ARMSupport

This file provides supporting functions for Analytical *R*-Matrix calculations.

Version history

1.0.0	Initial set-up – pulling functions from a nebulous cloud of files.
1.0.1	- Made error handling on coulombCorrection more flexible by allowing for customized ReportingFunction. - Fixed options handling on coulombCorrection (gave an error if no option was given).
1.0.2	Added v2Tolerance as an option for closestApproachTimesPath.
1.0.3	Fixed classicalClosestApproach - it gave wrong times for some reason.
1.0.4	Added new exception to path chooser - turning point on $-\pi/2 < \mathrm{Re}(\omega t) < \pi/2$ to help avoid $\mathrm{Re}\left(\boldsymbol{r}_{\mathrm{cl}}(t)^2\right) < 0$ regions.
1.0.5	Added rlnit support to trajectory functions.
1.0.6	Added non-standard t_s support to trajectory functions (i.e. forcets).
1.0.7	Added package export functionality.
1.0.8	Sealed off implementations inside `Private` contexts.

General functions

Sundry initialization

```
BeginPackage["ARMSupport`", {"EPToolbox`"}]
```

```
ARMSupport`
```

```
stdpars = {0.05, 0.055, 1.007};
```

```
r0 = {0, 0, 0};
```

This needs to be run before any parallel evaluation:

```
ParallelEvaluate[Needs["EPToolbox`",
      "/home /episanty/Work/CQD/Project/Code/EPToolbox/EPToolbox/EPToolbox.m "]];
```

t_s and relatives

```
ts::usage = "ts[{po, py, pp}, {F, ω, κ}] Returns the saddle point tₛ directly.

ts[pp, κ, ω, F, po, py] Returns the saddle point tₛ directly.";
t0::usage = "t0[{po, py, pp}, {F, ω, κ}] Returns t₀=Re[tₛ] directly.

t0[pp, κ, ω, F, po, py] Returns t₀=Re[tₛ] directly.";
τ::usage = "τ[{po, py, pp}, {F, ω, κ}] Returns τ_T=Im [tₛ] directly.

τ[pp, κ, ω, F, po, py] Returns τ_T=Im [tₛ] directly.";
tκ::usage =
    "tκ[{po, py, pp}, {F, ω, κ}] Returns the starting point t_κ directly.

tκ[pp, κ, ω, F, po, py] Returns the starting point t_κ directly.";
Begin["`Private`"]
```

$$\texttt{ts[pp\_, κ\_, ω\_, F\_, po\_, py\_]} := \frac{1}{\omega}\texttt{ArcSin}\left[\frac{\omega}{F}\texttt{pp} + i\frac{\omega}{F}\sqrt{\kappa^2 + \texttt{po}^2 + \texttt{py}^2}\right]$$

```
ts[{po_, py_, pp_}, {F_, ω_, κ_}] := ts[pp, κ, ω, F, po, py]

t0[{po_, py_, pp_}, {F_, ω_, κ_}] := Re[ts[pp, κ, ω, F, po, py]]
t0[pp_, κ_, ω_, F_, po_, py_] := Re[ts[pp, κ, ω, F, po, py]]

τ[{po_, py_, pp_}, {F_, ω_, κ_}] := Im [ts[pp, κ, ω, F, po, py]]
τ[pp_, κ_, ω_, F_, po_, py_] := Im [ts[pp, κ, ω, F, po, py]]
```

$$\texttt{tκ[pp\_, κ\_, ω\_, F\_, po\_, py\_]} := \texttt{ts[pp, κ, ω, F, po, py]} - i/\kappa^2$$

```
tκ[{po_, py_, pp_}, {F_, ω_, κ_}] := tκ[pp, κ, ω, F, po, py]
End[]
```

Transition times and momenta

Classical transition times are those times t_r for which a classical orbit has a recollision at zero velocity: $\boldsymbol{v}(t_r) = 0$ and $\mathrm{Re}\left[\int_{t_\kappa}^{t_r} \boldsymbol{p} + \boldsymbol{A}(\tau)\, d\tau\right] = 0$.

Classical transitions times and momenta

getClassical Transition returns exact numerical solutions.

getClassicalTransition

```
getClassicalTransition::usage =
    "getClassicalTransition[n, {F, ω, κ}] Returns pz and tr
        in atomic  units as a list of replacement  rules.
getClassicalTransition[range, {F, ω, κ}]
getClassicalTransition[n, F, ω, κ]";
```

```
Begin["`Private`"]
getClassicalTransition[n_, {F_, ω_, κ_}] := getClassicalTransition[n, F, ω, κ]
getClassicalTransition[range_List, {F_, ω_, κ_}] :=
  (getClassicalTransition[#, {F, ω, κ}] & /@range)
getClassicalTransition[n_, F_, ω_, κ_] := Module[{getTimes , t00, zinit},
    getTimes [pz_] := ({t0 → Re[#], τ → Im [#]} & [1/ω ArcSin[ω/F (pz + ⅈ κ)]]);
    t00[pz_?NumericQ ] := (t0 /. getTimes [pz]);
    zinit[pz_?NumericQ ] :=
      Re[F/ω^2 (Cos[ω t0] - Cos[ω (t0 + ⅈ τ - ⅈ/κ^2)]) /. getTimes [pz]];
    FindRoot[
      {pz (tr - t00[pz]) + F/ω^2 (Cos[ω tr] - Cos[ω t00[pz]]) + zinit[pz] == 0,
        pz - F/ω Sin[ω tr] == 0}
      , {{pz, 0}, {tr, (n + 1) π/ω}}
    ]
  ]
End[]
```

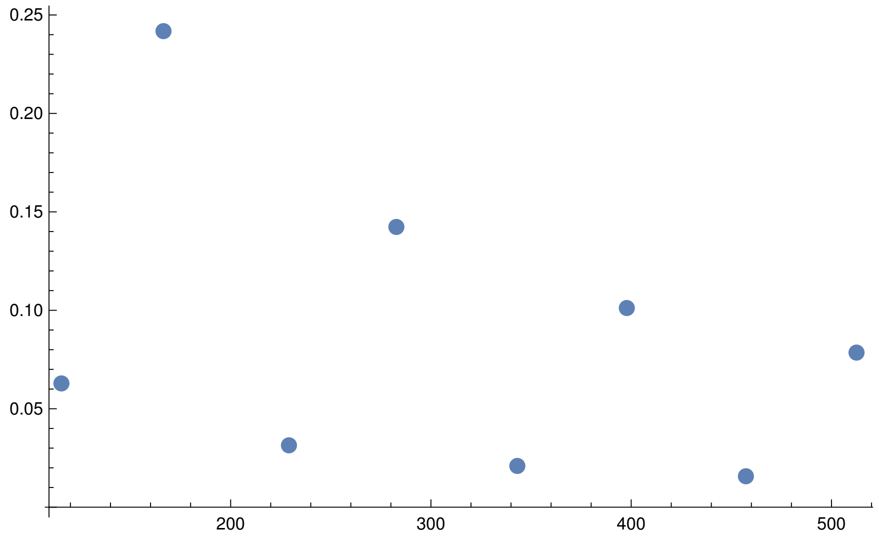
```
getClassicalTransition[Range[8], stdpars]
```

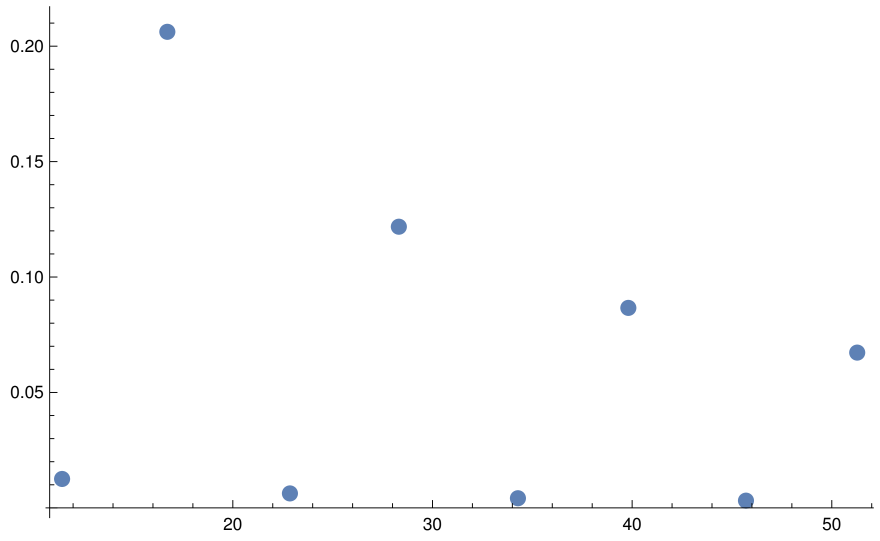
```
{{pz → 0.062865, tr → 115.498}, {pz → 0.241791, tr → 166.465},
  {pz → 0.0314275, tr → 229.108}, {pz → 0.142337, tr → 282.741},
  {pz → 0.0209511, tr → 343.138}, {pz → 0.101158, tr → 397.812},
  {pz → 0.0157131, tr → 457.273}, {pz → 0.0785167, tr → 512.507}}
```

Benchmarking

Momentum against time.

