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 autogenerated 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.

```
(*
This is the RB-SFA package for calculating high-
order harmonic generation within the Strong Field Approximation. For the
   notebook that generated this package file and additional documentaion ,
see https://github.com/episanty/RB-SFA.
*)
```

Implementation

Supporting functions

Initialization

```
BeginPackage | "RBSFA`" | ;
```

Version number

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

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

 $NotebookEventActions \rightarrow \{ \{ "MenuCommand ", "Save" \} \Rightarrow (NotebookSave[]), PassEventsDown \rightarrow True \} \}$

Timestamp

```
Begin["`Private`"];
$RBSFAtimestamp = "Tue 28 Feb 2017 11:48:14";
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]], {" " \rightarrow " \}],
      $RBSFAdirectory= StringReplace[DirectoryName [$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"}]]);
```

Standard function (re)definitions

ConstantArray

End[];

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. mm.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.

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

AssociationTranspose

```
ClearAll [AssociationTranspose
AssociationTranspose:usage =
    "AssociationTransposeassociation transposes the given two-level
         association of associations ";
AssociationTranspose:wrngshp = "Input `1` is the wrong shape; it must be
         an associationall of whose Values are valid associations ";
Begin["`Private`"];
AssociationTranspose association_? (
           And@@(AssociationQ/@Join[{#}, Values[#]]) &
         ) ] := GroupBy [
         Join@@Thread/@Normal //@association,
         {First@*Last, First}
      [A11, A11, 1, 2, 2];
AssociationTransposeassociation_] :=
  "Doesn't display; cf. mm .se/q/29321 for details"/;
    Message [AssociationTranspose:wrngshp, association]
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.

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

KeyValueMap

This exists in Mathematica 10.1 and later, but it's nice to have it on version 10.0 so this is a back-port for versions that do not have it.

```
If[
  $VersionNumber < 10.1,</pre>
 KeyValueMap::usage =
    "\!\(\*RowBox[{\"KeyValueMap\", \"[\", RowBox[{StyleBox[\"f\",\"TI\"], \",\",
       RowBox[{\"<|\",RowBox[{RowBox[{SubscriptBox[StyleBox[\"key\", \"TI\"],</pre>
       \"TI\"], StyleBox[\"1\", \"TR\"]]}], \",\",
       RowBox[{SubscriptBox[StyleBox[\"key\", \"TI\"], StyleBox[\"2\",
       \"TR\"]], \"->\", SubscriptBox[StyleBox[\"val\", \"TI\"], StyleBox[\"2\",
       \"TR\"]]}], \",\", StyleBox[\"...\", \"TR\"]}], \"|>\"}]], \"]\"}]\)
       gives the list \!\(\*RowBox[{\"{\", RowBox[{RowBox[{StyleBox[\"f\",
       \"TI\"], \"[\", RowBox[{SubscriptBox[StyleBox[\"key\", \"TI\"],
       StyleBox[\"1\", \"TR\"]], \",\", SubscriptBox[StyleBox[\"val\", \"TI\"],
       StyleBox[\"1\", \"TR\"]]}], \"]\"}], \",\", RowBox[{StyleBox[\"f\",
       \"TI\"], \"[\", RowBox[{SubscriptBox[StyleBox[\"key\", \"TI\"],
       \"TI\"], StyleBox[\"2\", \"TR\"]]}], \"]\"}], \",\", StyleBox[\"...\",
       \"TR\"]}], \"}\"}]\). (Note: function backported from v10.1+.)
operator form of KeyValueMap that can be applied to an expression.";
  KeyValueMap::invak = "The argument `1` is not a valid association";
]
Begin["`Private`"];
If[
  $VersionNumber < 10.1,</pre>
 KeyValueMap[f_, assoc_?AssociationQ := Map[Apply[f], Normal [assoc]];
 KeyValueMap[f_][assoc_?AssociationQ := KeyValueMap[f, assoc];
 KeyValueMap[f_, assoc__]:=
    "Doesn't display; cf. mm .se/q/29321 for details"/; Message KeyValueMap::invak, assoc];
End[];
```

Dipole transition matrix elements

Default DTME, for a hydrogenic 1s state

hydrogenicDTME::usage =

"hydrogenicDTME[p, κ] returns the dipole transition matrix element for a 1s hydrogenic state of ionization potential $I_p = \frac{1}{\kappa^2}$.

hydrogenicDTME[p, κ , {n,l,m}] returns the dipole transition matrix element for an n,1,m hydrogenic state of ground-state ionization potential $I_p = \frac{1}{x^2}$.

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

 $\label{eq:hydrogenicDTMERegularized:usage = "hydrogenicDTMERegularizedp, \kappa] returns the} \\$ dipole transition matrix element for a 1s hydrogenic state of ionization potential $I_p = \frac{1}{\kappa^2}$, regularized to remove the denominator of $1/(p^2+\kappa^2)^3$, where the saddle-point solutions are singular.

 $\label{eq:hydrogenicDTMERegularizedp, k, n,l,m} \ | \ \text{returns the dipole transition matrix element for} \\$ an n,1,m hydrogenic state of ground-state ionization potential $I_p = \frac{1}{2} \kappa^2$, regularized to remove factors of $(p^2 + \kappa^2)$ from the denominator .

 $\label{eq:local_power_$ n,1,m hydrogenic state of ground-state ionization potential $I_p = \frac{1}{2} \kappa^2$,

regularized to remove factors of $(p^2+\kappa^2)$ from the denominator."; Begin["`Private`"];

 $\label{eq:hydrogenicDTME} \text{hydrogenicDTME} \big[\textbf{p_List,} \; \kappa_{-} \big] := \frac{8 \, \text{i}}{\pi} \, \frac{\sqrt{2 \, \kappa^5} \; \textbf{p}}{\left(\text{Total} \left[\textbf{p}^2 \right] + \kappa^2 \right)^3}$

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

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

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

For a gaussian orbital

SolidHarmonicS

This function implements the solid harmonic $S_{l,m}$ (\mathbf{r}) = $r^l Y_{l,m}$ (θ , ϕ), 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 [1,m ,x,y,z] calculates the solid harmonic S_{lm} (x,y,z)=r^{l}Y_{lm} (x,y,z). SolidHarmonicS [1,m ,{x,y,z}] does the same ."; Begin["`Private`"]; SolidHarmonicS [\lambda_Integer, \mu_Integer, x_, y_, z_] /; \lambda \ge Abs[\mu] := sqrt\left[\frac{2\lambda+1}{4\pi}\right] sqrt\left[\frac{Gamma}{Gamma} \frac{\left[\lambda-Abs[\mu]+1\right]}{\left[\lambda+Abs[\mu]+1\right]}\right]^{2-\lambda} (-1)^{(\mu-Abs[\mu])/2} \times If\left[Rationalize(\mu]=0,1,(x+sign[\mu]iy)^{Abs[\mu]}\right] \times sum\left[ (-1)^{\mu+k}Binomial\left[\lambda,k\right]Binomial\left[2\lambda-2k,\lambda\right]Pochhammer \left[\lambda-Abs[\mu]-2k+1,Abs[\mu]\right] \times If\left[TrueQ[Pochhammer \left[\lambda-Abs[\mu]-2k+1,Abs[\mu]\right]=0\right],1, If\left[Rationalize(k)=0,1,(x^2+y^2+z^2)^k\right]If\left[Rationalize(\lambda-Abs[\mu]-2k\right]=0,1,z^{\lambda-Abs[\mu]-2k}\right] , \{k,0,Quotient[\lambda,2]\} SolidHarmonicS [\lambda_Integer, \mu_Integer, {x_,y_,z_}] /; \lambda \ge Abs[\mu] := SolidHarmonicS [\lambda_Integer, \mu_Integer, {x_,y_,z_}] /; \lambda \ge Abs[\mu] := SolidHarmonicS [\lambda_u, x, y, z]
```

