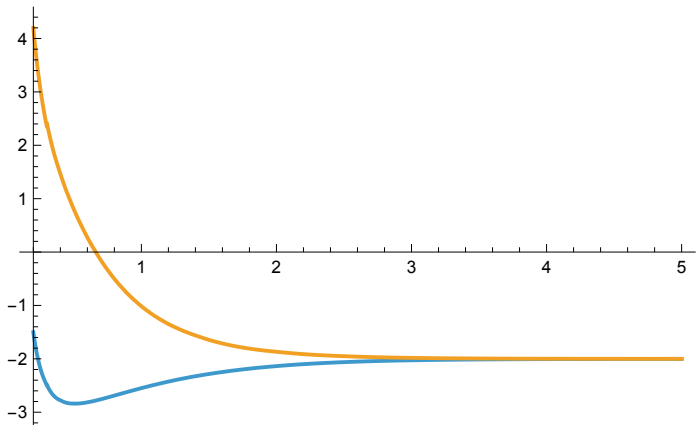
In[1]:=
```
(* this routine needs to run Vpots.nb *)
```

In[2]:=
```
geradeData =
  Import["/Users/zelimir/Work/Physics-Thesis/thesis-2/ZelimirOverleaf/
     MathematicaCodeFinal/gerade1sV3.mx"];
geradePotential = Table[{geradeData[[i, 1]], geradeData[[i, 3]]}, {i, 1, 27}];
ungeradeData =
  Import["/Users/zelimir/Work/Physics-Thesis/thesis-2/ZelimirOverleaf/
     MathematicaCodeFinal/ungerade1sV3.mx"];
ungeradePotential = Table[{ungeradeData[[i, 1]], ungeradeData[[i, 3]]}, {i, 1, 27}];
long[R_] := -2.0 - 0.082 / R^4;
geradefun = Interpolation[geradePotential];
ungeradefun = Interpolation[ungeradePotential];
(* Fit to a model *)
gdata = Drop[geradePotential, {5, 27}];
udata = Drop[ungeradePotential, {5, 27}];
model[R_, C1_, C2_, C3_] := C1 Exp[-C2 R] / R + C3;
gnlm = NonlinearModelFit[gdata, model[R, C1, C2, C3], {C1, C2, C3}, R];
unlm = NonlinearModelFit[udata, model[R, C1, C2, C3], {C1, C2, C3}, R];
gshort[R_] := model[R, C1, C2, C3] /. gnlm["BestFitParameters"];
ushort[R_] := model[R, C1, C2, C3] /. unlm["BestFitParameters"];
gpot[R_] = Piecewise[
   {{gshort[R], R ≤ 0.3}, {geradefun[R], 0.3 < R < 13.0}, {long[R], R ≥ 13.0}}];
upot[R_] = Piecewise[
   {{ushort[R], R ≤ 0.3}, {ungeradefun[R], 0.3 < R < 13.0}, {long[R], R ≥ 13.0}}];
Plot[{gpot[R], upot[R]}, {R, 0.2, 5}, PlotRange → All]

(*e=0.1/27.21;*)
μ = 1866.0 / 2.0;
(*k=√(2 μ e);*)
kB = 0.695 (* Boltzman in AU, cm^-1/K *)
(*λ=2π/k*)
a0 = 5.29188^-11;

r0 = 0.01;
rend = 100;

(*For a single partial wave m, energy e, and range r0 → rend*)
computePhaseShifts[m_, e_, r0_, rend_] :=
  Module[{k, eqG, eqU, solsG, solsU, fg, fu},
   k = √(2 μ e);
   equG := yg''[r] + yg'[r] / r - 2 μ (gpot[r] + 2) yg[r] - m^2 / r^2 yg[r] + 2 μ e yg[r];
   equU := yu''[r] + yu'[r] / r - 2 μ (upot[r] + 2) yu[r] - m^2 / r^2 yu[r] + 2 μ e yu[r];
```

```
solsG = Flatten[NDSolve[
    {equG == 0, yg[r0] == 0, yg'[r0] == 1}, yg, {r, r0, rend}, MaxSteps → 200 000]];
solsU = Flatten[NDSolve[
    {equU == 0, yu[r0] == 0, yu'[r0] == 1}, yu, {r, r0, rend}, MaxSteps → 200 000]];
fg[r_] = yg[r] /. solsG;
fu[r_] = yu[r] /. solsU;
If[((e > 0.002 && e < 0.003) || (e > 0.02 && e < 0.03)) &&
   (m == 40 || m == 5 || m == 0), Print["k=", k];
 Print[Plot[fg[r], {r, r0, rend}, PlotLabel → StringJoin["m=",
     ToString[m], ", e=", ToString[e], "eV"], AxesLabel → "R"]]];
ylogG[r_] := fg'[r] / fg[r];
ylogU[r_] := fu'[r] / fu[r];
(*Print[Plot[ylogG[r],{r,r0,rend}]];
Print[Plot[ylogU[r],{r,r0,rend}]];*)
sl[n_, r_] := BesselJ[n, k r];
cl[n_, r_] := HankelH1[n, k r];
slp[n_, r_] := Derivative[0, 1][sl][n, r];
clp[n_, r_] := Derivative[0, 1][cl][n, r];
bG[n_, r_] :=
 (-I)^(Abs[n]) (slp[n, r] - ylogG[r] × sl[n, r]) / (clp[n, r] - ylogG[r] × cl[n, r]);
bU[n_, r_] :=
 (-I)^(Abs[n]) (slp[n, r] - ylogU[r] × sl[n, r]) / (clp[n, r] - ylogU[r] × cl[n, r]);
If[m == 0,
 Return[{Abs[N[bG[m, rend]]], Abs[N[bG[m, rend] - bU[m, rend]]]^2}],
 Return[{2 Abs[N[bG[m, rend]]], 2 Abs[N[bG[m, rend] - bU[m, rend]]]^2}]]
];
(*computePhaseShifts[10,0.003,0.1,100]*)
```