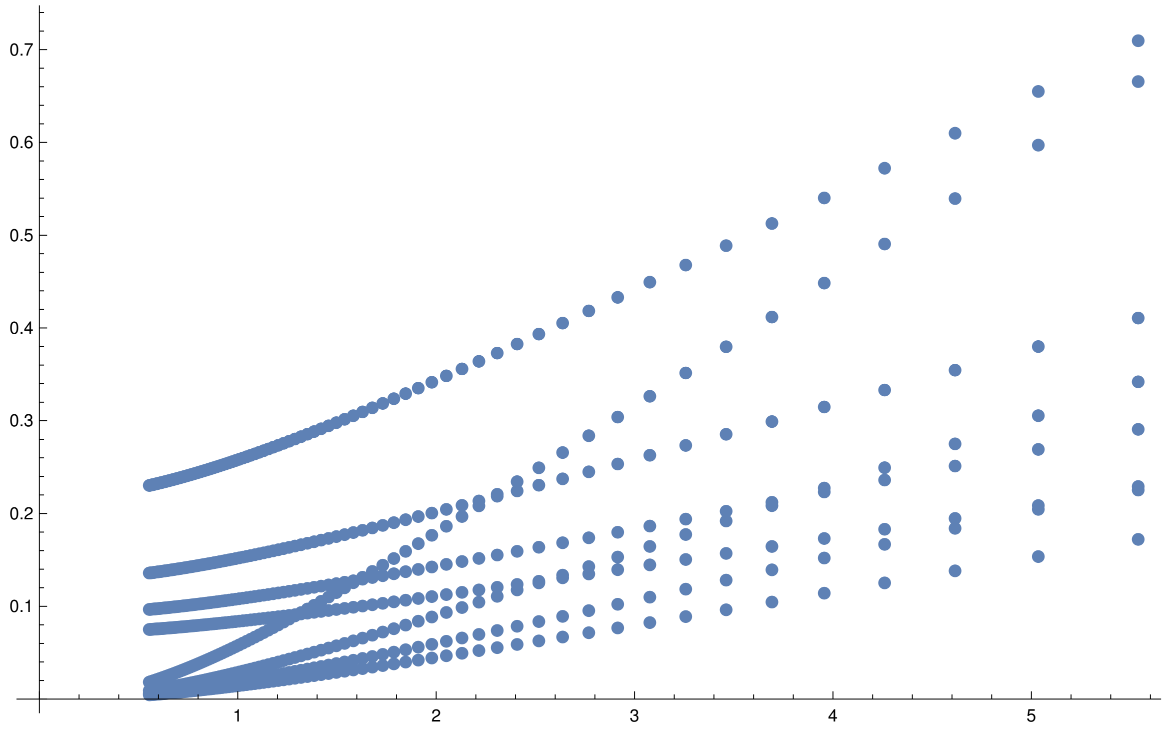
```
Row[{
    ListPlot[{tr, pz} /. getClassicalTransition[Range[8], {0.05, 0.055, 1.007}],
      ImageSize → 450],
    ListPlot[{tr, pz} /. getClassicalTransition[Range[8], {10 × 0.05, 10 × 0.055, 1.007}],
      ImageSize → 450]
  }]
```





Normalized momentum against γ.

```
ListPlot[
  Flatten[Table[
      Block[{ω = 0.055, κ = 1.007},
        {ωκ/F, ωpz/F} /. getClassicalTransition[Range[8], {F, ω, κ}]
      ]
      , {F, 0.01, 0.1, 0.001}], 1]
  , ImageSize → 600
]
```



Sandbox

You’re probably here to calculate classical transitions for some given parameters. Have a go.

```
pz /. getClassicalTransition[Range[4], {0.05, 45.6/3100, 1.07}]
```

```
{0.0240298, 0.755595, 0.0120147, 0.446211}
```

```
27.2 pz^2/2 /. getClassicalTransition[Range[4], {0.05, 45.6/3100, 1.07}]
```

```
{0.00785306, 7.76456, 0.0019632, 2.70781}
```

Linearized solutions.

These functions return classical transition times which have been linearized to first order in ***p***, i.e.

$p_z = \frac{F}{\omega}\frac{(-1)^n+\sqrt{1+\gamma^2}}{(n+1)\,\pi}$. The reduced results return $\frac{\omega}{F}\,\boldsymbol{p}$.

getLinearizedTransition

```
getLinearizedTransition::usage =
   "getLinearizedTransition[n, {F, ω, κ}] Returns pz and
      tr in atomic  units as a list of replacement  rules.
getLinearizedTransition[range, {F, ω, κ}]
getLinearizedTransition[n, F, ω, κ]";
```

```
Begin["`Private`"]
getLinearizedTransition[n_, {F_, ω_, κ_}] := getClassicalTransition[n, F, ω, κ]
getLinearizedTransition[range_List, {F_, ω_, κ_}] :=
  (getClassicalTransition[#, {F, ω, κ}] & /@range)
getLinearizedTransition[n_, F_, ω_, κ_] := {pz → F/ω getReducedLinearizedTransition[n, ωκ/F],
   tr → 1/ω ((n+1) π + ArcSin[getReducedLinearizedTransition[n, ωκ/F]])}
End[]
```

getReducedLinearizedTransition

```
getReducedLinearizedTransition::usage =
   "getReducedLinearizedTransition[n, {F, ω, κ}] Returns ωpz/F directly.
getReducedLinearizedTransition[range, {F, ω, κ}]
getReducedLinearizedTransition[n, F, ω, κ]";
```

```
Begin["`Private`"]
getReducedLinearizedTransition[range_List, γ_] :=
  (getReducedLinearizedTransition[#, γ] & /@range)
getReducedLinearizedTransition[n_, γ_] := ((-1)^n + Sqrt[1 + γ^2]) / (π (n+1))
End[]
```

Full transitions. getFullLinearizedTransition and getFullReducedLinearizedTransition.

i.e. without neglecting terms in ω/κ^2.

```
getFullLinearizedTransition::usage =
   "getFullLinearizedTransition[n, {F, ω, κ}] Returns pz and
      tr in atomic units as a list of replacement rules,
      for the linearized case without neglecting ω/κ^2.
getFullLinearizedTransition[range, {F, ω, κ}]
getFullLinearizedTransition[n, F, ω, κ]";
getFullReducedLinearizedTransition::usage =
   "getFullReducedLinearizedTransition[n, {F, ω, κ}] Returns ωpz/F directly.
getFullReducedLinearizedTransition[range, {F, ω, κ}]
getFullReducedLinearizedTransition[n, F, ω, κ]";

Begin["`Private`"]
getFullLinearizedTransition[n_, {F_, ω_, κ_}] :=
  getFullLinearizedTransition[n, F, ω, κ]
getFullLinearizedTransition[range_List, {F_, ω_, κ_}] :=
  (getFullLinearizedTransition[#, {F, ω, κ}] & /@range)
getFullLinearizedTransition[n_, F_, ω_, κ_] :=
```

$$\left\{pz \to \frac{F}{\omega}\text{getFullReducedLinearizedTransition}\left[n, \frac{\omega\kappa}{F}\right],\ tr \to \frac{1}{\omega}\left((n+1)\,\pi + \text{ArcSin}\left[\text{getReducedLinearizedTransition}\left[n, \frac{\omega\kappa}{F}\right]\right]\right)\right\}$$

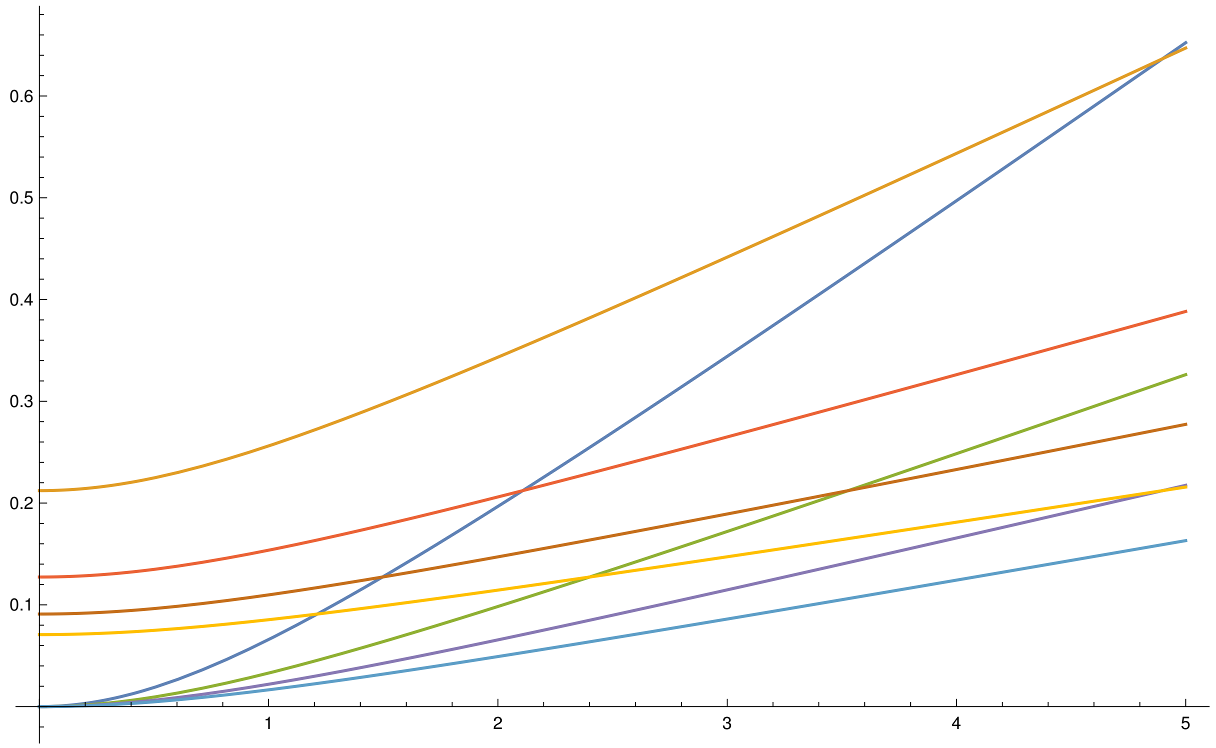
```
getFullReducedLinearizedTransition[range_List, F_, ω_, κ_] :=
  (getFullReducedLinearizedTransition[#, F, ω, κ] & /@range)
getFullReducedLinearizedTransition[n_, F_, ω_, κ_] :=
```

$$\frac{(-1)^n + \sqrt{1 + \left(\frac{\omega\kappa}{F}\right)^2}\ \text{Cosh}\left[\frac{\omega}{\kappa^2}\right] - \frac{\omega\kappa}{F}\text{Sinh}\left[\frac{\omega}{\kappa^2}\right]}{(n+1)\,\pi}$$

```
End[]
```

Benchmarking

```
Plot[Evaluate@getReducedLinearizedTransition[Range[8], γ], {γ, 0, 5}]
```



Complex-momentum solutions.