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 =
            "hydrogenic\Psi[n,1,m,\kappa,px,py,pz] calculates the momentum -space wavefunction
                        \Psi(p) = \langle p | nlm \rangle for a hydrogenic atom with ionization potential \kappa^2/2.
\label{eq:local_problem} \mbox{hydrogenic} \Psi[\mbox{n,l,m} \mbox{,} \kappa, \{\mbox{px,py,pz}\}] \mbox{ calculates the momentum} - \mbox{space wavefunction}
                        \Psi(p) = \langle p | nlm \rangle for a hydrogenic atom with ionization potential \kappa^2/2.";
Begin["`Private`"];
\label{eq:hydrogenic} \begin{aligned} &\text{hydrogenic} \Psi[\texttt{n}\_, \texttt{1}\_, \texttt{m}\_, \kappa\kappa\_, \texttt{ppx}\_, \texttt{ppy}\_, \texttt{ppz}\_] := \texttt{Block} \big[ \{\kappa, \texttt{px}, \texttt{py}, \texttt{pz}\}, \end{aligned}
                 hydrogenic\Psi[n, 1, m, \kappa_{-}, px_{-}, py_{-}, pz_{-}] = Simplify
                             -SolidHarmonics [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}}{\left(px^2+py^2+pz^2+\kappa^2\right)^{1+2}} \\ \text{GegenbauerC}\Big[n-1-1,\,1+1,\,\frac{px^2+py^2+pz^2-\kappa^2}{px^2+py^2+pz^2+\kappa^2}\Big]
                 hydrogenicΨ[n, l, m , κκ, ppx, ppy, ppz]
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.
hydrogenic TRegularized: usage =
            "hydrogenicYRegularizeqn,1,m, \kappa,px,py,pz] calculates the momentum
                                                                                                                                                                                                            -space
                       wavefunction \Psi(p) = \langle p | nlm \rangle for a hydrogenic atom with
                       ionization
potential \kappa^2/2, multiplied by (p^2+\kappa^2)^{n+1}
                       to remove any factors of p^2 + \kappa^2 in the denominator .
hydrogenicYRegularizeqn,1,m ,x,{px,py,pz}] calculates the momentum -space wavefunction
                       \Psi(p) = \langle p | \text{nlm} \rangle for a hydrogenic atom with ionization potential \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`"];
hydrogenic \P Regularized n_, l_, m_ , \kappa \kappa_, ppx_, ppy_, ppz_] := Block [\{\kappa, px, py, pz\}, ppx_] := Regularized n_, l_, m_ , \kappa \kappa_, ppx_, ppx_] := Regularized n_, l_, m_ , \kappa \kappa_, ppx_, ppx_] := Regularized n_, l_, m_ , \kappa \kappa_, ppx_, ppx_] := Regularized n_, l_, m_ , \kappa \kappa_, ppx_, ppx_, ppx_] := Regularized n_, l_, m_ , \kappa \kappa_, ppx_, ppx_, ppx_] := Regularized n_, l_, m_ , k \kappa_, ppx_, ppx_, ppx_] := Regularized n_, l_, m_ , k \kappa_, ppx_, ppx_, ppx_, ppx_] := Regularized n_, l_, m_ , k \kappa_, ppx_, ppx
                 hydrogenic \Psi Regularize (n, 1, m, \kappa_{-}, px_{-}, py_{-}, pz_{-}) = Simplify [Cancel]
                                   -SolidHarmonicS [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} \left( px^2 + py^2 + pz^2 + \kappa^2 \right)^{n-1-1} GegenbauerC \left[ n-1-1, 1+1, \frac{px^2 + py^2 + pz^2 - \kappa^2}{px^2 + py^2 + pz^2 + \kappa^2} \right]
                 hydrogenic TRegularizedn, 1, m , kk, ppx, ppy, ppz]
hydrogenic\PsiRegularizedn_,l_,m_ ,\kappa_, {px_,py_,pz_}]:=
           hydrogenicΨRegularizedn, l, m , κ, px, py, pz];
End[];
Upsilon function, given by Y(\mathbf{p}) = \left(\frac{1}{2}\mathbf{p}^2 + I_p\right)\Psi(\mathbf{p}) = \frac{1}{2}\left(\mathbf{p}^2 + \kappa^2\right)\langle\mathbf{p} \mid n, I, m\rangle, which can be used in the form
```

Y(p + A(t')) as a replacement for the ionization dipole $d(p + A(t')) \cdot F(t')$, 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,1,m ,\kappa,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,1,m ,\kappa,{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_{,}\kappa_{,}px_{,}py_{,}pz_{]}:=
     \frac{1}{2} \left( px^2 + py^2 + pz^2 + \kappa^2 \right) \text{ hydrogenic} \Psi[n, 1, m, \kappa, px, py, pz];
hydrogenicY[n_, l_, m_ , \kappa_, py_, pz_]] := hydrogenicY[n, l, m , \kappa, px, py, pz];
End[];
hydrogenicDTME for arbitrary states
Begin["`Private`"];
hydrogenicDTME[{px_,py_,pz_}, \kappa_, n, 1, m] =
          Simplify [Grad[hydrogenicY[n, 1, m , k, px, py, pz], {px, py, pz}]];
       hydrogenicDTME[{ppx, ppy, ppz}, κκ, n, 1, m]
\label{eq:hydrogenicDTME} \begin{aligned} &\text{hydrogenicDTME}[\{px_, py_, pz_\}, \kappa_-, \{n_-, 1_-, m_-\}] := &\text{hydrogenicDTME}[\{px, py_, pz\}, \kappa, n, 1, m_-\}; \end{aligned}
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_}, k_, n_, l_, m_ ] :=
     (px^2 + py^2 + pz^2 + \kappa^2)^{n+1} hydrogenicDTME[\{px, py, pz\}, \kappa, n, 1, m];
hydrogenicDTMERegularized {px, py, pz}, k, n, 1, m ];
End[];
```

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,
        \text{Piecewise}\Big\{\big\{\{0,\, t<0\}\,,\, \Big\{\text{Sin}\Big[\frac{\omega\,t}{4\,\text{nRamp}}\Big]^2\,,\, 0\leq t<\frac{2\,\pi}{\omega}\text{nRamp}\,\,\Big\}\,,\, \Big\{1\,,\, \frac{2\,\pi}{\omega}\text{nRamp}\,\,\leq t<\frac{2\,\pi}{\omega}\,\,(\text{num -nRamp })\Big\}\,,
                 \left\{ \sin \left[ \frac{\omega \left( \frac{2\pi}{\omega} \text{ num } - t \right)}{4\pi \text{ page}} \right]^2, \frac{2\pi}{\omega} \left( \text{num } - \text{nRamp } \right) \le t < \frac{2\pi}{\omega} \text{ num } \right\}, \left\{ 0, \frac{2\pi}{\omega} \text{ num } \le t \right\} \right\} \right] \right]
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}, num_{num}] := Function[t, 1 - Cos[\frac{\omega t}{2num}]^{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.";
CarrierFrequency::default = "Warning: no CarrierFrequency was
        specified, using \omega=1 a.u. as the default.";
$DefaultCarrierFrequency::usage = "Default CarrierFrequency to use
        when no explicit option is indicated ";
Protect[PointsPerCycle, TotalCycles, CarrierFrequency];
standardOptions = \{PointsPerCycle \rightarrow 90, TotalCycles \rightarrow 1, \}
      CarrierFrequency→Automatic , IntegrationPointsPerCycle→Automatic };
$DefaultCarrierFrequency= 0.057;
GetCarrierFrequency::usage = "GetCarrierFrequency[OptionValue[CarrierFrequency]] returns
        OptionValue[CarrierFrequency], unless it's set to Automatic, in
        which case it returns $DefaultCarrierFrequency and issues a warning.
GetCarrierFrequency[\omega] works for any input.";
Begin["`Private`"];
GetCarrierFrequency[optionvalue_] := If[
    optionvalue === Automatic ,
    Message[CarrierFrequency::default, $DefaultCarrierFrequency];
    $DefaultCarrierFrequency,
    optionvalue
End[]
RBSFA`Private`
```

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] =
      \label{local_condition} Join \big[ \texttt{standardOptions, } \big\{ \texttt{TargetLength} \rightarrow \texttt{Automatic , LengthCorrection} \rightarrow 1 \big\} \big] \,;
harmonicOrderAxis::target =
      "Invalid TargetLength option `1`. This must be a positive integer or Automatic .";
harmonicOrderAxis [OptionsPattern[]] :=
  Module | {num = OptionValue TotalCycles | , npp = OptionValue PointsPerCycle } ,
     Piecewise {
           \left\{\frac{1}{\text{num}} \text{Range}\left[0., \text{Round}\left[\frac{\text{npp num} + 1}{2.}\right] - 1 + \text{OptionValue}\left[\text{LengthCorrection}\right]\right],\right\}
              OptionValue[TargetLength] === Automatic },
           \left\{\frac{\text{Round}\left[\frac{\text{nppnum} \ +1}{2.}\right]}{\text{num}}\frac{\text{Range}\left[\text{0,OptionValue}\left[\text{TargetLength}\right]-1\right]}{\text{OptionValue}\left[\text{TargetLength}\right]},\right.
              IntegerQ[OptionValue[TargetLength]] &&OptionValue[TargetLength] \geq 0}
        Message[harmonicOrderAxis::target, OptionValue["TargetLength"]];
        Abort[]
End[];
```