Out[18]=



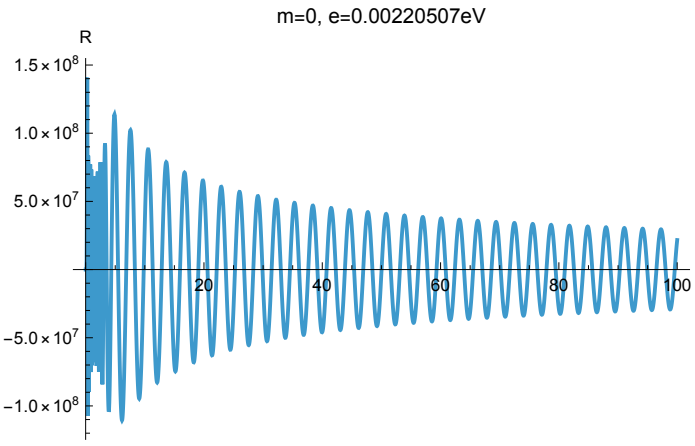
Out[20]=

```
0.695
```

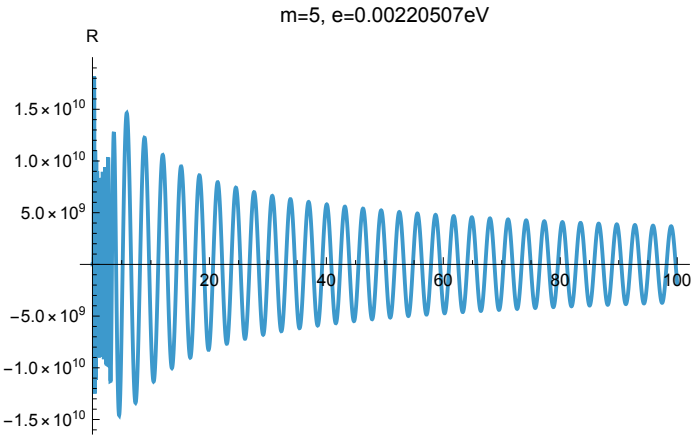
In[25]:=

```
(* e = collision energy in eV, r0, rend - R range *)
computeCrossSect[eV_, r0_, rend_] := Module[{allBs, eH, kk, crossSection},
   eH = eV / 27.21;  (* energy Hartree *)
   kk = √(2 μ eH);
   (* m - partial waves *)
   allBs = Table[{m, computePhaseShifts[m, eH, r0, rend]}, {m, 0, 40}];
   crossSection = 1/kk Total[allBs, {1}][[2]];
   {eV, crossSection}
  ];

crossSection = Table[computeCrossSect[e, r0, rend], {e, 0.01, 1, 0.01}];
crossSectionGraphSC =
 Interpolation[{crossSection[[All, 1]], crossSection[[All, 2]][[All, 1]]} // Transpose]
crossSectionGraphCT =
  Interpolation[{crossSection[[All, 1]], crossSection[[All, 2]][[All, 2]]} // Transpose];


Plot[crossSectionGraphSC[e], {e, 0.01, 1},
 AxesOrigin → {0, 0}, AxesLabel → {"eV", "σ (a0)"},
 PlotLabel → "Scattering Cross Section (a₀) vs Energy (eV)"]
Plot[crossSectionGraphCT[e], {e, 0.01, 1},
 AxesOrigin → {0, 0}, AxesLabel → {"eV", "σ (a₀)"},
 PlotLabel → "Resonant Charge Transfer Cross Section (a0) vs Energy (eV)"]
```

k=2.02846



k=2.02846



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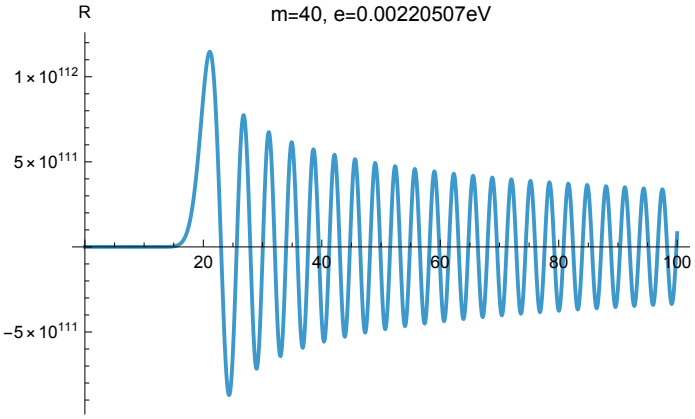

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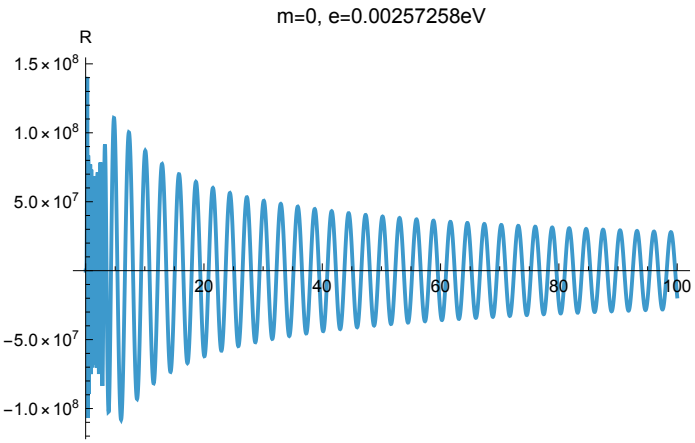

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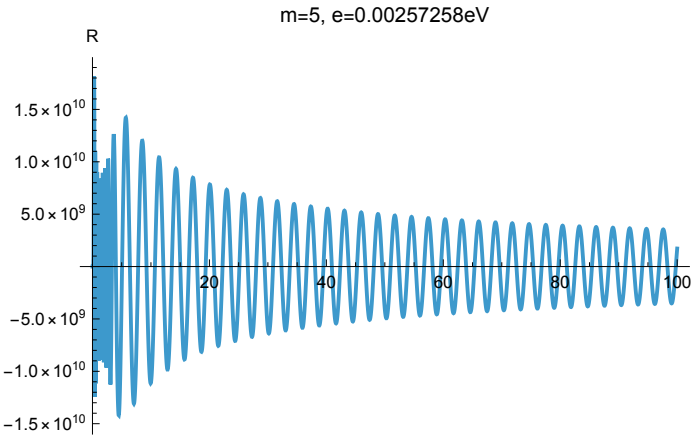

