValue[IndependentVariables] /.
    {"RecombinationTime" → "t", "ExcursionTime" → " $\tau$ ", "IonizationTime" → "tt"};
  depVar = First[DeleteCases[{ "t", " $\tau$ ", "tt" }, Alternatives@@indVars]];
  depVarRule = depVar /. {"tt" → {tt → t -  $\tau$ }, "t" → {t → tt +  $\tau$ }, " $\tau$ " → { $\tau$  → t - tt}};
  fullSeedVars[seed_] := <|"t" → seed[[1]], " $\tau$ " → seed[[2]], "tt" → seed[[1]] - seed[[2]]|>;
  equations = {D[S[t, tt], t] ==  $\Omega$ , D[S[t, tt], tt] == 0} /. depVarRule;
  tolerances = Which[
    ListQ[OptionValue[Tolerance]], OptionValue[Tolerance],
    True, ConstantArray[
      Which[
        NumberQ[OptionValue[Tolerance]], OptionValue[Tolerance],
        True, 10^If[NumberQ[OptionValue[WorkingPrecision]],
          2 - OptionValue[WorkingPrecision], 2 - $MachinePrecision]
      ]
    , 2]];

SortBy[
  DeleteDuplicates[
    Select[
      Table[
        Check[
          roots = ({t,  $\tau$ } /. depVarRule) /. (
            FindRoot[
              equations
              , {Symbol[#], fullSeedVars[seed][[#]]} & /@ indVars
              , Evaluate[Sequence@@FilterRules[{options}, Options[FindRoot]]]
            ]
          /. {{} → ({t,  $\tau$ } /. depVarRule) → {}))
          , Message[GetSaddlesFromSeeds::error,  $\Omega$ ]; roots
        ]
        , {seed, seedsList}]
      , Function[timesPair,
        OptionValue[SelectionFunction][timesPair[[1]], timesPair[[2]], S,  $\Omega$ ]]
    ]
    , Function[{timesPair1, timesPair2},
      And@@Thread[Abs[timesPair1 - timesPair2] < tolerances] ]
  ]
  , If[
    ListQ[OptionValue[SortingFunction]],
    Table[Function[timesPair, f[timesPair[[1]], timesPair[[2]], S,  $\Omega$ ]],
      {f, OptionValue[SortingFunction]}],
    Function[timesPair, OptionValue[SortingFunction][timesPair[[1]], timesPair[[2]], S,  $\Omega$ ]]
  ]
]
End[];

```

```

ClassifyQuantumOrbits::usage =
  "ClassifyQuantumOrbits [saddlePoints,f] sorts an indexed set of saddle points
    of the form  $\langle |\Omega_1 \rightarrow \{\{t_{11}, \tau_{11}\}, \{t_{12}, \tau_{12}\}, \dots\} \dots \rangle$  using a function f,
    which should turn  $f[t, \tau, \Omega]$  into an appropriate label, and returns an
    association of the form  $\langle |label_1 \rightarrow \langle |\Omega_1 \rightarrow \langle |1 \rightarrow \{t, \tau\}, 2 \rightarrow \{t, \tau\}, \dots \rangle, \dots \rangle, \dots \rangle$ .

ClassifyQuantumOrbits [saddlePoints,f,sortFunction] uses
  the function sortFunction to sort the sets of saddle points
   $\{\{t_{11}, \tau_{11}\}, \{t_{12}, \tau_{12}\}, \dots\}$  for each label and harmonic energy.

ClassifyQuantumOrbits [saddlePoints,f,sortFunction,DiscardedLabels $\rightarrow\{\text{label}_1, \text{label}_2, \dots\}$ ]
  specifies a list of labels to discard from the final output.";
DiscardedLabels::usage = "DiscardedLabels is an option for ClassifyQuantumOrbits
  which specifies a list of labels to discard from the final output.";

Begin["`Private`"];

Options[ClassifyQuantumOrbits] = {DiscardedLabels $\rightarrow\{\}$ };
Protect[DiscardedLabels];

ClassifyQuantumOrbits [saddlePointList_,
  classifierFunction_, sortingFunction_ : Sort, OptionsPattern[]] := Map[
  Composition [
    Association,
    MapIndexed[#2[[1]]  $\rightarrow$  #1 &],
    sortingFunction
  ],
  Delete[DeleteMissing[
    Query[Transpose][
      MapIndexed[
        GroupBy[classifierFunction@@# &][
          Flatten/@Transpose[{{#1, ConstantArray[#2[[{1}, 1], Length[#1]]}]}]] &
        , saddlePointList][[All, All, All, {1, 2}]]
      ], 2], List/@OptionValue[DiscardedLabels]]
  , {2}]