Complex-momentum solutions return complex times and momenta which are solutions to the complex equations $\boldsymbol{v}(t_r)=0$ and $\int_{t_\kappa}^{t_r}\boldsymbol{p}+\boldsymbol{A}(\tau)\,d\tau=0$.

getComplexTransition

```
getComplexTransition::usage =
    "getComplexTransition[n, {F, ω, κ}] Returns pz and tr
        in atomic units as a list of replacement rules.
getComplexTransition[range, {F, ω, κ}]
getComplexTransition[n, F, ω, κ]";
```

```
Begin["`Private`"]
getComplexTransition [n_, {F_, ω_, κ_}] := getComplexTransition [n, F, ω, κ]
getComplexTransition [range_List, {F_, ω_, κ_}] :=
  (getComplexTransition [#, {F, ω, κ}] & /@range)
getComplexTransition [n_, F_, ω_, κ_] := Module[{tκκ},
    tκκ[pz_] := ts[pz, κ, ω, F, 0, 0] - i/κ^2;
    FindRoot[
```

$$\frac{\omega pz}{F}\left((n+1)\,\pi+\mathrm{ArcSin}\left[\frac{\omega pz}{F}\right]-\omega\, t\kappa\kappa[pz]\right)+(-1)^{n+1}\sqrt{1-\left(\frac{\omega pz}{F}\right)^{2}}-\mathrm{Cos}[\omega\, t\kappa\kappa[pz]]==0$$

```
      , {pz, 0.0}]
  ]
End[]
```

```
getComplexTransition [Range[2], stdpars]
```

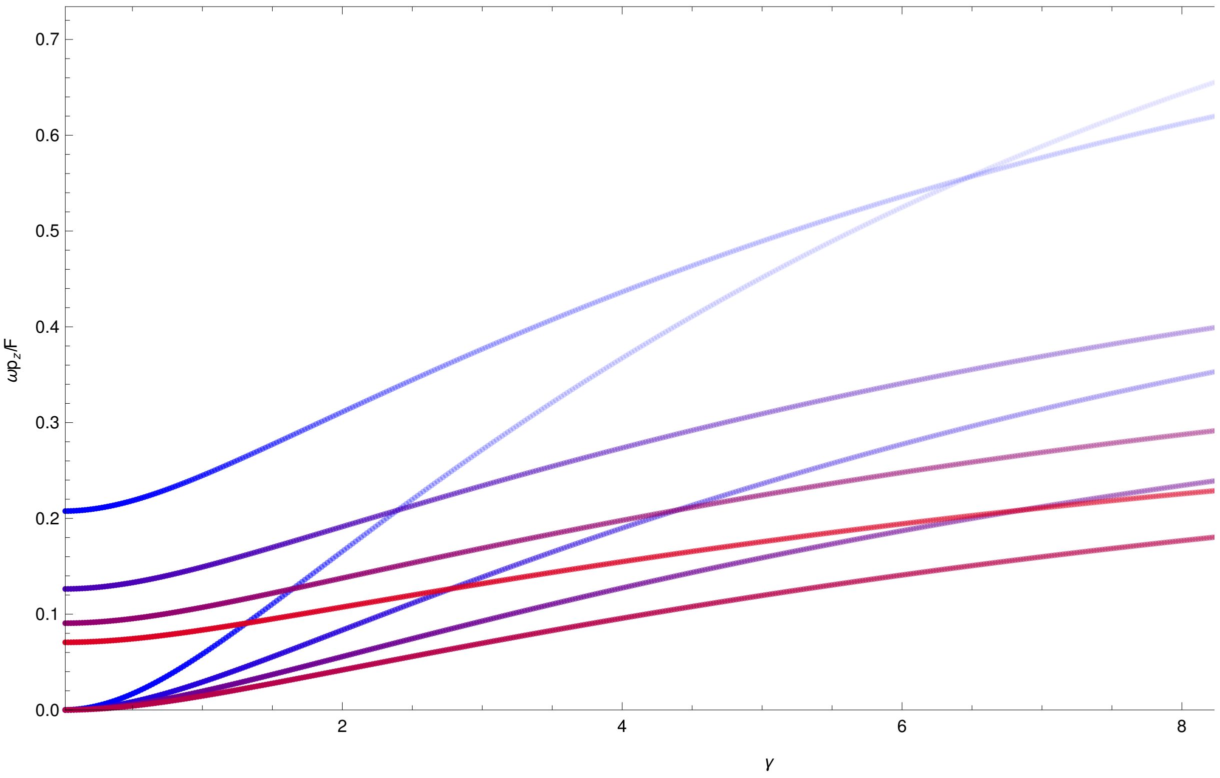
```
{{pz → 0.0627928 + 0.00212574 i}, {pz → 0.228599 + 0.00501516 i}}
```

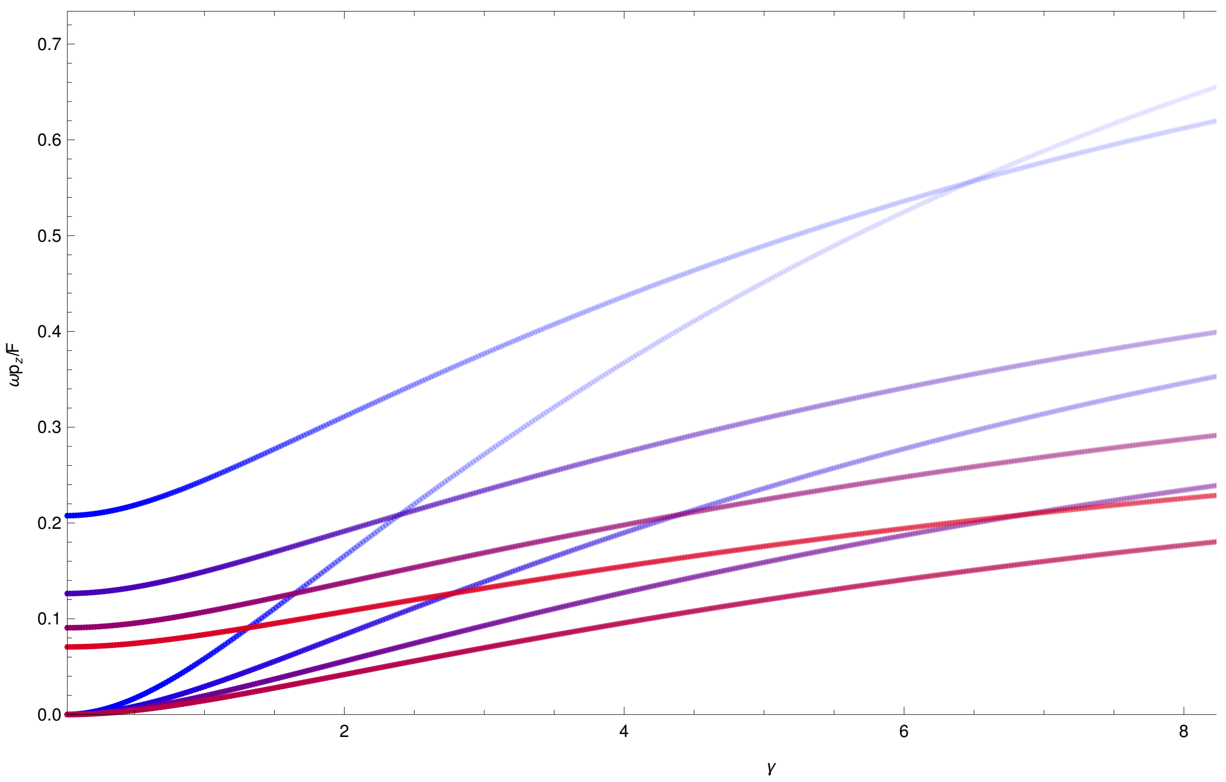
Benchmarking

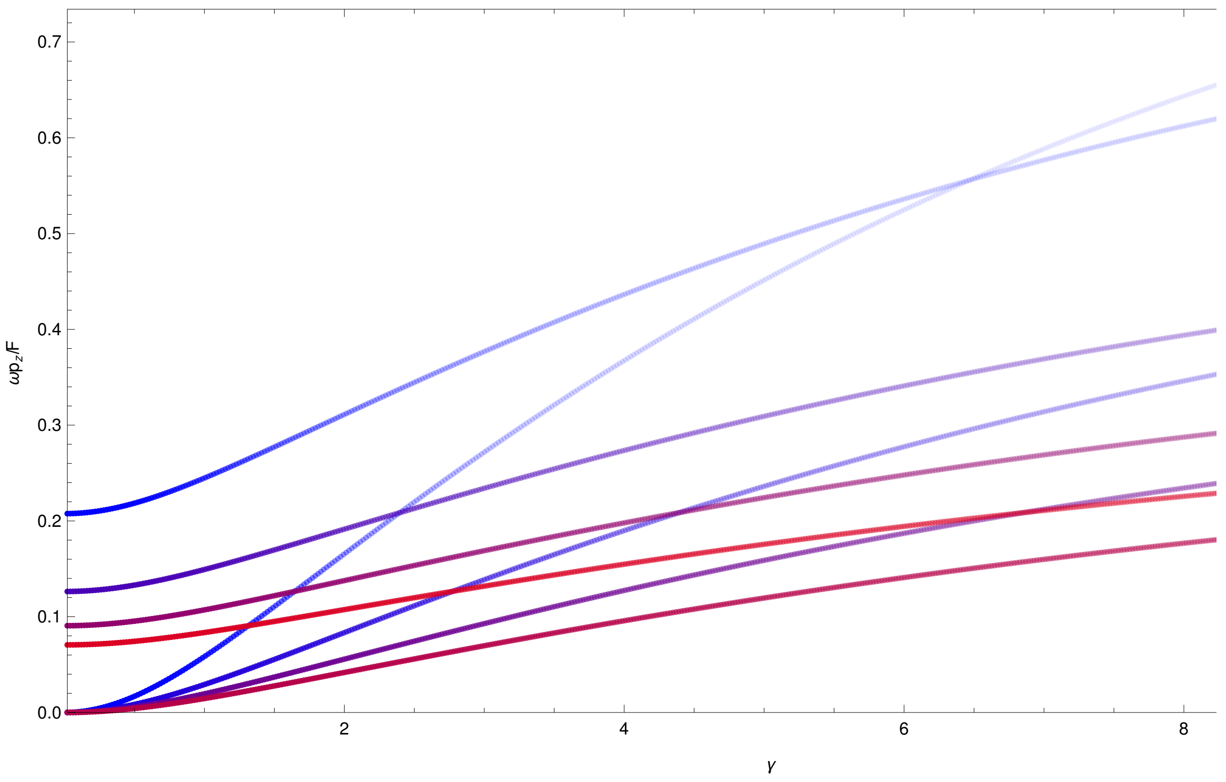
```
AbsoluteTiming [
  complexTransitionsBenchmarkingData  = Flatten[Table[
          Block[{F = 0.05, κ = 1.007},
            {"k" → k, "γ" → ωκ/F, "ωpF" → ωpz/F} /. getComplexTransition [k, {F, ω, κ}]
          ]
          , {k, 1, 8}, {ω, 0.001, 0.5, 0.001}], 1];
]
```

```
{3.329340, Null}
```