frequencyAxis

frequency Axis 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[]]:=
  GetCarrierFrequency[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\pi/\omega, \omega = GetCarrierFrequency | OptionValue | CarrierFrequency | \}, 
       num = OptionValue[TotalCycles], npp = OptionValue[PointsPerCycle]},
     Piecewise {
            {1, OptionValue[TimeScale ] === AtomicUnits },
            \left\{\frac{1}{T}, \text{OptionValue}[\text{TimeScale}] === \text{LaserPeriods}\right\}
         Message[timeAxis::scale, OptionValue[TimeScale]]; Abort[]
       |xTable | t
         , \left\{\text{t, 0, num } \frac{2\pi}{\omega}, \frac{\text{num }}{\text{num } \times \text{npp+OptionValue[PointNumberCorrection]}} \frac{2\pi}{\omega}\right\}
End[];
tInit=0;
    tFinal-tInit
num xnpp+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,
- \cdot 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 $\epsilon = \{1, \bar{\imath}\}$ and $\epsilon = \{1, -\bar{\imath}\}$ 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 $[\ddagger]^2$ & 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 = "DifferentiationOrderis 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 \rightarrow False, ComplexPart \rightarrow (\#\&), \}
          ωPower → 0, DifferentiationOrder→ 0}~Join~standardOptions;
getSpectrum ::diffOrd = "Invalid differentiationorder `1`.";
getSpectrum ::\omegaPow = "Invalid \omega power `1`.";
getSpectrum [dipoleList_OptionsPattern[]]:=Block|
     polarizationVector, differentiatedList depth, dimensions ,
       num = OptionValue[TotalCycles], npp = OptionValue[PointsPerCycle], \omega, \delta t = \frac{2\pi/\omega}{\pi m}
     },
     \tt differentiatedList=OptionValue[ComplexPart\ ][Piecewise]\{
                \left\{ \texttt{dipoleList}, \texttt{OptionValue} \middle[ \texttt{DifferentiationOrder} = 0 \right\},
               \Big\{\frac{1}{2\,\delta t} \left( \texttt{Most} \big[ \texttt{Most} \big[ \texttt{dipoleList} \big] \big] - \texttt{Rest} \big[ \texttt{Rest} \big[ \texttt{dipoleList} \big] \big] \right),
                  OptionValue[DifferentiationOrder == 1 },
               \left\{\frac{1}{\kappa+2}\left(\mathsf{Most}\big[\mathsf{Most}\big[\mathsf{dipoleList}\big]\big]-2\,\mathsf{Most}\big[\mathsf{Rest}\big[\mathsf{dipoleList}\big]\big]+\mathsf{Rest}\big[\mathsf{Rest}\big[\mathsf{dipoleList}\big]\big]\right),
                  OptionValue DifferentiationOrder = 2 } ,
             Message[getSpectrum ::diffOrd, OptionValue[DifferentiationOrder];
             Abort[]
          ]];
     Abort[] |;
     If [OptionValue[\omegaPower] \neq 0, \omega = GetCarrierFrequency[OptionValue[CarrierFrequency]], \omega = 1];
     (*If ωPower==
        0 the value of \omega doesn't matter and there's no sense in printing error messages *)
     num Table
          \left(\frac{\omega}{\text{num}}k\right)^{2 \text{ OptionValue}[\omega Power]}, \left\{k, 1, \text{Round}\left[\frac{\text{Length}\left[\text{differentiatedLis}^{\frac{1}{2}}\right]}{2}\right]\right\}
        |xIf
```

```
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]];
         Sum Abs
               Fourier
                    If [depth > 1, Re [differentiatedLis [All, i]]], Re [differentiatedLis [All]]]
                    , FourierParameters \rightarrow \{-1, 1\}
                 ] [1;; Round [\frac{Length[differentiatedList]}{2}]]
             ]<sup>2</sup>, {i, 1, dimensions }]
         , (*polarized spectrum *)
        Abs
             Transpose Table
                        Re[differentiatedLis[All, i]], FourierParameters \rightarrow {-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" \rightarrow 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 \rightarrow Full
    , PlotStyle \rightarrow Thick
    , Frame → True
    , Axes \rightarrow False
    , ImageSize \rightarrow 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 \begin{bmatrix} dipoleList, Polarization \rightarrow \{1, +ii\}, \end{bmatrix}
            Sequence@@FilterRules[{options}, Options[getSpectrum ]]],
          PlotStyle \rightarrow 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 % \left( 1\right) =\left( 1\right) +\left( 1\right
 LinearRampGate ::usage = "LinearRampGate [nGateRamp] specifies an integration gate
                                                              with a linear ramp , such that SineSquaredGate[nGateRamp ][\omegat,nGate]
                                                              has nGate flat periods and nGateRamp ramp periods.";
 Begin["`Private`"];
 SineSquaredGate[nGateRamp_ ][\omega\tau_, nGate_] := Piecewise \{\{1, \omega\tau \le 2\pi \text{ (nGate-nGateRamp )}\},
                                                \left\{ \sin \left[ \frac{2 \pi \text{nGate} - \omega \tau}{4 \text{nGateRamp}} \right]^2, 2 \pi \left( \text{nGate-nGateRamp} \right) < \omega \tau \le 2 \pi \text{nGate} \right\}, \left\{ 0, \text{nGate} < \omega \tau \right\} \right\} \right\}
LinearRampGate [nGateRamp_ ][\omega\tau_, nGate_] := Piecewise \{\{1, \omega\tau \le 2\pi \text{ (nGate-nGateRamp )}\},
                                                \left\{-\frac{\omega\tau-2\pi\left(\text{nGate}+\text{nGateRamp}\right.\right)}{2\pi\text{nGateRamp}},\,2\pi\left(\text{nGate}-\text{nGateRamp}\right.\right)<\omega\tau\leq2\pi\text{nGate}\right\},\,\left\{0\,,\,\text{nGate}<\omega\tau\right\}\right\}\right]
 End[];
```

getIonizationPotential