End[];

```

ReperiodSaddles

```

ClearAll[ReperiodSaddles]
ReperiodSaddles::usage =
  "ReperiodSaddles[{{t1, τ1}, {t2, τ2}, ...}, f] readjusts the assigned cycle of
    the saddle points {ti, τi}, returning the list {{t1+f[t1, τ1], τ1}, ...}.

ReperiodSaddles[ $\langle |\Omega_1 \rightarrow \{\{t_{11}, \tau_{11}\}, \dots\}, \Omega_2 \rightarrow \dots \rangle$ , f] reperiods
  saddle-point pairs in a harmonic -energy-indexed association

ReperiodSaddles[ $\langle |label_1 \rightarrow \langle |\Omega_1 \rightarrow \{\{t_{11}, \tau_{11}\}, \dots\}, \dots \rangle, \dots \rangle$ , f] reperiods
  saddle-point pairs of a classified set of saddle points.";

Begin["`Private`"];

ReperiodSaddles[pair_/; Depth[pair] == 2, f_] := {pair[[1]] + f[pair[[1]], pair[[2]]], pair[[2]]}
ReperiodSaddles[association_, f_] := Apply[f, association, {Depth[association] - 2}]

End[];

```

HessianRoot

HessianRoot::usage = "HessianRoot[S,t,τ] calculates the Hessian root $\sqrt{\frac{(2\pi)^2}{i^2 \text{Det}[\partial_{\{t,tt\}}^2 S]}}$.";

Begin["`Private`"];

HessianRoot[S_, t_, τ_] := $\sqrt{\frac{2\pi}{i \text{Derivative}[0, 2][S][t, t - \tau]}}$

$\sqrt{\left(\frac{2\pi \text{Derivative}[0, 2][S][t, t - \tau]}{i (\text{Derivative}[2, 0][S][t, t - \tau] \text{Derivative}[0, 2][S][t, t - \tau] - \text{Derivative}[1, 1][S][t, t - \tau]^2)}\right)}$

End[];

FindStokesTransitions

FindStokesTransitions::usage =

"FindStokesTransition[S, <|Ω₁→<|1→{t₁₁, τ₁₁}, 2→{t₁₂, τ₁₂}|>, Ω₂→<|1→{t₂₁, τ₂₁}, 2→{t₂₂, τ₂₂}|>, ...|>

] finds the set {{Ω_S},{Ω_{AS}},n} of the Stokes and anti-Stokes transition energies for the given set of saddle points, where Re(S) changes sign after the Ω_S and Im (S) changes sign after the Ω_{AS}, and n is the index of the member of the pair that should be chosen after the transition (taken as the member with a positive imaginary part of the action at the largest Ω_i in the given keys).

FindStokesTransition[S, <|label₁→<|Ω₁→...|>|>] finds the Stokes transitions for the given set of saddle-point curve pairs, and returns them labeled with the label_i .";

FindStokesTransitions::saddleno = "FindStokesTransitions called with `1` of `2` saddle-point sets of length different from 2, with set length structure `3`. Excluding those sets from the calculation .";

FindStokesTransitions::multipleS = "FindStokesTransitions found multiple Stokes transitions using `1` to return a single transition .";

FindStokesTransitions::multipleAS = "FindStokesTransitions found multiple anti-Stokes transitions using `1` to return a single transition .";

ChooserFunction::usage = "ChooserFunction is an option for FindStokesTransition that specifies which transition to take if there are multiple transitions in the given dataset. The default is Last and gives the one with higher energy; to get the full set of transitions found use Full or Identity .";

ReperiodingFunction::usage = "ReperiodingFunction is an option for FindStokesTransitions SPAdipole and UAdipole which specifies a function f[t,τ] of recombination time t and excursion time τ that will be used to re-period the pairs {t,τ} into the form {t+f[t,τ],τ}. The default is Function[0], but if pairs are split it can be useful to set ReperiodingFunction to

Function[{t,τ}, Floor[-Re[t-τ], $\frac{2\pi}{\omega}$]] for ω the carrier frequency. In general, however, it is preferable to do this in a single go using ReperiodSaddles .";

Begin["`Private`"];

Protect[ReperiodingFunction, ChooserFunction];

Options[FindStokesTransitions] =

{ReperiodingFunction → Function[{t, τ}, 0], ChooserFunction → Automatic};

FindStokesTransitions[S_,

deeperAssociation_ /; Depth[deeperAssociation] == 5, options: OptionsPattern[]] := Map[

FindStokesTransition[S, #, options] &,

deeperAssociation

]