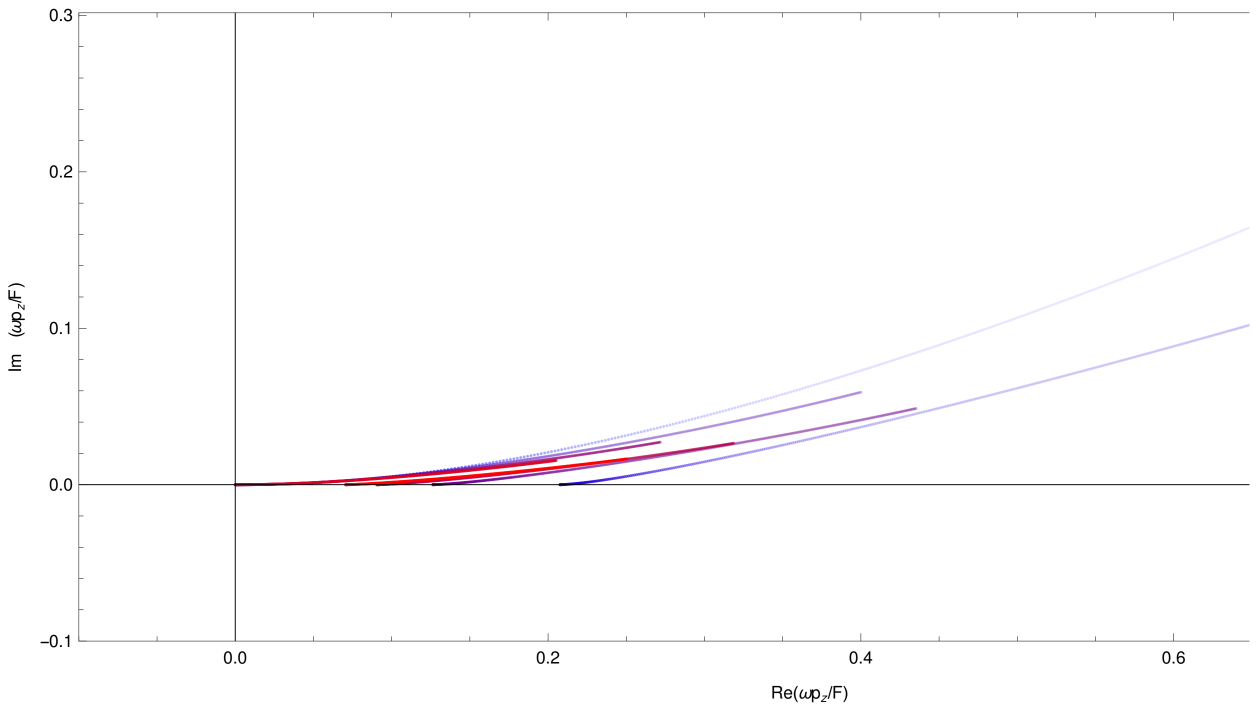
```
Show[
  Graphics[
    {Quiet[Blend[{Blue, Red}, ("k" - 2)/7]], Opacity[1 / (1 + Im ["ωpF"] / 0.01)],
        Point[{"γ", Re["ωpF"]}]} /. complexTransitionsBenchmarkingData
  ]
  , FrameLabel  → {"γ", "ωp_z/F"}, PlotRangePadding → None,
  Frame  → True, ImageSize  → {800, 400}, AspectRatio → 0.5
]
```

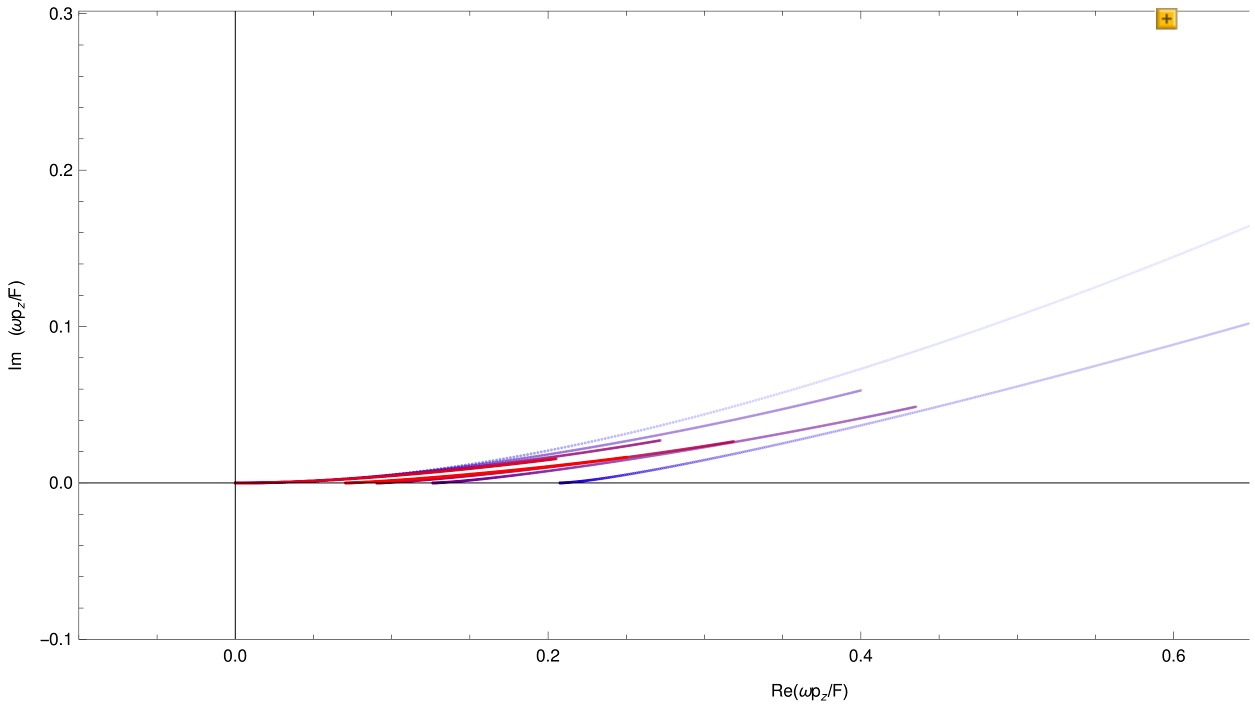



0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$\omega p_z/F$
2
4
6
8
γ


0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$\omega p_z/F$
2
4
6
8
γ

```
Graphics[
  {Quiet[Blend[{Blue, Red}, ("k" - 1)/7]], Opacity[1/(1 + Im ["ωpF"] / 0.01)], PointSize[0.002],
      Point[{Re["ωpF"], Im ["ωpF"]}]} /. complexTransitionsBenchmarkingData
  , PlotRangePadding→ 0.1, Frame  → True, Axes → {True, True}, AxesOrigin→ {0, 0},
  FrameLabel  → {"Re(ωp_z/F)", "Im  (ωp_z/F)"}, ImageSize  → 800
]
```