```
getIonizationPotential:usage =
    "getIonizationPotentia[Target] returns the ionizationpotential
        of an atomic target, e.g. \"Hydrogen\", in atomic units.
getIonizationPotentia[Target,q] returns the ionizationpotential
        of the q-th ion of the specified Target, in atomic units.
getIonizationPotentia[{Target,q}] returns the ionizationpotential
        of the q-th ion of the specified Target, in atomic units.";
Begin["`Private`"];
getIonizationPotentia[Target_, Charge_: 0] :=
  UnitConvert[ElementData [Target, "IonizationEnergies] [Charge+1] /
       (Quantity[1, "AvogadroConstant"] Quantity[1, "Hartrees"])]
\tt getIonizationPotentia[{Target\_, Charge\_: 0}] := \tt getIonizationPotentia[Target, Charge]
End[];
```

makeDipoleList: main numerical integrator

The main integration function is makeDipoleList, and its basic syntax is of the form makeDipoleList[VectorPoten : tial→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 \rightarrowpars.
        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 \rightarrow g, nGate \rightarrow 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 = "IonizationPotentialis an option for makeDipoleList
         which specifies the ionization potential Ip 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 secifies 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 ionizationand
         recombination dipoels, to be used in the form f[p,\kappa]=f[p,\sqrt{2I_p}].";
€Correction::usage = "€Correction is an option for makeDipoleList which specifies the
         regularization correction \epsilon, i.e. as used in the factor \frac{1}{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 \rightarrow SineSquaredGate[1/2], nGate \rightarrow 3/2, \epsilonCorrection \rightarrow 0.1,
         IonizationPotentia → 0.5,
         Target → Automatic , DipoleTransitionMatrixElement → hydrogenicDTME,
         PointNumberCorrection \rightarrow 0, Verbose \rightarrow 0, CheckNumericFields \rightarrow True,
         RunInParallel → Automatic ,
         Simplifier \rightarrow Identity, QuadraticActionTerms \rightarrow 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 ElectricField Automatic .";
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::runpar = "Wrong RunInParallel option `1`.";
makeDipoleList::carrfreq = "Non-numeric option CarrierFrequency `1`.";
makeDipoleList [OptionsPattern[]] := Block [
      num = OptionValue[TotalCycles], npp = OptionValue[PointsPerCycle], ω,
      dipoleRec, dipoleIon, k,
      A, F, GA, pi, ps, S,
      gate, tGate, setPreintegral,
      tInit, tFinal, \delta t, \delta tint, \epsilon = OptionValue[\epsilon Correction],
      AInt, A2Int, GAInt, GAdotAInt, AdotGAInt, GAIntInt,
      PScorrectionInt, constCorrectionInt, GAIntdotGAIntInt, QuadMatrix, q,
      simplifier, prefactor, integrand, dipoleList,
      TableCommand , SumCommand
    },
    A[t_] = OptionValue [VectorPotential] [t] //. OptionValue [FieldParameters];
      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
      ];
    ω = GetCarrierFrequency[OptionValue[CarrierFrequency]];
    Message [makeDipoleList::carrfreq, \omega];
      Abort[];
    tInit=0;
    tFinal = \frac{2\pi}{m}num;
    (*looping timestep *)
                        tFinal-tInit
        num xnpp+OptionValue[PointNumberCorrection];
    (*integration timestep *)
    δtint=If OptionValue IntegrationPointsPerCycle === Automatic ,
         \delta t, (tFinal-tInit) / (num xOptionValue IntegrationPointsPerCycle +
               OptionValue[PointNumberCorrection])];
    tGate = OptionValue[nGate] \frac{2\pi}{};
    (*Check potential and potential gradient for correctness.*)
    (*To do: change logic conditions to constructions on VectorQ[#, NumberQ ]&
      and MatrixQ.*)
    If [TrueQ [OptionValue | CheckNumericFields ]],
```

```
With [\{\omega t \text{Random} = \text{RandomReal} [\{\omega t \text{Init}, \omega t \text{Final}\}]\},
     If [!And@@ (NumberQ /@A [\omegatRandom /\omega]), Message [makeDipoleList::pot,
          OptionValue [VectorPotential], \omegatRandom, A [\omegatRandom]];
        Abort[];
     If [!And@@(NumberQ/@Flatten[GA[\omegatRandom/\omega]]), Message[makeDipoleList::gradpot,]]
          OptionValue[VectorPotentialGradient], wtRandom , GA[wtRandom ]];
        Abort[]|;
     If [ ! And@@ (NumberQ /@F [\omegatRandom /\omega]), Message [makeDipoleList :: efield,
          OptionValue[ElectricField, \omegatRandom, F[\omegatRandom]];
        Abort[];
  ]];
gate [\omega \tau_{-}] := OptionValue[Gate] [\omega \tau, OptionValue[nGate]];
\label{eq:with_andom} \textbf{With} \big[ \big\{ \omega \, \texttt{tInit}, \, \omega \, \texttt{tFinal} \big\} \big] \big\} \, ,
  If [!TrueQ[NumberQ [gate \omegatRandom]]],
     Message makeDipoleList::gate,
        OptionValue[Gate], \omegatRandom , OptionValue[nGate], gate[\omegatRandom]];
     Abort[]
];
(*Target setup*)
Which
  OptionValue[Target] === Automatic , \kappa = \sqrt{2 \, \text{OptionValue}[\text{IonizationPotentia}]} ,
  True, \kappa = \sqrt{2 \text{ getIonizationPotentia}} OptionValue[Target]
With [\dim = Length [A[RandomReal [\{\omega tInit, \omega tFinal\}]]]],
   (*Explicit conjugation of the
     recombination matrix element to keep the integrand analytic.*)
  Which
        Head[OptionValue[DipoleTransitionMatrixElement]] === List,
        dipoleIon[\{p1_, p2_, p3_\}[1;; dim], \kappa\kappa] =
          First[OptionValue[DipoleTransitionMatrixElement]][{p1, p2, p3}[1;; dim ], kk];
        dipoleRec[{p1_, p2_, p3_}[[1;; dim]], κκ_] =
          Assuming |\{p1, p2, p3, \kappa\kappa\} \in \text{Reals}\}, Simplify |
                Conjugate Last OptionValue DipoleTransitionMatrixElement
                     {p1, p2, p3} [1;; dim ], κκ]]
             ]];
        , True,
        dipoleIon[{p1_, p2_, p3_}[1;; dim], κκ_] =
          OptionValue[DipoleTransitionMatrixElement] [{p1, p2, p3} [1;; dim ], xx];
        dipoleRec[\{p1_, p2_, p3_\}[1;; dim], \kappa\kappa_] =
          Assuming [\{p1, p2, p3, \kappa\kappa\} \in Reals\}, Simplify [
                Conjugate OptionValue DipoleTransitionMatrixElement
                     {p1, p2, p3} [1;; dim ], \(\kappa\kappa\)]
             ]];
     ];
];
simplifier = OptionValue[Simplifier];
q = Boole[TrueQ[OptionValue[QuadraticActionTerms]]];
setPreintegral integral Variable, preintegrand,
     dimensions_ , integrateWithoutGradient, parametric_ ] := Which[
```

```
(*Vector potential gradient specified
     or integral variable does not depend on it, so integrate*)
    Which
          OptionValue[Preintegrals] == "Analytic",
          integralVariable[t_, tt_] = simplifier[
                 ((\#/. \{\tau \to t\}) - (\#/. \{\tau \to tt\})) \& [Integrate[preintegrand[\tau, tt], \tau]]];
          , OptionValue[Preintegrals] == "Numeric ",
         Which
               TrueQ[Not[parametric]],
              Block [{innerVariable},
                    integral Variabl \verb||[t_-, tt_-]| = \Big( inner Variabl \verb||[t_-]| - inner Variabl \verb||[t_-]| /. First [
                             NDSolve[\{innerVariable'[\tau] = preintegrand[\tau],\}]
                                  innerVariabletInit == ConstantArray [0, dimensions]},
                                innerVariable, \{\tau, \text{tInit}, \text{tFinal}\}, MaxStepSize\rightarrow 0.25/\omega
                           1)
                 ];
               , 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+\tau pre \le tFinal}, 0],
                                     innerVariable[##][0, tt] == 0
                                   }, innerVariable[##]
                                   , {tpre, 0, tFinal-tInit}, {tt, tInit, tFinal}
                                   , MaxStepSize\rightarrow 0.25/\omega
                        &, 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]&
    GAInt
                          GA[#1] &
   GAdotAInt
                          GA[#1].A[#1]&
   AdotGAInt
                          A[#1].GA[#1]&
   GAIntInt
                          GAInt[#1, #2] &
   PScorrectionInt
                          GAdotAInt[#1, #2] + A[#1] .GAInt[#1, #2] - qGAInt[#1, #2] .GAdotAInt[#1, #
                         qGAInt[#1, #2]^{T}.GAInt[#1, #2] &
   GAIntdotGAIntInt
   constCorrectionInt (A[#1] - \frac{\alpha}{\alpha}GAdotAInt[#1, #2]). GAdotAInt[#1, #2] &
```