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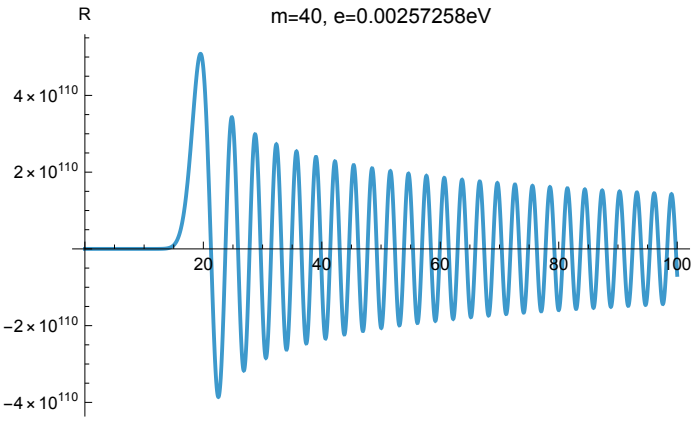

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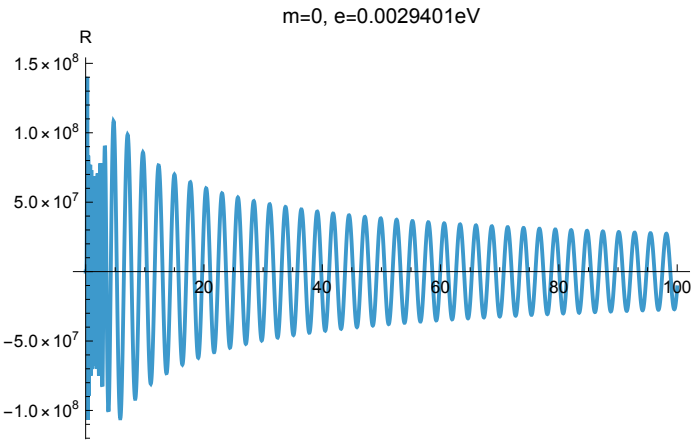

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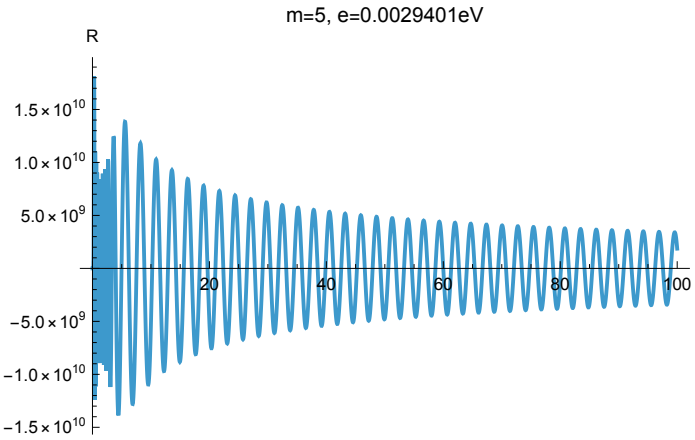

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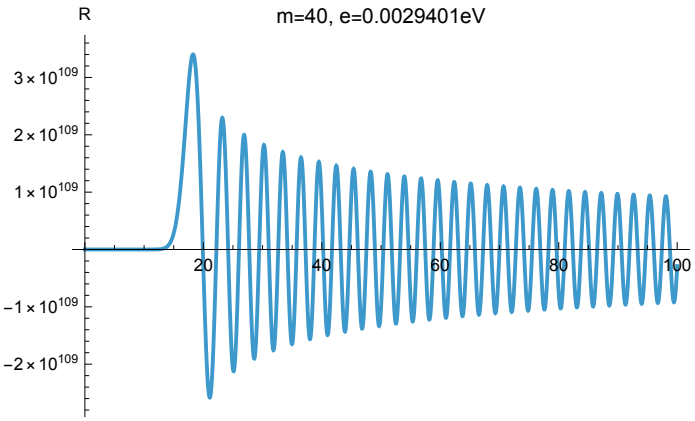

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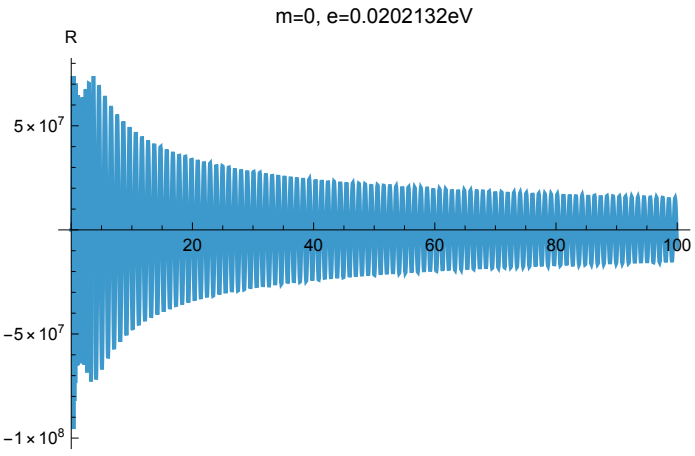

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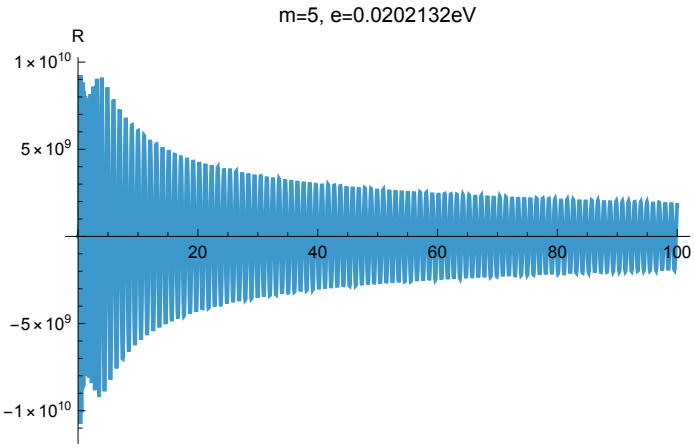