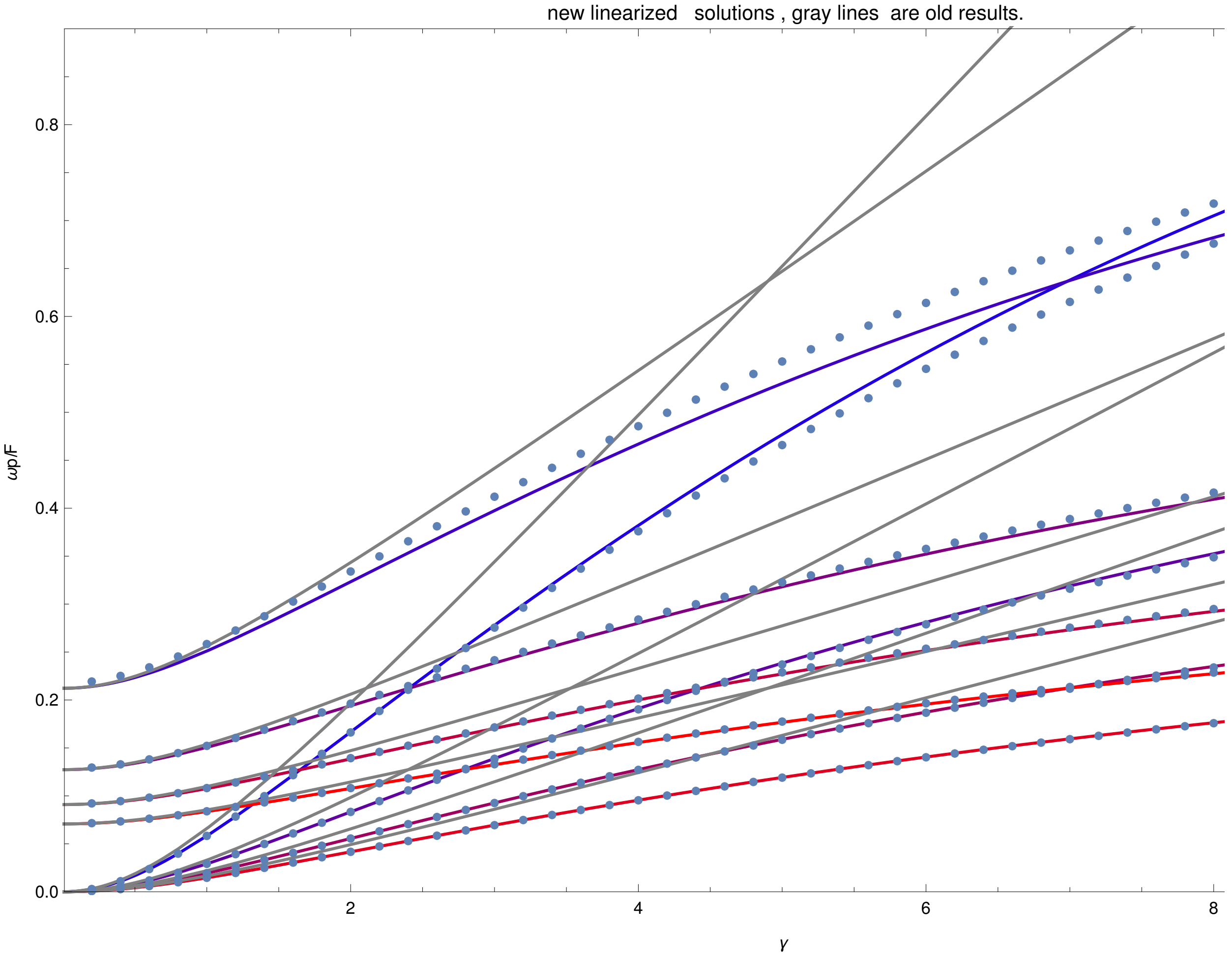



0.3
0.2
0.1
0.0
−0.1
0.0
0.2
0.4
0.6
Im $(\omega p_z/F)$
Re$(\omega p_z/F)$

Comparison

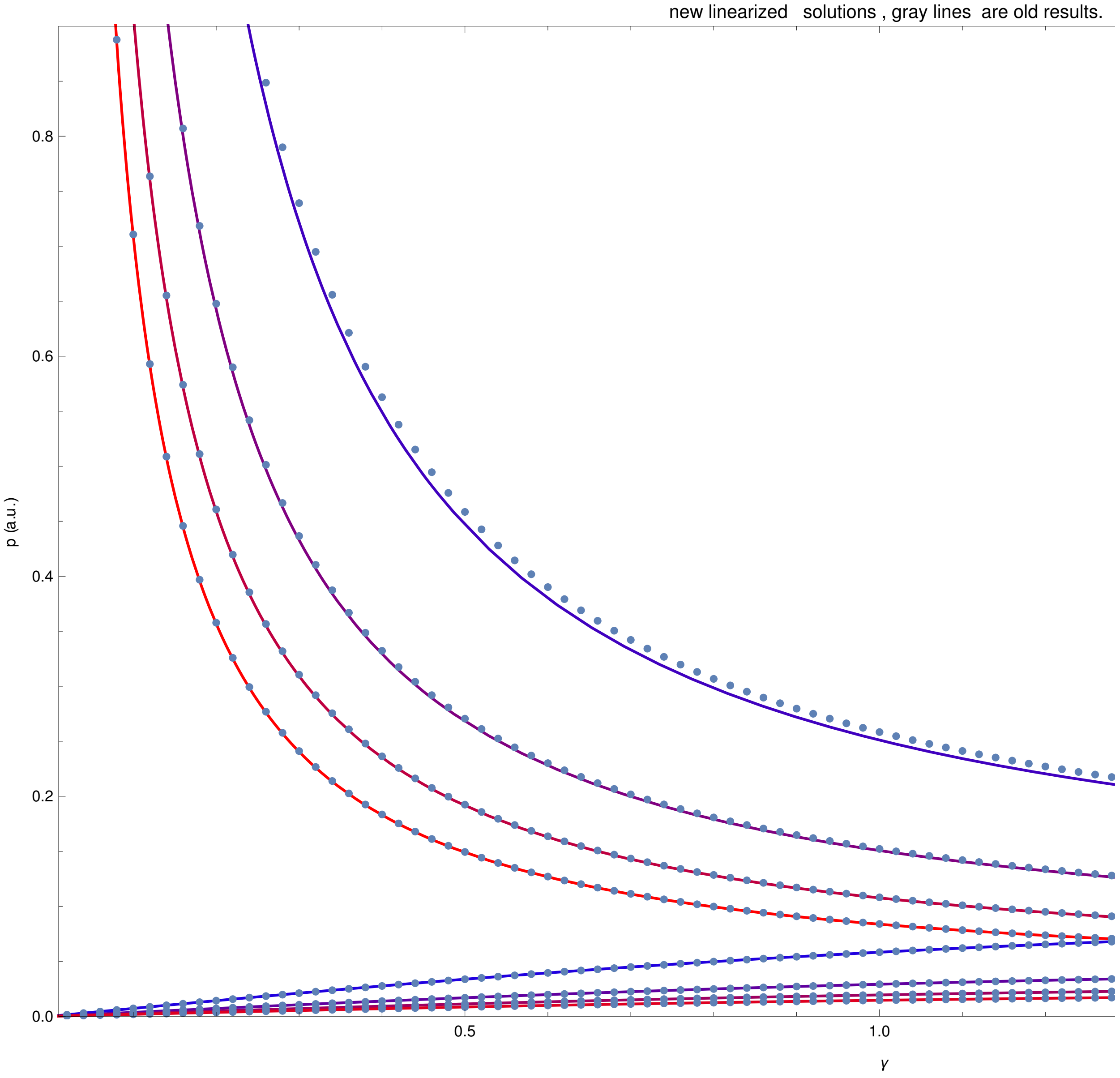
```
Block[{F = 0.05, κ = 1}, Show[Table[
        ParametricPlot [
          Tooltip[
            {ωκ/F, getFullReducedLinearizedTransition[n, F, ω, κ]}
            , n]
          , {ω, 0.0, 0.5}, PlotStyle → Blend[{Blue, Red}, n / 8]
          , Frame  → True, PlotRangePadding → None, Axes → False,
          AspectRatio → 0.6, ImageSize  → 800, FrameLabel  → {"γ", "ωp/F"}
          , PlotLabel → "κ=1, F=0.05, ω∈[0,0.5]. Dots are exact solutions,
                coloured lines are\n new linearized
                solutions, gray lines are old results."
        ]
        , {n, 1, 8}] ~Join~ Table[
        ParametricPlot [
          Tooltip[
            {ωκ/F, getReducedLinearizedTransition[n, ωκ/F]]}
            , n]
          , {ω, 0.0, 0.5}, PlotStyle → Gray
        ]
        , {n, 1, 8}] ~Join~ {
        ListPlot[
          Flatten[Table[
              {ωκ/F, ωpz/F} /. getClassicalTransition[Range[8], {F, ω, κ}]
              , {ω, 0.01, 0.5, 0.01}], 1]
          , PlotStyle → PointSize[Medium ]
        ]
      }, PlotRange → {{0.01, 10}, {0, 0.9}}]]
```

κ=1, F=0.05, $\omega\in$[0,0.5]. Dots are exact solutions , coloured lines are new linearized solutions , gray lines are old results.



```
Block[{F = 0.05, κ = 1}, Show[Table[
        ParametricPlot [
          Tooltip[
            {ωκ/F, F/ω getFullReducedLinearizedTransition[n, F, ω, κ]}
            , n]
          , {ω, 0.0, 0.1}, PlotStyle → Blend[{Blue, Red}, n / 8]
          , Frame  → True, PlotRangePadding → None, Axes → False,
          AspectRatio → 0.6, ImageSize  → 1000, FrameLabel  → {"γ", "p  (a.u.)"}
          , PlotLabel → "κ=1, F=0.05, ω∈[0,0.5]. Dots are exact solutions,
                coloured lines are\n new linearized
                solutions, gray lines are old results."
        ]
        , {n, 1, 8}] ~Join~ {
        ListPlot[
          Flatten[Table[
              {ωκ/F, F/ω ωpz/F} /. getClassicalTransition[Range[8], {F, ω, κ}]
              , {ω, 0.001, 0.1, 0.001}], 1]
          , PlotStyle → PointSize[Medium ]
        ]
      }, PlotRange → {{0.01, 2}, {0, 0.9}}]]
```

κ=1, F=0.05, ω∈[0,0.5]. Dots are exact solutions , coloured line
new linearized solutions , gray lines are old results.



Trajectories

complexTrajectory

Returns $\boldsymbol{r}_{\text{cl}}(t) = \int_{t_s}^{t_r} \boldsymbol{p} + \boldsymbol{A}(\tau)\, d\tau$.

```
complexTrajectory ::usage =
    "complexTrajectory [t,{px,py,pz},{F,ω,κ}] Returns the vector-valued
        complex  trajectory r_cl(t)=∫_{t_s}^{t} (p+A(τ))ⅆτ.

complexTrajectory [t,pz,{F,ω,κ}] Returns the z component
        of the complex  trajectory z_cl(t)=∫_{t_s}^{t} (p_z+A(τ))ⅆτ.";

rInit::usage =
    "rInit is an option for complexTrajectory  and classicalTrajectory which
        specifies the initialposition for the trajectory at time  t_s.";
zInit::usage = "zInit is an option for complexTrajectory  and classicalTrajectory
        which specifies the initialz position for the trajectory at time  t_s.";
forcets::usage = "forcets is an option for complexTrajectory  and
        classicalTrajectory which specifies a start time  t_s to
        use for the trajectory, or uses the Automatic  one.";
Protect[rInit, zInit, forcets];

Begin["`Private`"]
Options[complexTrajectory ] = {zInit→0, rInit→{0, 0, 0}, forcets→Automatic };
complexTrajectory [t_, pz_, {F_, ω_, κ_}, OptionsPattern[]] :=
  With[{tss = If[OptionValue[forcets] === Automatic ,
          ts[{0, 0, pz}, {F, ω, κ}], OptionValue[forcets]]},
    OptionValue[zInit] + pz (t - tss) + F/ω^2 (Cos[ω t] - Cos[ω tss])
  ]
complexTrajectory [t_, {px_, py_, pz_}, {F_, ω_, κ_}, OptionsPattern[]] :=
  With[{tss = If[OptionValue[forcets] === Automatic ,
          ts[{px, py, pz}, {F, ω, κ}], OptionValue[forcets]]},
    OptionValue[rInit] + {px, py, pz} (t - tss) + {0, 0, 1} F/ω^2 (Cos[ω t] - Cos[ω tss])
  ]
End[]
```

classicalTrajectory

Returns $\mathrm{Re}[\boldsymbol{r}_{\mathrm{cl}}(t)] = \mathrm{Re}\left[\int_{t_s}^{t_r} \boldsymbol{p} + \boldsymbol{A}(\tau)\, d\tau\right]$.

```
classicalTrajectory::usage =
    "classicalTrajectory[t, {px, py, pz}, {F, ω, κ}] Returns the real part of the
        vector-valued complex  trajectory, Re(r_cl(t))=Re(∫_{t_s}^{t} (p+A(τ))ⅆτ).

classicalTrajectory[t, pz, {F, ω, κ}] Returns the real part of the z component
        of the complex  trajectory, Re(z_cl(t))=Re(∫_{t_s}^{t} (p_z+A(τ))ⅆτ).";
```

```
Begin["`Private`"]
classicalTrajectory[t_, pz_, {F_, ω_, κ_}, OptionsPattern[zInit→0]] :=
  Re[complexTrajectory [t, pz, {F, ω, κ}, zInit→OptionValue[zInit]]]
classicalTrajectory[t_?NumericQ , {px_, py_, pz_},
    {F_, ω_, κ_}, OptionsPattern[rInit→0]] :=
  Re[complexTrajectory [t, {px, py, pz}, {F, ω, κ}, rInit→OptionValue[rInit]]]
End[]
```