OptionValue VectorPotentialGradient = != None | | TrueQ integrateWithoutGradient,

```
(\star \left\{ \int_{t_0}^t A\left(\tau\right) d\tau, \int_{t_0}^t A\left(\tau\right)^2 d\tau, \int_{t_0}^t \nabla A\left(\tau\right) d\tau, \int_{t_0}^t \nabla A\left(\tau\right) d\tau, \int_{t_0}^t \nabla A\left(\tau\right) d\tau, \int_{t_0}^t A\left(\tau\right) \cdot \nabla A\left(\tau\right) d\tau, \int_{t_0}^t \nabla A\left(\tau\right) d\tau \right\} \right\} = (\star + 1)^{-1} \left\{ \int_{t_0}^t A\left(\tau\right) d\tau, \int_{t_0}^t A\left(\tau\right) d\tau, \int_{t_0}^t \nabla A\left(\tau\right) d\tau, \int_{t_0}^t \nabla A\left(\tau\right) d\tau, \int_{t_0}^t A\left(\tau\right) d\tau \right\} \right\} = (\star + 1)^{-1} \left\{ \int_{t_0}^t A\left(\tau\right) d\tau, \int_{t_0}^t A\left(\tau
                    \int_{t^{\cdot}}^{t} \int_{t^{\cdot}}^{\tau} \partial_{j} A_{k}(\tau') A_{k}(\tau') d\tau' + A_{k}(\tau) \int_{t^{\cdot}}^{\tau} \partial_{k} A_{j}(\tau') d\tau' - \int_{t^{\cdot}}^{\tau} \partial_{i} A_{j}(\tau') d\tau' \int_{t^{\cdot}}^{\tau} \partial_{i} A_{k}(\tau') A_{k}(\tau') d\tau' d\tau,   \int_{t^{\cdot}}^{t} \int_{t_{0}}^{t} \partial_{i} A_{j}(\tau') A_{j}(\tau') d\tau' \int_{t_{0}}^{t} \partial_{i} A_{k}(\tau') A_{k}(\tau') d\tau' d\tau, 
                   \int_{t^{+}}^{t}\left(A_{k}\left(\tau\right)-\frac{1}{2}\int_{t^{+}}^{\tau}\partial_{k}A_{i}\left(\tau^{+}\right)A_{i}\left(\tau^{+}\right)d\tau^{+}\right)\cdot\int_{t^{+}}^{\tau}\partial_{k}A_{j}\left(\tau^{+}\right)A_{j}\left(\tau^{+}\right)d\tau^{+}d\tau^{+}\};\star)
  (*Displaced momentum
 pi[p_, t_, tt_] := p+A[t] - GAInt[t, tt].p-GAdotAInt[t, tt];
  (*Quadratic coefficient in nondipole action*)
 \label{eq:QuadMatrix} \text{QuadMatrix[t\_, tt\_]} := \frac{\text{GAIntInt[t, tt]} + \text{GAIntInt[t, tt]}^\intercal}{2} - \frac{1}{2} \\ \text{GAIntdotGAIntInt[t, tt]};
  (*Stationary momentum
                                                                                                            and action*)
ps[t_{,}tt_{]}:=ps[t,tt]=\\ -\frac{1}{t-tt-i\epsilon}Inverse\Big[IdentityMatrix[Length[A[tInit]]]-\frac{1}{t-tt-i\epsilon}2QuadMatrix[t,tt]\Big].
 S[t_, tt_] := simplifier
                   \frac{1}{2}\left(\text{Total}\left[\text{ps}[t, tt]^{2}\right] + \kappa^{2}\right)\left(t - tt\right) + \text{ps}[t, tt].\text{AInt}[t, tt] + \frac{1}{2}\text{A2Int}[t, tt] - \left(\frac{1}{2}\right)
                                     ps[t, tt].QuadMatrix[t, tt].ps[t, tt]+
                                              ps[t, tt].PScorrectionInt[t, tt]+constCorrectionInt[t, tt]
           ];
prefactor[t_{-}, \tau_{-}] := i \left(\frac{2\pi}{\epsilon + i \tau}\right)^{3/2} dipoleRec[pi[ps[t, t-\tau], t, t-\tau], \kappa] \times
                    dipoleIon[pi[ps[t, t-\tau], t-\tau, t-\tau], \kappa].F[t-\tau];
 integrand[t_, \tau_] := prefactor[t, \tau] Exp[-iS[t, t-\tau]] gate[\omega \tau];
  (*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"], \tau = Symbol ["\tau"],
                                     \texttt{p} = \big\{ \texttt{Symbol} \ ["p1"], \ \texttt{Symbol} \ ["p2"], \ \texttt{Symbol} \ ["p3"] \big\} \big[\![1\,;; \ \texttt{Length} \big[ \texttt{A} \big[ \omega \, \texttt{tInit} \big] \big] \big]\!\big] \big\},
                             \{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, τ]}]],
      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;
      OptionValue RunInParallel === True, TableCommand = ParallelTable;
                     = Sum ;,
      SumCommand
      True, TableCommand = OptionValue[RunInParallel][1];
      SumCommand = OptionValue[RunInParallel][2];
    ];
    (*Numerical integration loop*)
    dipoleList=Table
         OptionValue ReportingFunction [
           \deltatintSum [(
                  integrand[t, τ]
                ), {τ, 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 EPToolbox package, which is located and better documented at https://github.com/episanty/EPToolbox, 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 rectancle 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, \infty\} \} \};
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,\infty).";
MessageGroups = Join[MessageGroups, {"FindComplexRoots "} {FindRoot::lstol}}]
Protect[Seeds];
Protect SeedGenerator;
Compiler :→ Compile::cpf, Compile::cpapot, Compile::cpbool, Compile::cpdsts,
      Compile::cpint, Compile::cpintlt, Compile::cpintlt2, Compile::cpiter,
      Compile::cplist, Compile::cpout, Compile::cppat, Compile::cpts,
      Compile::cptype, Compile::cret, Compile::nocomp, Compile::part, Compile::cxcoerce,
      Compile::realcoerce, CompiledFunction::cfex, CompiledFunction::cflist,
      CompiledFunction::cfn, CompiledFunction::cfnlts, CompiledFunction::orank,
      CompiledFunction::cfsa, CompiledFunction::cfse, CompiledFunction::cfta,
      CompiledFunction::cfte, CompiledFunction::cfsec, CompiledFunction::cftec},
  CompilerWarnings :→ {Compile::noinfo, CompiledFunction::npext,
      CompiledFunction::prng, CompiledFunction::pext, CompiledFunction::plrng,
      CompiledFunction::psbrng, CompiledFunction::prngd},
  Graphics:→ {General::plnr, General::pp3tr, General::pptr, General::pwfailed,
      General::nfunfail, Compiled::deprec, System`Dump`ContourPlot3D::njnum,
      System `Dump `ParametricPlot3D::njnum, System `Dump `Plot3D::njnum,
      System `Dump `RegionPlot3D::njnum, General::accbend, System `Dump `ContourPlot::accbend,
      System `Dump `ContourPlot3D::accbend, System `Dump `DensityPlot::accbend,
      LogLinearPlot::accbend, LogLogPlot::accbend, LogPlot::accbend,
      System `Dump `ParametricPlot::accbend, System `Dump `ParametricPlot3D::accbend,
      System `Dump `Plot::accbend, System `Dump `Plot3D::accbend,
      PolarPlot::accbend, System `Dump `RegionPlot3D::accbend },
  Obsolete:→ {General::obs, General::obspkg, General::newpkg},
  Packing:→ {General::unpack, General::punpack,
      General::punpack1, General::punpack1, General::punpack11},
  Spelling:→ {General::spell, General::spell1},
  Symbolics ⇒ {Integrate::gener, Maximize::nopmet, Minimize::nopmet, Series::esss},
  FindComplexRoots :→ {FindRoot::lstol}}
Begin["`Private`"];
FindComplexRoots [equations_List, domainSpecifiers__, ops:OptionsPattern[]]:=
  Block[{seeds, tolerances},
    If [! IntegerQ [Rationalize OptionValue Seeds]]] | OptionValue Seeds] \le 0,
```

```
If [!] (OptionValue Tolerance === Automatic || OptionValue Tolerance \ge 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::lstol]] /. {
         Hold[messageSequence___ ] :> Quiet[
              DeleteDuplicates
                Select|
                   Check
                          FindRoot[
                            , 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]] \le Re[
                                 [j, 1] \leq 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 } ] }
\label{eq:complexRoots} \ \left[ \texttt{e1}\_\texttt{==e2}\_, \left\{ \texttt{z}\_, \texttt{zmin}\_, \texttt{zmax}\_ \right. \right\}, \texttt{ops:OptionsPattern[]} \right] \texttt{:=}
  FindComplexRoots [{e1 == e2}, {z, zmin, zmax}, ops]
End[];
```