```

FindStokesTransition[S_, saddlesAssociation_, options:OptionsPattern[]] :=
Block[{reducedSaddlesAssociation, actionList, signsList, s, processor},
  reducedSaddlesAssociation= KeySort[Select[saddlesAssociation, Length[#] == 2 &]];
  If[Length[saddlesAssociation] - Length[reducedSaddlesAssociation] > 0,
    Message[FindStokesTransitions::saddleno,
      Length[saddlesAssociation] - Length[reducedSaddlesAssociation],
      Length[saddlesAssociation], First/@Tally/@Split[Values[Length/@saddlesAssociation]]
    ]
  ];
  actionList= ReIm [
    Map[(#reduces each  $\Omega \rightarrow \langle 1 \rightarrow S_1, 2 \rightarrow S_2 \rangle$  to  $\Omega \rightarrow (S_1 - S_2) *$ )
      Apply[Subtract],
      MapIndexed[(#reduces each  $\Omega \rightarrow \langle 1 \rightarrow \{t_1, \tau_1\}, 2 \rightarrow \{t_2, \tau_2\} \rangle$  to  $\Omega \rightarrow \langle 1 \rightarrow S_1, 2 \rightarrow S_2 \rangle *$ )
        With[{t = #1[[1]] + OptionValue[ReperiodingFunction][#1[[1]], #2[[2]]],
               $\tau = \#1[[2]]$ ,  $\Omega = \#2[[1, 1]]$ },
          S[t, t -  $\tau$ ] -  $\Omega t$ 
        ] &
      , reducedSaddlesAssociation, {2}
    ]
  ];
  signsList= Sign[Times [
    Rest[actionList],
    AssociationThread[Rest[Keys[actionList]], Most[Values[actionList]]]
  ]];
  processor = OptionValue[ChooserFunction] /. {Automatic -> Last, Full -> Identity};
  If[Length[Keys[Select[signsList, #[[1]] < 0 &]]] > 1,
    Message[FindStokesTransitions::multipleS, processor]];
  If[Length[Keys[Select[signsList, #[[2]] < 0 &]]] > 1,
    Message[FindStokesTransitions::multipleAS, processor]];
  {
    processor[Keys[Select[signsList, #[[1]] < 0 &]] /. {{}} -> {Missing["No transition"]}],
    processor[Keys[Select[signsList, #[[2]] < 0 &]] /. {{}} -> {Missing["No transition"]}],
    Sign[Last[actionList][[2]]] /. {1 -> 2, -1 -> 1}
  }
]

End[];

```

SPAdipole

```

SPAdipole::usage =
  "SPAdipole[S,prefactor, $\Omega$ , {t, $\tau$ }] returns the saddle-point approximation amplitude
  corresponding to action  $S[t,t-\tau]-\Omega t$  and the given prefactor[t,t- $\tau$ ].

SPAdipole[S,prefactor, $\Omega$ , <|1→{t1, $\tau$ 1},2→{t2, $\tau$ 2},...|>]
  returns the total harmonic -dipole contribution in the
  saddle-point approximation from the specified saddle points.

SPAdipole[S,prefactor, $\Omega$ , <|1→{t1, $\tau$ 1},2→{t2, $\tau$ 2}|>,transition] uses the given Stokes transition
  set to drop the relevant saddle after the anti-Stokes transition";
SPAdipole::wrongno = "SPAdipole called with a Stokes transition but with
  an input association of length `1` at harmonic
  energy  $\Omega=2$ . Reverting to unstructured evaluation.";
SPAdipole::invldtrns = "SPAdipole called with invalid Stokes transition
  set `1`. Reverting to unstructured evaluation.";

Begin["`Private`"];

Options[SPAdipole] = {ReperiodingFunction->Function[{t,  $\tau$ }, 0]};