Closest Approach times

Classical t_{CA}s

classicalClosestApproach

Returns a list of the classical closest approach times in the specified Range, in atomic units. These are solutions of the equation $\mathrm{Re}[\boldsymbol{r}_{\mathrm{cl}}(t)]\cdot\boldsymbol{v}(t) = \mathrm{Re}\left[\boldsymbol{r}_{\mathrm{init}} + \int_{t_s}^{t}\boldsymbol{p} + \boldsymbol{A}(\tau)\,d\tau\right]\cdot\boldsymbol{v}(t) = 0$ and are all real valued.

```
classicalClosestApproach::usage =
    "classicalClosestApproach[{px, py, pz}, {F, ω, κ}] Returns tCA, such that
        Re[rcl(tCA)]·v(tCA)=0, for the given momentum   and parameters .
        Accepts \"rules\" as an option, as well as \"Range\" in the
        format  {t1, t2}, where both can contain the laser period \"T\".";
```

```
Begin["`Private`"]
Options[classicalClosestApproach] = {"rules" → Automatic , "Range" → {0, 2 "T"}};
classicalClosestApproach[{px_, py_, pz_}, {F_, ω_, κ_}, OptionsPattern[]] := Module[
    {tstart, zinit},
    tstart = If[NumberQ [OptionValue["rules"]],
        "t0" /. OptionValue["rules"],
        Re[1/ω ArcSin[ω/F (pz + ⅈ Sqrt[κ^2 + px^2 + py^2])]]
      ];
    zinit= F/ω^2 Cos[ω tstart] - F/ω^2 Re[Cos[ArcSin[ω/F (pz + ⅈ Sqrt[κ^2 + px^2 + py^2])]]];
    If[Length[#] > 0, t /. #, {}] &@Quiet[
        NSolve[{
            {px, py, pz - F/ω Sin[ω t]}.classicalTrajectory[t, {px, py, pz}, {F, ω, κ}] == 0,
            Evaluate[
              OptionValue["Range"][[1]] < t < OptionValue["Range"][[2]] /. {"T" → 2 π/ω}]
          }, t]
      ]
  ]
End[]
```

rDotV

Returns the value of $\mathrm{Re}[\boldsymbol{r}_{\mathrm{cl}}(t)]\cdot\boldsymbol{v}(t) = \mathrm{Re}\left[\boldsymbol{r}_{\mathrm{init}} + \int_{t_s}^{t}\boldsymbol{p}+\boldsymbol{A}(\tau)\,d\tau\right]\cdot\boldsymbol{v}(t)$ for the specified time, momentum and parameters. Useful mainly as a cleaner way to plot its zero contours - i.e. the surfaces formed by the t_{CA} on different geometrical spaces.

```
rDotV::usage = "rDotV[t, px, pz, {F, ω, κ}] Returns the classical
        r(t)·v(t) for the given momentum   and parameters .";
```

```
Begin["`Private`"]

rDotV[t_, {px_, py_, pz_}, {F_, ω_, κ_}] := Module[{tss, zinit= F/ω^2 (1 - Sqrt[1 + (κ ω/F)^2])},

    tss = If[NumberQ [OptionValue["rules"]],
        "t0" /. OptionValue["rules"],
        Re[1/ω ArcSin[ω/F (pz + ⅈ Sqrt[κ^2 + px^2 + py^2])]]
      ];
    (px^2 + py^2) (t - tss) + (pz (t - tss) + F/ω^2 (Cos[ω t] - Cos[ω tss]) + zinit) (pz - F/ω Sin[ω t])
  ]
End[]
```

Two-dimensional version memoized for efficiency:

```
Begin["`Private`"]
rDotV[t_, px_, pz_, {F_, ω_, κ_}] :=
  rDotV[t, px, pz, {F, ω, κ}] = rDotV[t, {px, 0, pz}, {F, ω, κ}]
End[]
```

d2r2

Returns the second derivative $\frac{d^2}{dt^2}\left[\boldsymbol{r}_{\mathrm{cl}}(t)^2\right] = \frac{d^2}{dt^2}\left[\mathrm{Re}\left(\boldsymbol{r}_{\mathrm{init}} + \int_{t_s}^{t} \boldsymbol{p} + \boldsymbol{A}(\tau)\, d\tau\right)^2\right]$.

```
d2r2::usage = "d2r2[t, {px, py, pz}, {F, ω, κ}] Returns the classical second time
        derivative d^2/dt^2 r_cl^2 at the given momentum  and parameers .";
```

```
Begin["`Private`"]
d2r2[t_, {px_, py_, pz_}, {F_, ω_, κ_}] :=
  d2r2[t, {px, py, pz}, {F, ω, κ}] = 2 (Norm [{px, py, pz} - {0, 0, 1} F/ω Sin[ω t]]^2 -
          classicalTrajectory[t, pz, {F, ω, κ}] F Cos[ω t])
End[]
```

Quantum t_{CA}s

are the complex solutions of $\boldsymbol{r}_{\mathrm{cl}}(t)\cdot\boldsymbol{v}(t) = \left(\boldsymbol{r}_{\mathrm{init}} + \int_{t_s}^{t} \boldsymbol{p} + \boldsymbol{A}(\tau)\, d\tau\right)\cdot\boldsymbol{v}(t) = 0$.

allQuantumClosestApproachTimes

```
allQuantumClosestApproachTimes  ::usage =
    "allQuantumClosestApproachTimes  [{px, py, pz}, {F, ω, κ}, {xinit,
        yinit, zinit}] returns the quantum  tCAs as a list of
        complex  values. It accepts as options an explicit \"ts\"
        and a \"Range\", set to {-2ⅈτ, T+2ⅈτ} by default, as
        well as all the options of EPToolbox`FindComplexRoots .";
tCA::usage = "tCA represents a closest approach time  t_CA.";

Begin["`Private`"]
Options[allQuantumClosestApproachTimes  ] =
    Join[Options[FindComplexRoots ], {"rules" → Automatic , "Range" → Automatic }];
allQuantumClosestApproachTimes  [{po_, py_, pp_}, {F_, ω_, κ_},
    {xinit_, yinit_, zinit_}, options:OptionsPattern[]] := Module[
    {tss, range, rules},
    tss = If[OptionValue["rules"] === Automatic ,
        ts[pp, κ, ω, F, po, py], "ts" /. OptionValue["rules"]];
    rules = If[OptionValue["rules"] === Automatic ,
        {"tκ" → tss - ⅈ/κ^2, "ts" → tss, "t0" → Re[tss], "τ" → Im [tss], "T" → 2 π/ω},
        OptionValue[rules]
      ];
    range = Which[
        MatchQ[OptionValue["Range"] /. rules,
          {a_?NumericQ , b_?NumericQ } /; Im [b-a] ≤ 0],
        (OptionValue[Range] /. rules) + {-2 ⅈ Im [tss], 2 ⅈ Im [tss]},
        MatchQ[OptionValue["Range"] /. rules, {_?NumericQ , _?NumericQ }],
        (OptionValue[Range] /. rules),
        True, {-2 ⅈ Im [tss], 2π/ω + 2 ⅈ Im [tss]}
      ];
    Sort@FindComplexRoots [
        2 ({xinit, yinit, zinit} + {po, py, pp} (tCA - tss) + {0, 0, F/ω^2 (Cos[ω tCA] - Cos[ω tss])}).
            {po, py, pp - F/ω Sin[ω tCA]} == 0
        , {tCA, range[[1]], range[[2]]}
        , Sequence@@FilterRules[{options}, Options[FindComplexRoots ]]
        , Seeds → 200
        , Tolerance → 10^(4 - $MachinePrecision)
      ]
  ]
End[]
```

makeCircuitTCAsFromCircuit

Takes a ready-made circuit, in the format $\{\{n_1, \{p_{x\,1}, p_{y\,1}, p_{z\,1}\}\}, \ldots, \{n_N, \{p_{x\,N}, p_{y\,N}, p_{z\,N}\}\}\}$, and calculates all the relevant t_{CA}s for it, returning the tags and the momentum in the output, which is of the form $\{\{n_1, \{p_{x\,1}, p_{y\,1}, p_{z\,1}\}, t_{\text{CA}\,1,1}\}, \{\{n_1, \{p_{x\,1}, p_{y\,1}, p_{z\,1}\}, t_{\text{CA}\,1,2}\}, \ldots, \{\{n_N, \{p_{x\,N}, p_{y\,N}, p_{z\,N}\}, t_{\text{CA}\,N,k}\}\}$.

```
makeTCAsFromCircuit ::usage =
   "makeTCAsFromCircuit [{{n1, {px1, py1, pz1}}, ..., {nN, {pxnN, pynN, pznN}}},
      {F, ω, κ}, {xinit, yinit, zinit}] Calculates the tCAs for the given
      circuit and parameters . The ni can be any tags which are returned
      with the output, which is of the form {{n1, {px1, py1, pz1},
      tCA11}, {n1, {px1, py1, pz1}, tCA12}, ..., {nN, {pxnN, pynN, pznN},
      tCAnNk}}, with all the appropriate tCA in separate entries. Same
      \"rules\" and \"Range\" options as allQuantumClosestApproachTimes .";
```

```
Begin["`Private`"]
Options[makeTCAsFromCircuit ] =
    Join[{"rules" → Automatic , OptionValue["Range"] → Automatic ,
        PlotRange → Automatic }, Options[allQuantumClosestApproachTimes ]];
makeTCAsFromCircuit [circuit_, {F_, ω_, κ_}, {xinit_, yinit_, zinit_},
    options: OptionsPattern[]] := Module[
    {range, rules, tss, n, pvec},
    Flatten[ParallelTable[
        {n, pvec} = element ;
        Needs["EPToolbox`",
          "/home /episanty/Work/CQD/Project/Code/EPToolbox/EPToolbox/EPToolbox.m "]
        tss = If[OptionValue["rules"] === Automatic ,
            ts[pvec⟦1⟧, κ, ω, F, pvec⟦1⟧], "ts" /. OptionValue["rules"]];
        rules = If[OptionValue["rules"] === Automatic ,
            {"tκ" → tss - i/κ^2, "ts" → tss, "t0" → Re[tss], "τ" → Im [tss], "T" → 2π/ω},
            OptionValue[rules]
          ];
        range = Automatic ;
        range = Which[
            MatchQ[OptionValue["Range"] /. rules, {_?NumericQ , _?NumericQ }],
            OptionValue["Range"] /. rules,
            MatchQ[OptionValue[PlotRange] /. rules,
              {{_?NumericQ , _?NumericQ }, {_?NumericQ , _?NumericQ }}],
            Complex @@@ (OptionValue[PlotRange]^T /. rules),
            True, {-2 i Im [tss], 2π/ω + 2 i Im [tss]}
          ];
        (*ugly logic inside the Table because
          range depends on tss which depends on p*)
        {n, pvec, tCA} /. allQuantumClosestApproachTimes [
            {pvec⟦1⟧, 0, pvec⟦2⟧}, {F, ω, κ}, {xinit, yinit, zinit}
            , Sequence @@ FilterRules[{options},
                Options[allQuantumClosestApproachTimes ]], "Range" → range
          ]
        , {element , circuit}], 1]
  ]
End[]
```