Message[FindComplexRoots ::seeds, OptionValue[Seeds]]];

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[randomsList ,
      pairsList[All, 1] + Complex @@@Times [
             ReIm [pairsList[All, 2]]-pairsList[All, 1]],
    ],
       \texttt{SeedRandom}^{\texttt{L}}[\texttt{Method} \rightarrow \{\texttt{"MKL", Method} \rightarrow \{\texttt{"Sobol", "Dimension"} \rightarrow 2 \texttt{Length}[\texttt{pairsList}]\}];
       SeedRandom [];
      RandomReal [{0, 1}, {number , Length[pairsList], 2}]
RandomSobolComplexes [{zmin_ ?NumericQ , zmax_ ?NumericQ }, number_ ] :=
  RandomSobolComplexes [\{\{zmin, zmax\}\}, number][All, 1]
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[randomsList ,
        pairsList[All, 1] + Complex @@@Times [
                ReIm [pairsList[All, 2]]-pairsList[All, 1]],
     BlockRandom
        SeedRandom
          \texttt{Method} \rightarrow \left\{ \texttt{"MKL", Method} \rightarrow \left\{ \texttt{"Niederreiter", "Dimension"} \rightarrow 2 \, \texttt{Length} \left[ \texttt{pairsList} \right] \right\} \right];
        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, gridPointBasisk},
      \texttt{sep} = \texttt{NestWhile} \Big[ \texttt{0.99 \# \&, Min} \Big[ \texttt{Flatten} \Big[ \texttt{ReIm} \; \Big[ \texttt{pairsList} \Big[ \texttt{All, 2} \Big] - \texttt{pairsList} \Big[ \texttt{All, 1} \Big] \Big] \Big] \Big] , 
          Times @@\frac{1}{0.99 \, \text{#}}Floor[Flatten[ReIm [pairsList[All, 2]]-pairsList[All, 1]]]], 0.99 #] \le \frac{1}{0.99 \ \text{#}}
     separationsList=Round [ 1 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[2j-1]+ik[2j], \{j, 1, Length[pairsList]\}],
          Evaluate [Sequence@@Table[{k[j],gridPointBasi[j]}], {j,1,2Length[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[\Omega,S,{tmin ,tmax },{tmin ,tmax }] finds a list of solutions {t,\tau}
                           of the HHG temporal saddle-point equations at harmonic energy \Omega
                           for action S, in the range {tmin, tmax} of recombination time and
                           \{tmin , tmax \} of excursion time , where both ranges should be the
                           lower-left and upper-right corners of rectangles in the complex plane.
GetSaddlePoints[\OmegaRange,S,{tmin ,tmax },{tmin ,tmax }] finds solutions of
                           the HHG temporal saddle-point equations for a range of harmonic
                           energies \Omega Range, and returns an Association with each harmonic
                           energy \Omega indexing a list of saddle-point solution pairs \{t, \tau\}.
GetSaddlePoints[Ωspec,S,{{{tmin 1,tmax 1}},{tmin 1,tmax 1}},{{tmin 2,tmax 2},{tmin 2,tmax 2}},
                           ...}] uses multiple time domains and combines the solutions.
\texttt{GetSaddlePoints}[\Omega \texttt{spec,S,} \{\{\texttt{urange,vrange}\}, ...\}, \texttt{IndependentVariables} \{\texttt{u,v}\}] \text{ uses the explicit } \{\texttt{u,v}\} = \texttt{u,v} = 
                           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 \"t\" resp.";
SortingFunction: usage = "SortingFunction is an option of GetSaddlePoints
                           which sets a function f, to be used as f[t,\tau,S,\Omega]\,, 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,\tau,S,\Omega],
                           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 \"\tau\", respectively), to be used in solving the
                    saddle-point equations, and which range over the given regions.";
FiniteDifference:usage =
          "FiniteDifferenceis 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 \rightarrow (#2 \&), SelectionFunction \rightarrow (True \&), IndependentVariables \rightarrow (#2 \&),
                          {"RecombinationTime ", "ExcursionTime"}}, Options[FindComplexRoots ]];
Protect SortingFunction, SelectionFunction, IndependentVariables, FiniteDifference;
\texttt{GetSaddlePoints}[\Omega \texttt{spec}\_, \texttt{S}\_, \{\texttt{tmin}\_, \texttt{tmax}\_\}, \{\texttt{tmin}\_, \texttt{tmax}\_\}, \texttt{options:OptionsPattern}[]] :=
     GetSaddlePoints Ωspec, S, {{{tmin , tmax }, {τmin , τmax }}}, options
GetSaddlePoints[\Omega_{,}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"→"t", "IonizationTime"→"tt"};
          depVar = First[DeleteCases[{"t", "t", "tt"}, Alternatives@@indVars]];
          depVarRule = depVar / . \{"tt" \rightarrow \{tt \rightarrow t-\tau\}, "t" \rightarrow \{t \rightarrow tt+\tau\}, "\tau" \rightarrow \{\tau \rightarrow t-tt\}\};
          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
                    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 \rightarrow RandomSobolComplexes
                                                                  , Seeds \rightarrow 50
                                                             ]/. \{\{\} \rightarrow (\{t, \tau\} /. depVarRule) \rightarrow \{\}\})\}
                                                        (*to deal with empty results*)
                                        , Message [GetSaddlePoints::error, Ω]; roots
                                    , Function timesPair,
```

```
OptionValue[SelectionFunction [timesPair [1], timesPair [2], S, \Omega]
                   , {range, timeRanges } ], 1
             , Function[{timesPair1, timesPair2},
                And@@Thread[Abs[timesPair1 - timesPair2] < tolerances] ]</pre>
           , 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, Ω]]
        1
   GetSaddlePoints[ΩRange_List, S_, timeRanges_ , options: OptionsPattern[]]:=
     Association Parallel Table
          \Omega \rightarrow \text{GetSaddlePoints}[\Omega, S, \text{timeRanges , options}]
           , \{\Omega, Sort[\Omega Range]\}
   End[];
GetSaddlesFromSeeds
   GetSaddlesFromSeeds ::usage =
        "GetSaddlesFromSeeds [\{\{t_1, \tau_1\}, \{t_2, \tau_2\}, ...\}, \Omega, S] finds a list of solutions \{t, \tau\}
             of the HHG temporal saddle-point equations at harmonic energy
             \Omega for action S, using the given \{t_i,\tau_i\} as seeds for the process.
   \texttt{GetSaddlesFromSeeds} \ \ [ < |\Omega_1 \rightarrow \{ \{t_{11}, \tau_{11}\}, \{t_{12}, \tau_{12}\}, \ldots \}, \Omega_2 \rightarrow \{ \{t_{21}, \tau_{21}\}, \{t_{22}, \tau_{22}\}, \ldots \}, \ldots | >, \Omega, S ] \}
             finds solutions of the HHG temporal saddle-point equations,
             using the seeds list from the \Omega_{\rm i} that's closest to
             \Omega, or as specified by the value of KeyChooserFunction.
   GetSaddlesFromSeeds [seeds, \{\Omega_1, \Omega_2, ...\}, 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,...\},\Omega], should return the indices \{\Omega_i,\Omega_j,...\}
             corresponding to the seed sets \{\{\{t_{i1},\tau_{i1}\},...\},\{\{t_{j1},\tau_{j1}\},...\}\}
             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 \Omega 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 Ω=`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] =
        \label{localculateRoots} \mbox{\it Join} \left[ \left\{ \mbox{\it RecalculateRoots} \rightarrow \mbox{\it False}, \mbox{\it SeedsChooserFunction} \rightarrow \mbox{\it Nearest} \right\}, \mbox{\it Options} \left[ \mbox{\it GetSaddlePoints} \right] \right];
```