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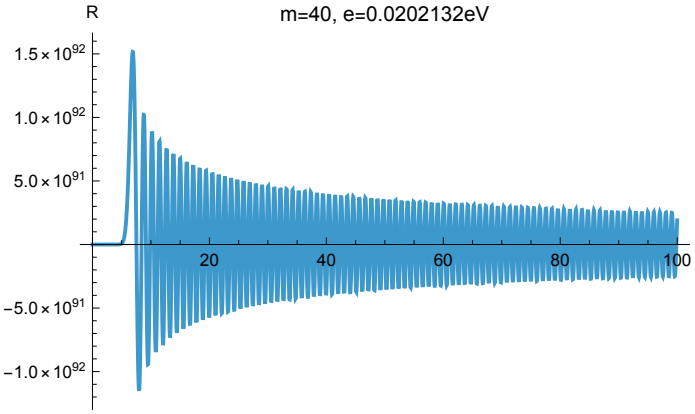

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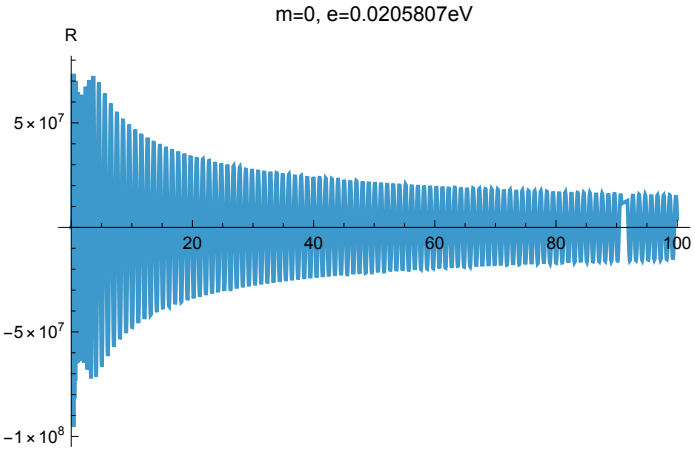

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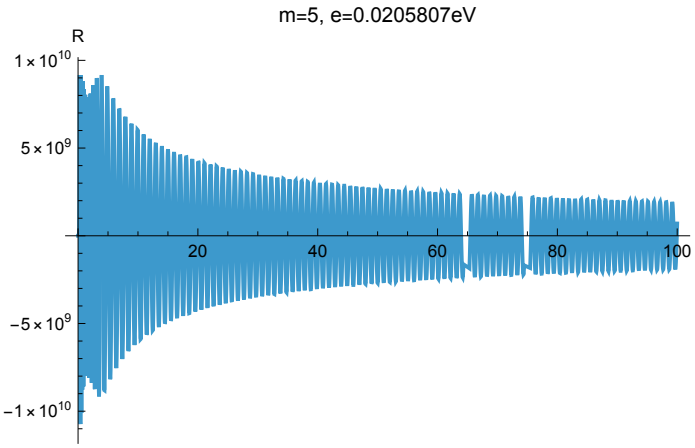

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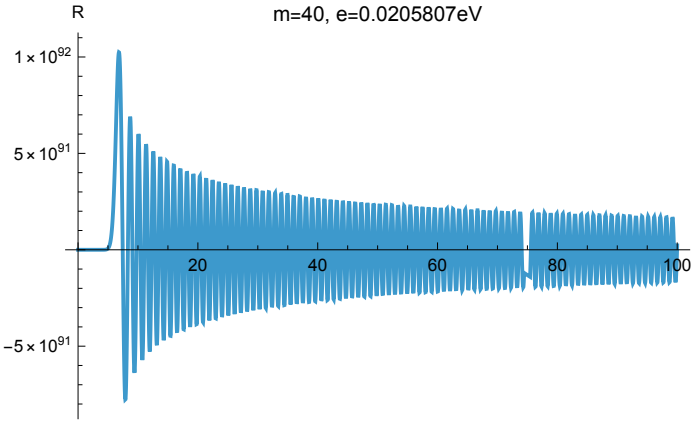

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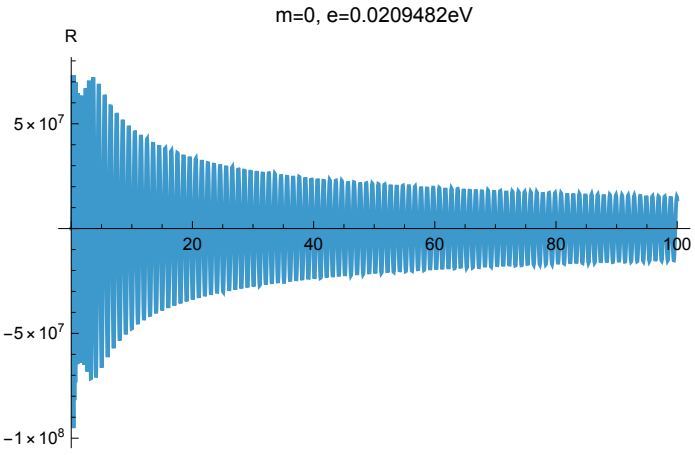