makeTCAsFromRange

Takes a specific range of momentum and gets all the relevant t_{CA}s for a rectangular grid of those specifications.

```
makeTCAsFromRange  ::usage =
    "makeTCAsFromRange  [{pomin , pomax , δpo}, {ppmin , ppmax , δpp},
        fixedMomenta , {F, ω, κ}, {xinit, yinit, zinit}, \"Range\"→{t1, t2}]
        Returns a list with elements  of the form  {{po, py, pp}, tCA} for a
        rectangular grid in momentum    with the given spans and separations.
        fixedMomenta  should be a list of replacement  rules such as {py→0}.";

Begin["`Private`"]
Options[makeTCAsFromRange  ] = Join[{"rules" → Automatic , OptionValue["Range"]},
      Options[allQuantumClosestApproachTimes  ]];
makeTCAsFromRange  [{pomin_ , pomax_ , δpo_}, {ppmin_ , ppmax_ , δpp_}, fixedMomenta_ ,
    {F_, ω_, κ_}, {xinit_, yinit_, zinit_}, options: OptionsPattern[]] := Module[
    {range, rules, tss},
    tss = If[OptionValue["rules"] === Automatic ,
        ts[pp, κ, ω, F, po, py], "ts" /. OptionValue["rules"]];
    rules = If[OptionValue["rules"] === Automatic ,
        {"tκ" → tss - i/κ^2, "ts" → tss, "t0" → Re[tss], "τ" → Im [tss], "T" → 2π/ω},
        OptionValue[rules]
      ];
    Flatten[
      Table[
        range = Which[
              MatchQ[OptionValue["Range"] /. rules /. fixedMomenta ,
                {_?NumericQ , _?NumericQ }], OptionValue["Range"] /. rules,
              MatchQ[OptionValue[PlotRange] /. rules /. fixedMomenta ,
                {{_?NumericQ , _?NumericQ }, {_?NumericQ , _?NumericQ }}],
              Complex @@@ (OptionValue[PlotRange]ᵀ /. rules),
              True, {-2 i Im [tss], 2π/ω + 2 i Im [tss]}
            ] /. fixedMomenta ;
        (*ugly logic inside the Table
          because range depends on tss which depends on p*)
        {{po, py, pp} /. fixedMomenta , tCA} /. allQuantumClosestApproachTimes  [
            {po, py, pp} /. fixedMomenta , {F, ω, κ}, {xinit, yinit, zinit}
            , "Range" → range, Sequence@@FilterRules[{options},
                Options[allQuantumClosestApproachTimes  ]]
          ]
        , {po, pomin , pomax , δpo}, {pp, ppmin , ppmax , δpp}]
      , {1, 2, 3}]
  ]
End[]
```

closestApproachTimesPath

uses magic to choose the appropriate t_{CA}'s the integration contour should pass through. Output is the same as allQuantumClosestApproachTimes.

```
closestApproachTimesPath ::usage =
  "closestApproachTimesPath [{px, py, pz}, {F, ω, κ}, {xinit, yinit, zinit}]
      Returns a selected and ordered list of complex  tCAs as
      replacement  rules, in atomic  units. Accepts the same  \"rules\"
      and \"Range\" options as allQuantumClosestApproachTimes  .";
v2Tolerance::usage = "v2Tolerance is an option for closestApproachTimesPath
    which determines  the tolerance v2tol to be used when selecting tCAs
    for the path. Time  tCA is included in the path if Re[v[tCA]^2]≥-v2tol.";
Protect[v2Tolerance];

Begin["`Private`"]
Options[closestApproachTimesPath ] = Join[{v2Tolerance → Automatic },
    Options[allQuantumClosestApproachTimes  ], Options[ListPlot]];
closestApproachTimesPath [{po_, py_, pp_}, {F_, ω_, κ_},
  {xinit_, yinit_, zinit_}, options: OptionsPattern[]] := Module[
  {tss, r, v, range, rules, v2tol},
  tss = If [OptionValue["rules"] === Automatic ,
     ts[pp, κ, ω, F, po, py], "ts" /. OptionValue["rules"]];
  rules = If [OptionValue["rules"] === Automatic ,
     {"tκ" → tss - i/κ^2, "ts" → tss, "t0" → Re[tss], "τ" → Im [tss], "T" → 2 π / ω},
     OptionValue[rules]
    ];
  v2tol = Which[OptionValue[v2Tolerance] === Automatic ,
     10^-8, True, OptionValue[v2Tolerance]];
  r[tt_] := ({xinit, yinit, zinit} + {po, py, pp} (tt - tss) +
       {0, 0, F/ω^2 (Cos [ω tt] - Cos [ω tss])});
  v[tt_] := ({po, py, pp} + {0, 0, -F/ω Sin[ω tt]});
  range = Which[
     MatchQ[OptionValue["Range"] /. rules, {_?NumericQ , _?NumericQ }],
     OptionValue["Range"] /. rules,
     MatchQ[OptionValue[PlotRange] /. rules,
       {{_?NumericQ , _?NumericQ }, {_?NumericQ , _?NumericQ }}],
     Complex @@@ (OptionValue[PlotRange]^T /. rules),
     True, {-2 i Im [tss], 2 π/ω + 2 i Im [tss]}
    ];
  Select[
   Sort[
     allQuantumClosestApproachTimes  [{po, py, pp}, {F, ω, κ}, {xinit, yinit, zinit}
       , "Range" → range
       , Sequence @@
         FilterRules[{options}, Options[allQuantumClosestApproachTimes  ]]
       , Tolerance → 10 ^ (4 - $MachinePrecision)],
            ((Re[tCA] /. #1) < (Re[tCA] /. #2)) &
          ],
          (Or[
                    And[1/4 2π/ω < Re[tCA] < 3/4 2π/ω, Im [tCA] > 0],
                    And[-1/4 2π/ω < Re[tCA] < 1/4 2π/ω, Im [tCA] ≥ 0, Im [Sin[ω tCA]] < ω κ / F],
                    And[(-0.3 Im [tss] ≤ Im [tCA] < Im [tss] - 1/κ²),
                      (Re[tCA] - 0.1 2π/ω > Re[tss]), (Re[v[tCA].v[tCA]] ≥ -v2tol)]
                ] /. # &)
        ]
      ]
    End[]
    (*closestApproachTimesPath [{0.05,0,1.2},
      stdpars,{0,0,0},"Range"→{-5i,5.6"T"+30i}]*)
```

Amplitude-related functions

Volkov exponent

```
volkovExponent::usage = "volkovExponent[{po, py,
          pp}, {F, ω, κ}] calculates Re(i∫_0^{t_s} (I_p+1/2(p+A(τ))²)dτ).";
```

```
Begin["`Private`"]
(*FullSimplify[Re[
    ⅈ Integrate[κ^2/2+1/2(po^2+py^2)+1/2(pp-F/ω Sin[ω t])^2,{t,0,1/ω ArcSin[ω/F(pp+ⅈ Sqrt[κ^2+po^2+py^2])]}]/.
      {Sin[2u_]->2Sin[u]Cos[u]}
  ]]*)
volkovExponent[{po_, py_, pp_}, {F_, ω_}, κ_] :=
```

$$-\frac{1}{8}\mathrm{Im}\left[\frac{1}{\omega^3}\left(2F\omega\left(-4\,pp+3\,pp\sqrt{1+\frac{\left(-\mathrm{i}\,pp+\sqrt{po^2+py^2+\kappa^2}\right)^2\omega^2}{F^2}}-\mathrm{i}\sqrt{po^2+py^2+\kappa^2}\sqrt{1+\frac{\left(-\mathrm{i}\,pp+\sqrt{po^2+py^2+\kappa^2}\right)^2\omega^2}{F^2}}\right)+2\left(F^2+2\left(po^2+pp^2+py^2+\kappa^2\right)\omega^2\right)\mathrm{ArcSin}\left[\frac{\left(pp+\mathrm{i}\sqrt{po^2+py^2+\kappa^2}\right)\omega}{F}\right]\right)\right]$$

```
volkovExponent[{po_, py_, pp_}, {F_, ω_, κ_}] := volkovExponent[{po, py, pp}, {F, ω}, κ]
End[]
```

coulombCorrection

Numerically integrates $\int_C \frac{1}{\sqrt{r_{\rm cl}(t)^2}}\,dt$ over the specified complex integration path C. Sows parameters when integration errors are encountered, and allows for softening of the Coulomb kernel if required.