```
Protect[SeedsChooserFunction, RecalculateRoots];
GetSaddlesFromSeeds [seedsSpec_, \OmegaRange_List, S_, options: OptionsPattern[]] :=
         Association Parallel Table
                             \Omega \rightarrow \text{GetSaddlesFromSeeds} \text{ [seedsSpec, } \Omega, \text{ S, options]}
                             , \{\Omega, Sort[\Omega Range]\}
\texttt{GetSaddlesFromSeeds} \ \left[ \texttt{seedsAssociation\_Association} \Omega\_\texttt{,} \ \texttt{S\_,} \ \texttt{options:OptionsPattern[]} \right] := \texttt{SeedsAssociation\_Association} \cap \texttt{Sociation\_Association} \cap \texttt{Sociat
         \label{eq:with_section} 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], Ω, S, options
          1
\texttt{GetSaddlesFromSeeds} \ \left[ \texttt{seedsList\_List}, \ \Omega\_? \texttt{NumberQ} \ , \ S\_, \texttt{options:OptionsPattern[]} \right] := \texttt{Block} \left[ \texttt{seedsList\_List}, \ \Omega\_? \texttt{NumberQ} \right] := \texttt{Block} \left[ \texttt{seedsList\_List}, \ \Omega\_? \texttt{seedsList\_List} \right] := \texttt{Block} \left[ \texttt{seeds
                    {equations, roots, t = Symbol ["t"], tt = Symbol ["tt"],
                             τ = Symbol ["τ"], indVars, depVar, depVarRule, fullSeedVars, tolerances},
                    indVars = OptionValue IndependentVariables /.
                                      {"RecombinationTime "→"t", "ExcursionTime"→"t", "IonizationTime"→"tt"};
                   depVar = First[DeleteCases [{"t", "τ", "tt"}, Alternatives@@indVars]];
                   \texttt{depVarRule} = \texttt{depVar} \, / \, \{ \texttt{"tt"} \rightarrow \{\texttt{tt} \rightarrow \texttt{t-\tau} \}, \, \texttt{"t"} \rightarrow \{\texttt{t} \rightarrow \texttt{tt+\tau} \}, \, \texttt{"t"} \rightarrow \{\texttt{t} \rightarrow \texttt{t-tt} \} \};
                   \texttt{fullSeedVars} \big[ \texttt{seed}_{\_} \big] := \langle \big| \texttt{"t"} \rightarrow \texttt{seed} [\![1]\!], \texttt{"t"} \rightarrow \texttt{seed} [\![2]\!], \texttt{"tt"} \rightarrow \texttt{seed} [\![1]\!] - \texttt{seed} [\![2]\!] \big| \rangle;
                   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)
                                                                                                         /. \{ \{ \} \rightarrow (\{t, \tau\} /. depVarRule) \rightarrow \{ \} ) \} )
                                                                   , Message [GetSaddlesFromSeeds :: error, \Omega]; roots
                                                         , {seed, seedsList}]
                                                , Function timesPair,
                                                        OptionValue[SelectionFunction [timesPair [1], timesPair [2], S, Ω]]
                                       , Function[{timesPair1, timesPair2},
                                               And@@Thread[Abs[timesPair1 - timesPair2] < tolerances] ]
```

```
, If[
             ListQ[OptionValue[SortingFunction]],
              Table \big[ Function \big[ \texttt{timesPair} \;, \; f \big[ \texttt{timesPair} \; [\![1]\!] \;, \; \texttt{timesPair} \; [\![2]\!] \;, \; S, \; \Omega \big] \big] \;, 
                {f, OptionValue[SortingFunction]}],
             Function [timesPair, OptionValue SortingFunction [timesPair [1], timesPair [2], S, Ω]]
   End[];
ClassifyQuantumOrbits
   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}\}, ...\} \rangle using a function f,
             which should turn f[t,\tau,\Omega] into an appropriate label, and returns an
             association of the form \langle | \text{label}_1 \rightarrow \langle | \Omega_1 \rightarrow \langle | 1 \rightarrow \{t, \tau\}, 2 \rightarrow \{t, \tau\}, ... | \rangle, ... | \rangle.
   ClassifyQuantumOrbits [saddlePoints, f, sortFunction] uses
              the function sortFunction to sort the sets of saddle points
              \{\{t_{11}, t_{11}\}, \{t_{12}, t_{12}\}, ...\} for each label and harmonic energy.
   ClassifyQuantumOrbits [saddlePoints, f, sortFunction, DiscardedLabels→{label<sub>1</sub>, label<sub>2</sub>,...}]
              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→ {}};
   Protect[DiscardedLabels];
   ClassifyQuantumOrbits [saddlePointList,
        classifierFunction, sortingFunction_:Sort, OptionsPattern[]]:=Map[
        Composition [
          Association,
          MapIndexed[#2[1]] \rightarrow #1 &],
           sortingFunction
        ],
        Delete[
           AssociationTranspose
             MapIndexed
                   GroupBy[classifierFunction@# &][
                        Flatten/@Transpose[\{#1, ConstantArray[#2[{1}, 1], Length[#1]]\}] &
                   , saddlePointList All, All, {1, 2}
```

, List/@OptionValue[DiscardedLabels]]

, {2}]

End[];

ReperiodSaddles

```
ClearAll | ReperiodSaddles |
ReperiodSaddles::usage =
         "ReperiodSaddles[\{\{t_1,\tau_1\},\{t_2,\tau_2\},...\},f] readjusts the assigned cycle of
                  the saddle points \{t_i, t_i\}, returning the list \{\{t_1+f[t_1, t_1], t_1\}, ...\}.
\texttt{ReperiodSaddles}[\, \langle |\, \Omega_1 \! \rightarrow \! \{ \{t_{11}, \tau_{11}\}, \ldots \}, \Omega_2 \! \rightarrow \! \ldots | \rangle, \texttt{f} ] \text{ reperiods}
                  saddle-point pairs in a harmonic -energy-indexed association
\texttt{ReperiodSaddles}[ < | \texttt{label}_1 \rightarrow < | \Omega_1 \rightarrow \{ \{t_{11}, \tau_{11}\}, \ldots \}, \ldots | >, \ldots | >, f ] \text{ reperiods}
                  saddle-point pairs of a classified set of saddle points.";
Begin["`Private`"];
 \begin{split} & \texttt{ReperiodSaddles}[\texttt{pair}\_/; \texttt{Depth}[\texttt{pair}] == 2, \texttt{f}\_] := \{\texttt{pair}[\![1]\!] + \texttt{f}[\texttt{pair}[\![1]\!], \texttt{pair}[\![2]\!]], \texttt{pair}[\![2]\!]\} \\ & \texttt{ReperiodSaddles}[\texttt{association}\_, \texttt{f}\_] := \texttt{Apply}[\texttt{f}, \texttt{association}, \{\texttt{Depth}[\texttt{association}] - 2\}] \end{split}
End[];
```

HessianRoot

```
 \text{HessianRoot::usage = "HessianRoot[S,t,\tau] calculates the Hessian root } \sqrt{\frac{(2\pi)^2}{\dot{\mathtt{i}}^2 \operatorname{Det}\left[\partial_{\{\mathtt{t},\mathtt{tt}\}}^2 S\right]}} \;."; 
Begin["`Private`"];
HessianRoot[S_{,t_{,\tau_{,l}}}] := \sqrt{\frac{2\pi}{iDerivative[0,2][S][t,t-\tau]}}
       \sqrt{(2\pi \text{Derivative}[0,2][S][t,t-\tau])/(i(\text{Derivative}[2,0][S][t,t-\tau])}
                                    Derivative[0, 2][S][t, t-\tau]-Derivative[1, 1][S][t, t-\tau]<sup>2</sup>)))
End[];
```

FindStokesTransitions