SPAdipole[S_, prefactor_,  $\Omega$ _, {t_,  $\tau$ _}, options:OptionsPattern[]] :=
  Block[{tr = t + OptionValue[ReperiodingFunction][t,  $\tau$ ]},
    HessianRoot[S, tr,  $\tau$ ] prefactor[tr, tr -  $\tau$ ] Exp[-i S[tr, tr -  $\tau$ ] + i  $\Omega$  tr]
  ]
SPAdipole[S_, prefactor_,  $\Omega$ _, times_Association, options:OptionsPattern[]] := Block[{},
  Total[SPAdipole[S, prefactor,  $\Omega$ , #, options] &/@times ]
]

SPAdipole[S_, prefactor_,  $\Omega$ _, times_Association,
  transition_, options:OptionsPattern[]] := Block[{},
  If[!NumberQ[transition[[2]]], Message[SPAdipole::invldtrns, transition];
    Return[SPAdipole[S, prefactor,  $\Omega$ , times ]]];
  If[Length[times ] ≠ 2, Message[SPAdipole::wrongno, Length[times ],  $\Omega$ ];
    Return[SPAdipole[S, prefactor,  $\Omega$ , times , options]]];
  If[ $\Omega$  < transition[[2]],
    SPAdipole[S, prefactor,  $\Omega$ , times , options],
    SPAdipole[S, prefactor,  $\Omega$ , KeySelect[times , # == transition[[3]] &], options]
  ]
]

End[];

```

UAdipole

```

UAdipole::usage =
  "UAdipole[S,prefactor,Ω,<|1→{t1,τ1},2→{t2,τ2},...|>,transition] returns the total
    harmonic -dipole contribution in the uniform approximation from the
    specified saddle points, using the action S[t,t-τ]-Ωt and prefactor[t,t-τ],
    and taking the given Stokes transitionset as a reference.";
UAdipole::saddleno = "UAdipole called with `1` time pairs at Ω=`2`.
  Reverting to the saddle-point approximation for this set.";
UAdipole::invldtrns = "UAdipole called with invalid Stokes transitionset `1`.
  Reverting to the saddle-point approximation for this set.";

Begin["`Private`"];

Options[UAdipole] = {ReperiodingFunction->Function[{t, τ}, 0]};

UAdipole[S_, prefactor_, Ω_, times_ , transition_, options:OptionsPattern[]] := (
  If[Length[times] ≠ 2, Message[UAdipole::saddleno, Length[times] , Ω];
    Return[SPAdipole[S, prefactor, Ω, times] ]];
  If[!NumberQ [transition[[2]]], Message[UAdipole::invldtrns, transition];
    Return[SPAdipole[S, prefactor, Ω, times] ]];
  Block[
    {A1, A2, S1, S2, Ss, Sm , z,
      t1 = times [1] [[1]] + OptionValue[ReperiodingFunction][times [1] [[1]], times [1] [[2]]],
      τ1 = times [1] [[2]],
      t2 = times [2] [[1]] + OptionValue[ReperiodingFunction][times [2] [[1]], times [2] [[2]]],
      τ2 = times [2] [[2]]},
    A1 = HessianRoot[S, t1, τ1] prefactor[t1, t1-τ1];
    S1 = S[t1, t1-τ1] - Ω t1;
    A2 = HessianRoot[S, t2, τ2] prefactor[t2, t2-τ2];
    S2 = S[t2, t2-τ2] - Ω t2;
    Ss =  $\frac{S1+S2}{2}$ ; Sm =  $\frac{S1-S2}{2}$ ;
    If[Ω < transition[[2]], z =  $\left(-\frac{3}{2}Sm\right)^{2/3}$ ,
      z =  $\left(-\frac{3}{2}Sm\right)^{2/3} \text{Exp}\left[\text{i} \left(\text{transition}[[3]] /. \{2 \rightarrow -1, 1 \rightarrow 1\}\right) \frac{2\pi}{3}\right]$ ;
       $\sqrt{6\pi Sm} \text{Exp}\left[-\text{i} Ss + \text{i} \frac{\pi}{4}\right] \left(\frac{A1 - \text{i} A2}{2} \frac{\text{AiryAi}[-z]}{\sqrt{z}} + \text{i} \frac{A1 + \text{i} A2}{2} \frac{\text{AiryAi}'[-z]}{z}\right)$ 
    ]
  )

End[];

```

Package closure

End of package

```
EndPackage[];
```

Add to distributed contexts.

```
DistributeDefinition["RBSFA`"];
```