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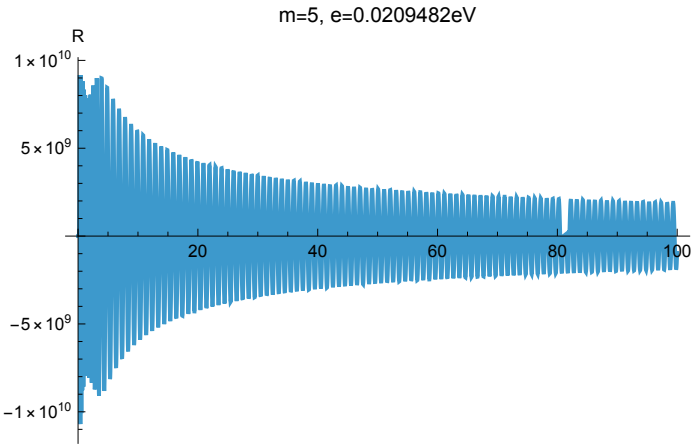

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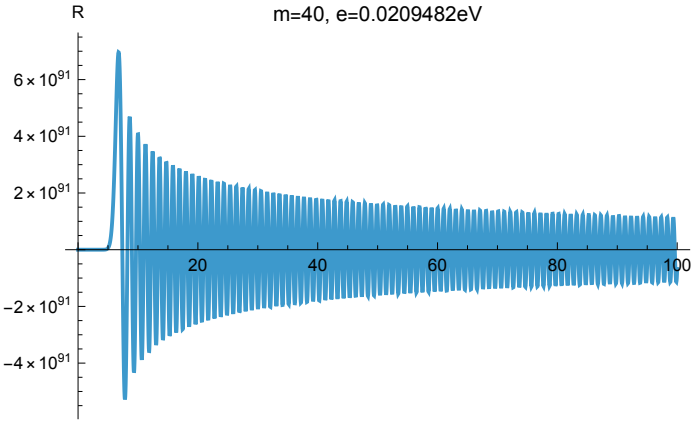

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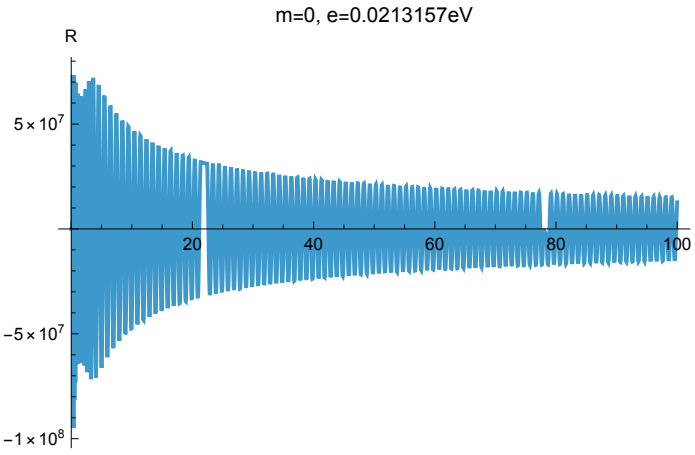

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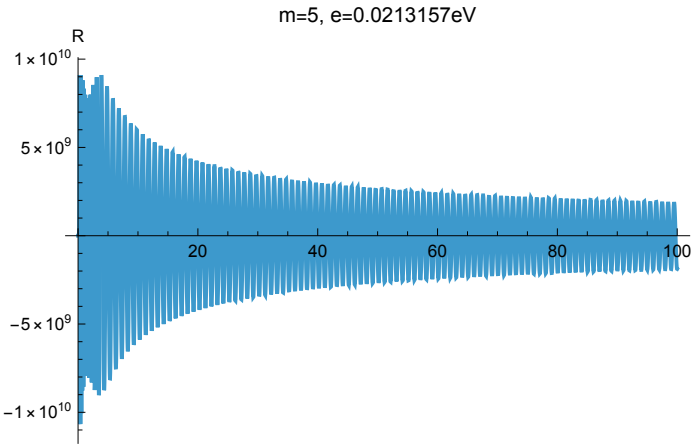

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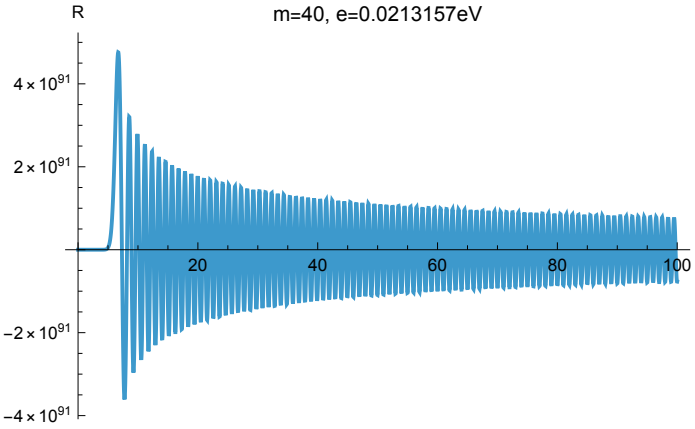

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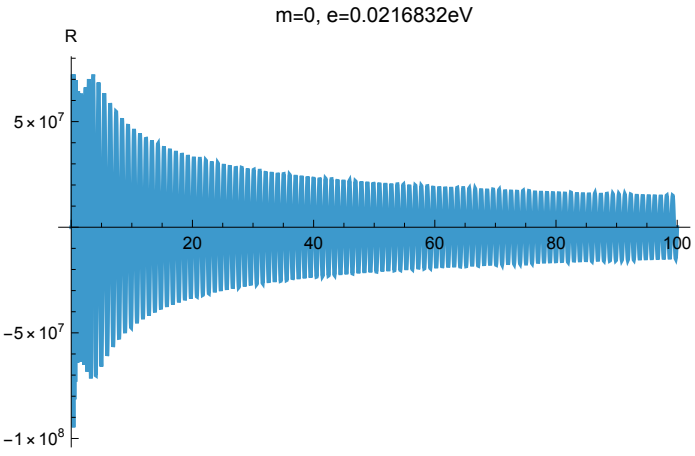