```
FindStokesTransitions:usage =
     "FindStokesTransition \S S, <|\Omega_1 \rightarrow <|1 \rightarrow \{t_{11}, \tau_{11}\}, 2 \rightarrow \{t_{12}, \tau_{12}\}|>, \Omega_2 \rightarrow <|1 \rightarrow \{t_{21}, \tau_{21}\}, 2 \rightarrow \{t_{22}, \tau_{22}\}|>, \ldots|>
          ] finds the set \{\{\Omega_{\text{S}}\},\{\Omega_{\text{AS}}\},n\} of the Stokes and
          anti-Stokes transition energies for the given set of saddle points,
          where Re(S) changes sign after the \Omega_S and Im (S) changes sign after
          the \Omega_{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 \Omega_i in the given keys).
FindStokesTransition\SS, \langle | \text{label}_1 \rightarrow \langle | \Omega_1 \rightarrow ... | \rangle | \rangle | finds the Stokes transitions for the given set
          of saddle-point curve pairs, and returns them labeled with the labeli.";
FindStokesTransitions:saddleno = "FindStokesTransitionscalled 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 = "FindStokesTransitionsfound multiple
          Stokes transitions using `1` to return a single transition";
FindStokesTransitions:multipleAS = "FindStokesTransitionsfound multiple
          anti-Stokes transitions using `1` to return a single transition";
ChooserFunction::usage = "ChooserFunction is an option for FindStokesTransitionsthat
          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 = "ReperiodingFunctionis an option for FindStokesTransitions
                        SPAdipole and UAdipole which specifies a function f[t, \tau] of recombination
                        time t and excursion time t that will be used to re-period the
                       pairs \{t,\tau\} into the form \{t+f[t,\tau],\tau\}. The default is Function[0],
                       but if pairs are split it can be useful to set ReperiodingFunctionto
                       Function[\{t,\tau\}, Floor[-\text{Re}[t-\tau], \frac{2\pi}{}]] for \omega 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, \tau}, 0], ChooserFunction Automatic };
FindStokesTransition$S_,
            deeperAssociation_/; Depth [deeperAssociation] == 5, options: OptionsPattern[]] := Map[
            FindStokesTransition $5, #, options &,
            deeperAssociation
FindStokesTransition$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 | ,
                             \texttt{MapIndexed} \left[ (*\texttt{reduces each } \Omega \rightarrow <|1 \rightarrow \{t_1, \tau_1\}, 2 \rightarrow \{t_2, \tau_2\}| > \texttt{to } \Omega \rightarrow <|1 \rightarrow S_1, 2 \rightarrow S_2| > \star) \right]
                                   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=SignTimes
                             Rest[actionList],
                             AssociationThreadRest[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]];
                     \texttt{processor} \big[ \texttt{Keys} \big[ \texttt{Select} \big[ \texttt{signsList}, \#[\![1]\!] < 0 \& \big] \big] /. \\ \big\{ \{ \} \rightarrow \big\{ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\    \texttt{processor} \big[ \texttt{Keys} \big[ \texttt{Select} \big[ \texttt{signsList}, \#[\![2]\!] < 0 \& \big] \big] /. \\ \big\{ \{ \} \rightarrow \big\{ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\    \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\    \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\    \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\    \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\    \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\    \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\   \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\   \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{"No transition"} \big] \big\} \big\} \big], \\   \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big] \big], \\  \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big] \big], \\  \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big] \big], \\  \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big] \big], \\  \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\  \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\  \texttt{processor} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\  \texttt{missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big[ \texttt{Missind} \big] \big], \\ \\ \texttt{Missind} \big[ \texttt{Missind} \big] \big[ \texttt{Missind} \big[ \texttt{Missind} \big], \\ \\ \texttt{Missind} \big[ \texttt{Mi
                  Sign[Last[actionList][2]] /. \{1 \rightarrow 2, -1 \rightarrow 1\}
      1
```

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, \langle |1 \rightarrow \{t_1, \tau_1\}, 2 \rightarrow \{t_2, \tau_2\}, ... | \rangle]
                    returns the total harmonic -dipole contribution in the
                    saddle-point approximation from the specified saddle points.
SPAdipole[S,prefactor,\Omega,\langle 1\rightarrow \{t_1,\tau_1\},2\rightarrow \{t_2,\tau_2\}]\rangle, 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]};
Block \{tr = t + Option Value | Reperioding Function [t, \tau] \},
          \texttt{HessianRoot[S, tr, }\tau]\texttt{ prefactor[tr, tr-}\tau]\texttt{ Exp[-iS[tr, tr-}\tau]+i\Omega tr]}
SPAdipole[S_{n}, prefactor_{n}, \Omega_{n}, times_{n}, association, options: OptionsPattern[]] := Block[\{\}, association, options option option options option 
          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, Ω, times ]];
          If [Length[times] \neq 2, Message [SPAdipole: wrongno, Length[times], <math>\Omega];
               Return [SPAdipole[S, prefactor, \Omega, times, options]]];
          If [\Omega < \text{transition}[2]],
               SPAdipole[S, prefactor, \Omega, times, options],
               SPAdipole S, prefactor, Ω, KeySelect [times , # == transition[3] &], options
End[];
```

UAdipole

```
UAdipole::usage =
      "UAdipole[S,prefactor,\Omega, \langle |1 \rightarrow \{t_1, \tau_1\}, 2 \rightarrow \{t_2, \tau_2\}, ... | \rangle, transition returns the total
            harmonic -dipole contribution in the uniform approximation from the
            specified saddle points, using the action S[t,t-\tau]-\Omega t and prefactor[t,t-\tau],
            and taking the given Stokes transition set as a reference.";
UAdipole::saddleno = "UAdipole called with `1` time pairs at \Omega= `2`.
            Reverting to the saddle-point approximation for this set.";
UAdipole::invldtrns = "UAdipole called with invalidStokes transition set `1`.
            Reverting to the saddle-point approximation for this set.";
Begin["`Private`"];
Options[UAdipole] = {ReperiodingFunction} Function[\{t, \tau\}, 0]};
VAdipole[S_{,prefactor_{,\Omega_{,times_{,transition_{,toptions: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, \Omega, times]]];
      Block
         {A1, A2, S1, S2, Ss, Sm , z,
            t1 = times [1] [1] + Option Value Reperioding Function [times [1] [1], times [1] [2]],
            \tau 1 = times [1][2],
            t2 = times [2] [1] + OptionValue Reperioding Function (times [2] [1], times [2] [2] ),
            \tau 2 = \text{times } [2][2],
         A1 = HessianRoot[S, t1, \tau1] prefactor[t1, t1 - \tau1];
         S1 = S[t1, t1 - \tau 1] - \Omega t1;
         A2 = HessianRoot[S, t2, \tau2] prefactor[t2, t2 - \tau2];
         S2 = S[t2, t2 - \tau2] - \Omega t2;
         Ss = \frac{S1 + S2}{2}; Sm = \frac{S1 - S2}{2};
         If \left[\Omega < \text{transition}[2]\right], z = \left(-\frac{3}{2}Sm\right)^{2/3},
            \mathbf{z} = \left(-\frac{3}{2}\operatorname{Sm}\right)^{2/3}\operatorname{Exp}\left[\operatorname{i}\left(\operatorname{transition}[3]\right]/.\left\{2 \to -1, 1 \to 1\right\}\right)\frac{2\pi}{3}\right];
         \sqrt{6\pi \text{Sm}} \operatorname{Exp}\left[-i \operatorname{Ss} + i \frac{\pi}{4}\right] \left(\frac{\operatorname{A1} - i \operatorname{A2}}{2} \frac{\operatorname{AiryAi}[-z]}{\sqrt{z}} + i \frac{\operatorname{A1} + i \operatorname{A2}}{2} \frac{\operatorname{AiryAi'}[-z]}{z}\right)
End[];
```

Package closure

End of package

EndPackage[];

Add to distributed contexts.

DistributeDefinition[s'RBSFA`"];