Definition

```
coulombCorrection ::usage =
    "coulombCorrection [{px, py, pz}, {F, ω, κ}, path] Calculates the Coulomb
        correction integral over the specified path. The path is a list
        which may  contain \"tκ\", \"ts\", \"t0\", \"τ\", \"tCApath\"
        and \"T\", which will be replaced by the appropriate points.";
coulombCorrection ::intErrors = "Integration errors obtained at
        input {{po, py, pp}, {F, ω, κ}, path}=`1`";
Softening::usage = "Softening is an option for coulombCorrection  which
        specifies whether the Coulomb  kernel should be softened by
        a length σ. It is set by default to None (σ=0), and it can
        be changed to Automatic  (σ=1/κ) or a numeric  value for σ.";
ReportingFunction::usage = "ReportingFunction is an option for coulombCorrection
        to specify the reporting of error-producing inputs. It should
        speficy a function f, set by default to Sow, which will be called as
        f[{{po, py, pp}, {F, ω, κ}, path}] if the inputs produce any errors
        during the NIntegrate call. To print to a file use ReportToFile.";
ReportToFile::usage = "ReportToFile[directory, file] returns a function
        which can be used as a value for ReportingFunction inside
        coulombCorrection .\n\nReportToFile[directory, file][expr]
        adds a line with expr (properly parsed to ASCII for
        spaces, backslashes and quote marks ) to directory/file.";
```

```
Begin["`Private`"]
SetSharedFunction[Sow];
Quiet[ReportingFunction= ReportingFunction; Softening= Softening;]
Protect[ReportingFunction]; Protect[Softening];

Options[coulombCorrection] = Join[{Softening→None, ReportingFunction→Sow},
      Options[closestApproachTimesPath]];
coulombCorrection[{po_, py_, pp_}, {F_, ω_, κ_}, path_: {"tκ", "t0"},
    options:OptionsPattern[]] := Block[
    {tss, iterator, rules, range, tCApath, int, σ},
    σ = Which[NumberQ [OptionValue[Softening]], OptionValue[Softening],
        OptionValue[Softening] === Automatic , 1/κ, True, 0];
    (*Coulomb  softening*)
    tss = ts[pp, κ, ω, F, po, py];
    rules = {"tκ" → tss - i/κ^2, "ts" → tss, "t0" → Re[tss], "τ" → Im [tss], "T" → 2π/ω};
    range = ({Re[First[path]] - 2 i "τ", Re[Last[path]] + 2 i "τ"} /. rules);
    If[
      !FreeQ[path, "tCApath"],
      tCApath =
        Chop[tCA /. closestApproachTimesPath [{po, py, pp}, {F, ω, κ}, {0, 0, 0},
              Sequence@@FilterRules[{options}, Options[closestApproachTimesPath]],
              "Range" → range]];
      If[Length[tCApath] > 0,
        AppendTo[rules, "tCApath" → Apply[Sequence, tCApath]],
        AppendTo[rules, "tCApath" → (## &[])]
      ]
    ]; (*Print[rules];*)
    iterator= {t, Sequence@@Evaluate[path /. rules]};
    (*Print[iterator];*)
    Check[
      int= NIntegrate[
```
$$-\left(\left(po^2+py^2\right)(t-tss)^2+\left(pp\,(t-tss)+\frac{F}{\omega^2}(\mathrm{Cos}[\omega t]-\mathrm{Cos}[\omega\, tss])\right)^2+\sigma^2\right)^{-1/2},$$
```
          Evaluate@iterator],
      OptionValue[ReportingFunction][Chop[{{po, py, pp}, {F, ω, κ}, path}]];
      Message[coulombCorrection ::intErrors, Chop[{{po, py, pp}, {F, ω, κ}, path}]];
      int
    ]
  ]
End[]
```

```
Begin["`Private`"]
ReportToFile[directory_, file_] :=
  Function[expr, Run["cd "<>directory<>" && echo "<>
        StringReplace[ToString[expr /. {s_String:→ StringJoin["\"", s, "\""]},
             CharacterEncoding→ "ASCII"], {" "→"\\ ", "\\"→"\\\\", "\""→"\\\""}] <>
        " >> "<>StringReplace[file, {" "→"\\ ", "\\"→"\\\\", "\""→"\\\""}]]]
End[]
```

Tests of the error handling

For a single evaluation

```
Reap[
  coulombCorrection [{2, 0, 0}, {0.05, 0.055, 1.007}, {"tκ", "t0"}]
]
```

```
NIntegrate::slwcon :
  Numerical integration converging too slowly; suspect one of the following: singularity, value of
      the integration is 0, highly oscillatory integrand, or WorkingPrecision too small. ≫

NIntegrate::ncvb :
  NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in t near {t} = {0. + 25.8533 ⅈ}.
      NIntegrate obtained 2.67192 + 2.68596 ⅈ and 0.061081270393484745`
      for the integral and error estimates. ≫

coulombCorrection::intErrors :
  Integration errors obtained at input {{po, py, pp}, {F, ω, κ}, path}={{2, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}}
{2.67192 + 2.68596 ⅈ, {{{{2, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}}}}}
```

Test of the error handling inside a Parallelized Table.

```
(*This needs to be run before any parallel evaluation.*)
ParallelEvaluate[Needs["EPToolbox`",
      "/home /episanty/Work/CQD/Project/Code/EPToolbox/EPToolbox/EPToolbox.m "]];
```

```
Reap[
    ParallelTable[
      Quiet@coulombCorrection [{po, 0, 0}, {0.05, 0.055, 1.007}, {"tκ", "t0"}]
      , {po, -2, 2, 0.1}]
  ][[2, 1]]
(*Generates about 2 pages of errors if not
  Quieted. This shows the Reaped trouble inputs only.*)
```

```
{{{-1.7, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.4, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.1, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-0.8, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-2., 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.6, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.3, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1., 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-0.7, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.9, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.5, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.2, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-0.9, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-0.6, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{0.7, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{0.9, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.8, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{0.6, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{0.8, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1., 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.9, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.1, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.3, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.5, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.7, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{2., 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.2, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.4, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.6, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.8, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}}}
```

Print errors to file:

```
coulombCorrection [{0.01, 0, 0.5}, stdpars, {"tκ", 2 "T"},
  ReportingFunction→ReportToFile[NotebookDirectory[], "test.txt"]]
```

```
NIntegrate::slwcon :
  Numerical integration converging too slowly; suspect one of the following: singularity, value of
      the integration is 0, highly oscillatory integrand, or WorkingPrecision too small. >>
NIntegrate::ncvb : NIntegrate failed to converge to prescribed accuracy
      after 9 recursive bisections in t near {t} = {75.9294 + 11.9 i}. NIntegrate obtained
      -7.48256 + 3.89417 i and 0.004771979130395705` for the integral and error estimates. >>
coulombCorrection::intErrors :
  Integration errors obtained at input {{po, py, pp}, {F, ω, κ}, path}={{0.01, 0, 0.5}, {0.05, 0.055, 1.007}, {tκ, 2 T}}
-7.48256+3.89417 i
```

and then reimport from the file

```
ToExpression[Import [NotebookDirectory[] <> "test.txt"]]
coulombCorrection @@%
```

```
{{0.01, 0, 0.5}, {0.05, 0.055, 1.007}, {tκ, 2 T}}
```

```
NIntegrate::slwcon :
  Numerical integration converging too slowly; suspect one of the following: singularity, value of
      the integration is 0, highly oscillatory integrand, or WorkingPrecision too small. >>
NIntegrate::ncvb : NIntegrate failed to converge to prescribed accuracy
      after 9 recursive bisections in t near {t} = {75.9294 + 11.9 i}. NIntegrate obtained
      -7.48256 + 3.89417 i and 0.004771979130395705` for the integral and error estimates. >>
coulombCorrection::intErrors :
  Integration errors obtained at input {{po, py, pp}, {F, ω, κ}, path}={{0.01, 0, 0.5}, {0.05, 0.055, 1.007}, {tκ, 2 T}}
-7.48256+3.89417 i
```

Printing to file from inside a parallelized environment. Note that parallelized kernels have no FrontEnd and therefore cannot access NotebookDirectory[].

```
Block[{directory= NotebookDirectory[]},
  ParallelTable[
      Quiet@coulombCorrection [{po, 0, 0}, {0.05, 0.055, 1.007}, {"tκ", "t0"},
          ReportingFunction→ReportToFile[directory, "test.txt"]]
      , {po, -2, 2, 0.1}];
]
ToExpression/@Import [NotebookDirectory[] <> "test.txt", "List"]
coulombCorrection @@@%
```

```
{{{-1.4, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.7, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.1, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-0.8, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.3, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.6, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-2., 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1., 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.2, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-0.7, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.5, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-0.9, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.9, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-0.6, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{0.7, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{0.9, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.1, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.7, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{-1.8, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.5, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{0.8, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1., 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.3, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.2, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.8, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{0.6, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.6, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.4, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{1.9, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}},
  {{2., 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}}}
```

```
NIntegrate::ncvb :
  NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in t near {t} = {0. + 18.639 ⅈ}.
      NIntegrate obtained 2.37932 + 3.44132 ⅈ and 0.07476695623809278`
      for the integral and error estimates. ≫

coulombCorrection::intErrors :
  Integration errors obtained at input {{po, py, pp}, {F, ω, κ}, path}={{–1.4, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}}

NIntegrate::ncvb :
  NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in t near {t} = {0. + 22.5694 ⅈ}.
      NIntegrate obtained 2.5598 + 3.02543 ⅈ and 0.05200239804482814`
      for the integral and error estimates. ≫

coulombCorrection::intErrors :
  Integration errors obtained at input {{po, py, pp}, {F, ω, κ}, path}={{–1.7, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}}

NIntegrate::slwcon :
  Numerical integration converging too slowly; suspect one of the following: singularity, value of
      the integration is 0, highly oscillatory integrand, or WorkingPrecision too small. ≫
```

```
NIntegrate::ncvb :
  NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in t near {t} = {0. + 13.7753 ⅈ}.
      NIntegrate obtained 2.12149 + 3.84551 ⅈ and 0.040628351055489696`
      for the integral and error estimates. ≫

General::stop : Further output of NIntegrate::ncvb will be suppressed during this calculation. ≫

coulombCorrection::intErrors :
  Integration errors obtained at input {{po, py, pp}, {F, ω, κ}, path}={{-1.1, 0, 0}, {0.05, 0.055, 1.007}, {tκ, t0}}

General::stop : Further output of coulombCorrection::intErrors will be suppressed during this calculation. ≫

NIntegrate::slwcon :
  Numerical integration converging too slowly; suspect one of the following: singularity, value of
      the integration is 0, highly oscillatory integrand, or WorkingPrecision too small. ≫

NIntegrate::slwcon :
  Numerical integration converging too slowly; suspect one of the following: singularity, value of
      the integration is 0, highly oscillatory integrand, or WorkingPrecision too small. ≫

General::stop : Further output of NIntegrate::slwcon will be suppressed during this calculation. ≫

{2.37932 + 3.44132 ⅈ, 2.5598 + 3.02543 ⅈ, 2.12149 + 3.84551 ⅈ,
  1.60378 + 4.39982 ⅈ, 2.33519 + 3.5208 ⅈ, 2.50409 + 3.16691 ⅈ, 2.67192 + 2.68596 ⅈ,
  1.98033 + 4.00272 ⅈ, 2.23833 + 3.67126 ⅈ, 1.34139 + 4.5624 ⅈ, 2.47792 + 3.24468 ⅈ,
  1.85702 + 4.16404 ⅈ, 2.63455 + 2.79829 ⅈ, 0.931087 + 4.7784 ⅈ,
  1.34139 + 4.5624 ⅈ, 1.85702 + 4.16404 ⅈ, 2.12149 + 3.84551 ⅈ, 2.5598 + 3.02543 ⅈ,
  2.61225 + 2.91755 ⅈ, 2.47792 + 3.24468 ⅈ, 1.60378 + 4.39982 ⅈ, 1.98033 + 4.00272 ⅈ,
  2.33519 + 3.5208 ⅈ, 2.23833 + 3.67126 ⅈ, 2.61225 + 2.91755 ⅈ, 0.931087 + 4.7784 ⅈ,
  2.50409 + 3.16691 ⅈ, 2.37932 + 3.44132 ⅈ, 2.63455 + 2.79829 ⅈ, 2.67192 + 2.68596 ⅈ}
```

End of package

```
EndPackage[]
```