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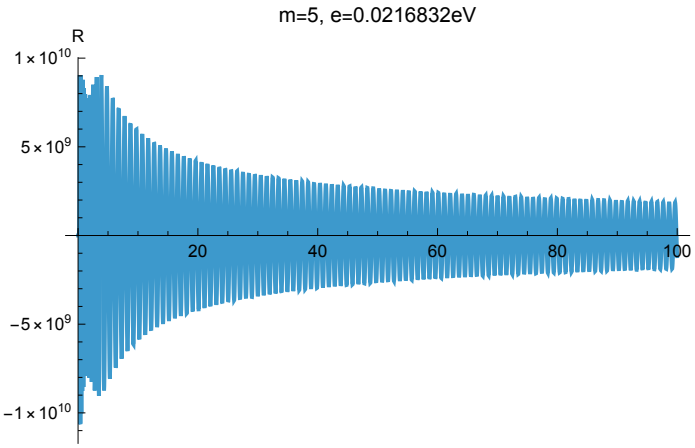

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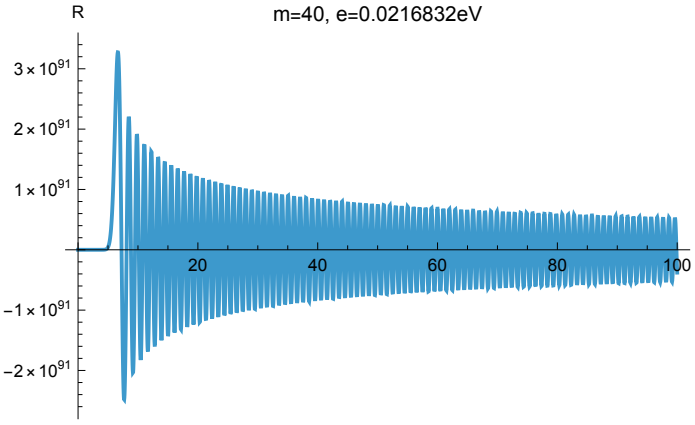

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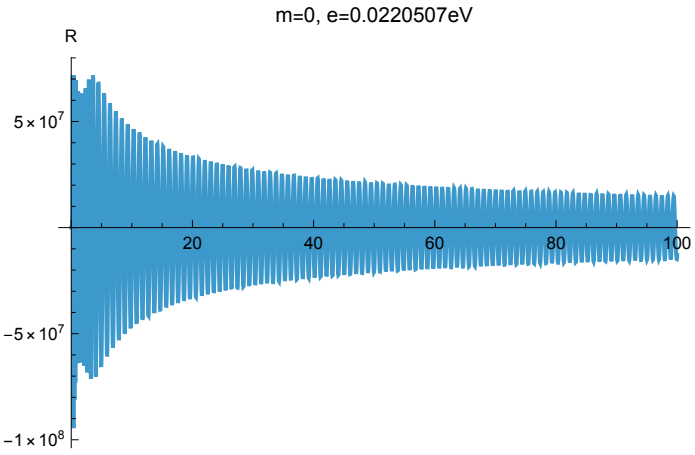

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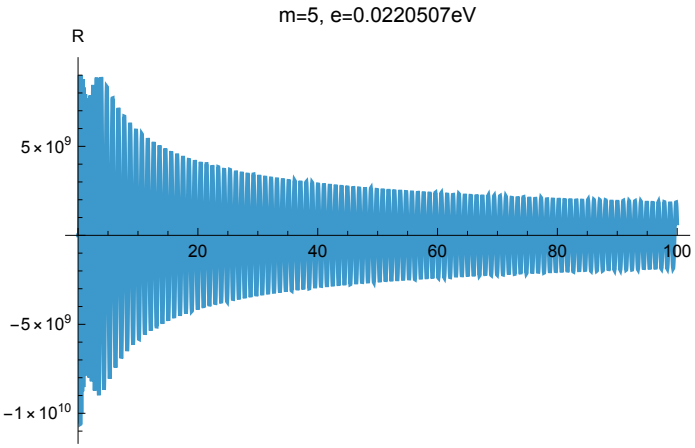

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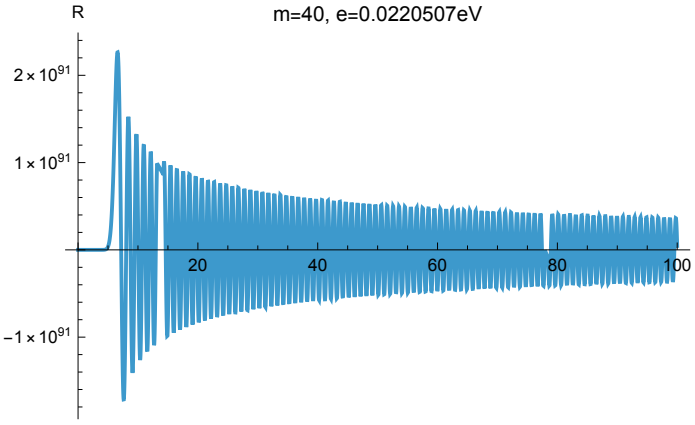

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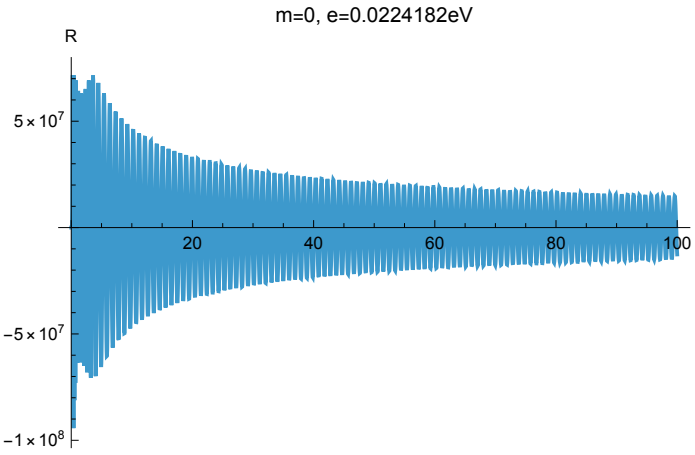

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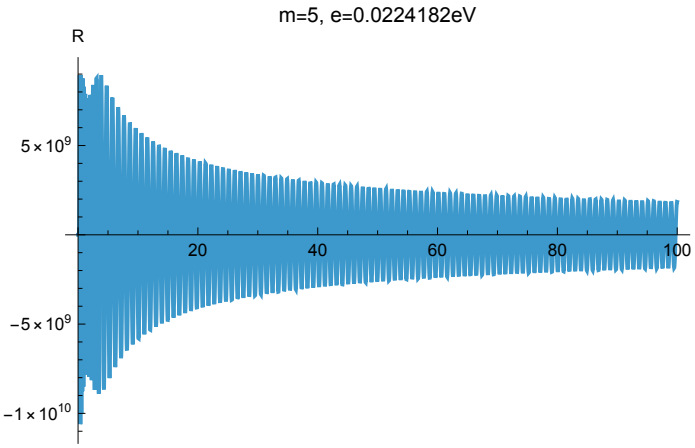

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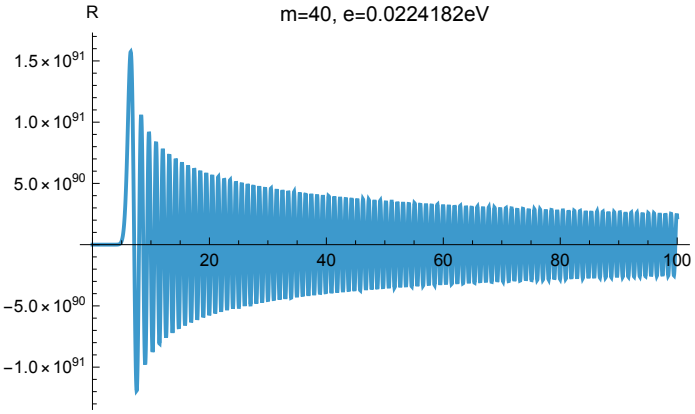

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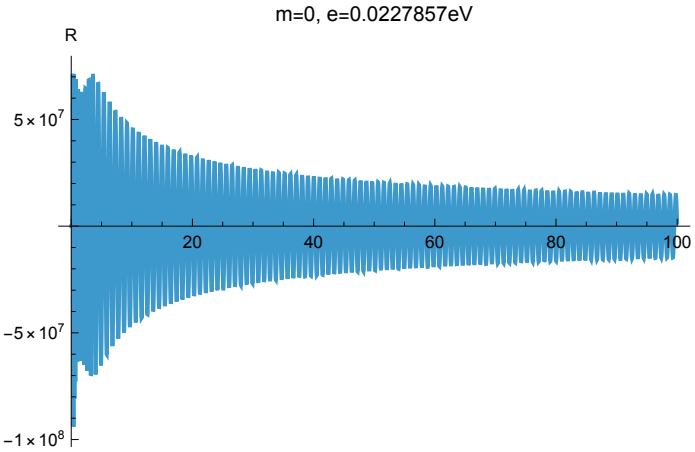

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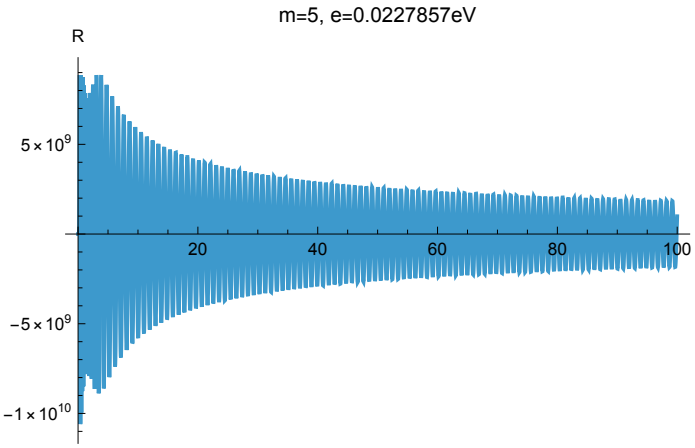

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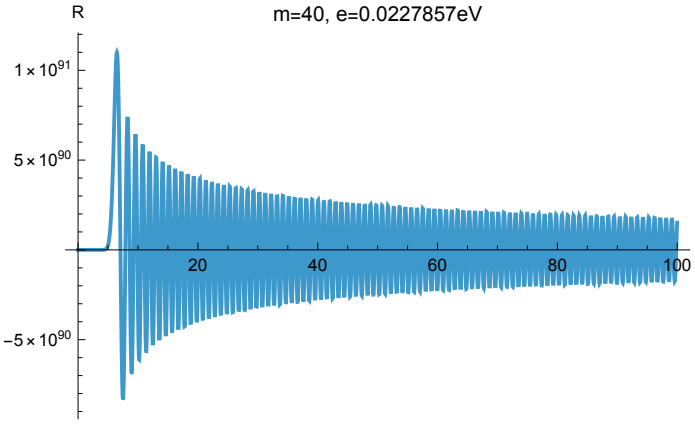

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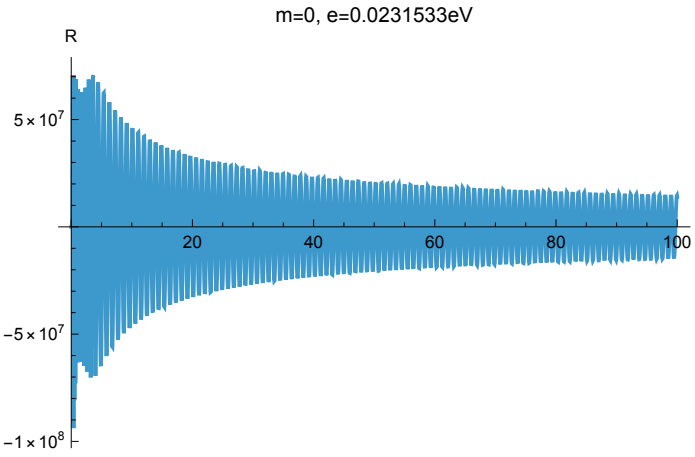

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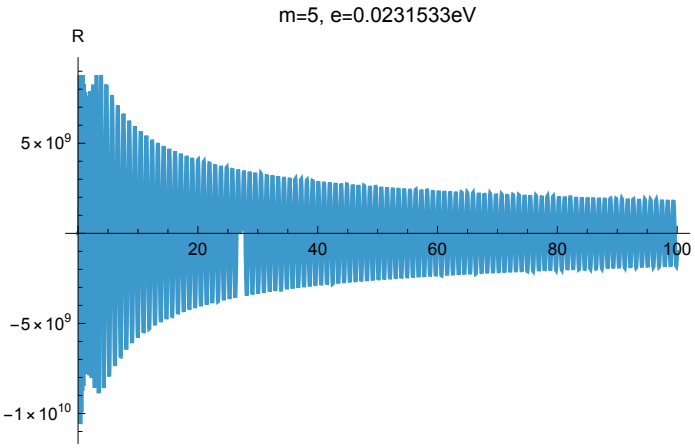

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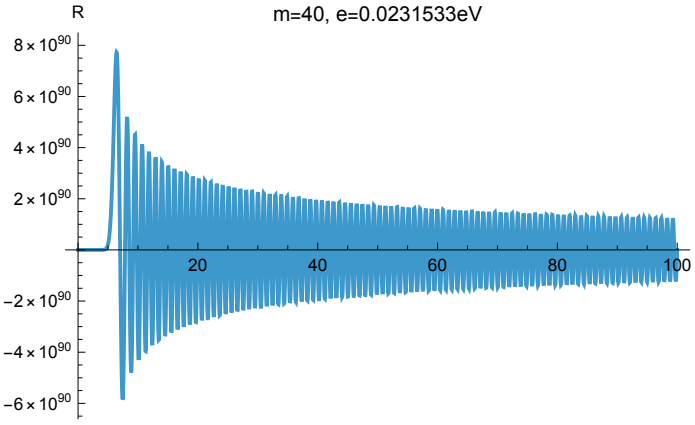

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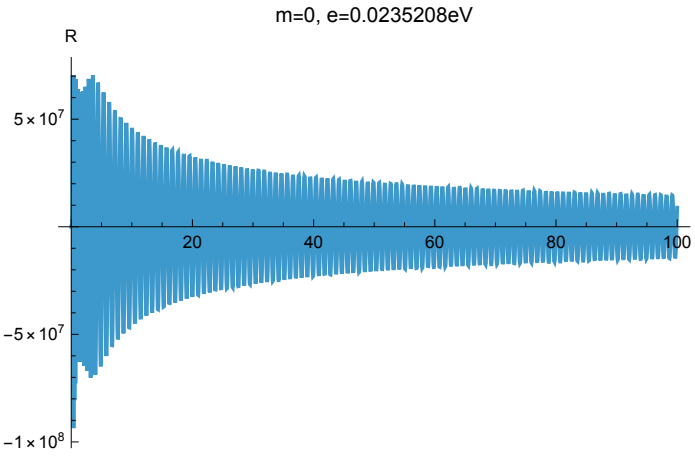

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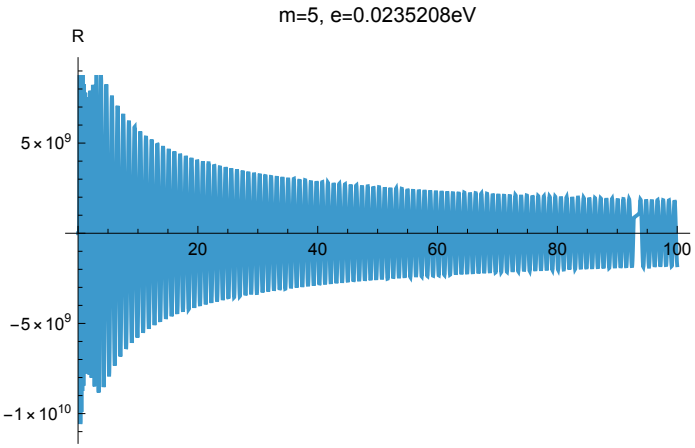

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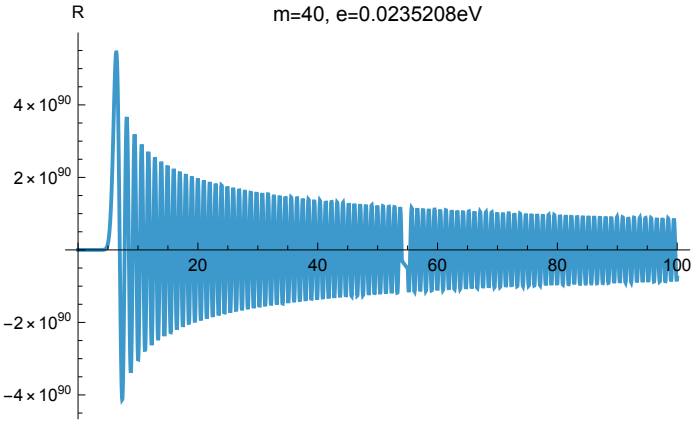

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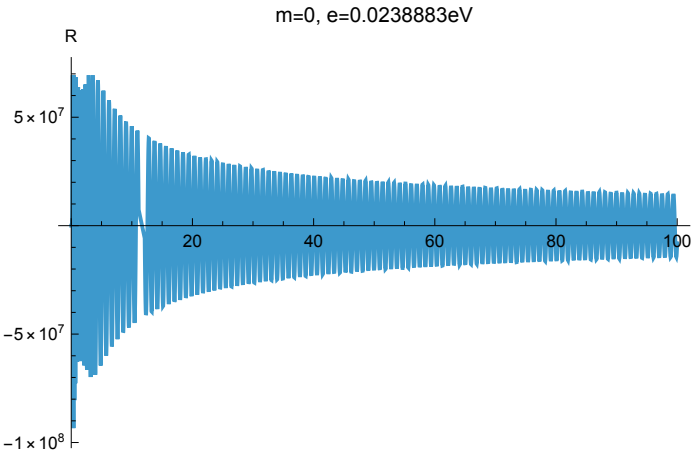

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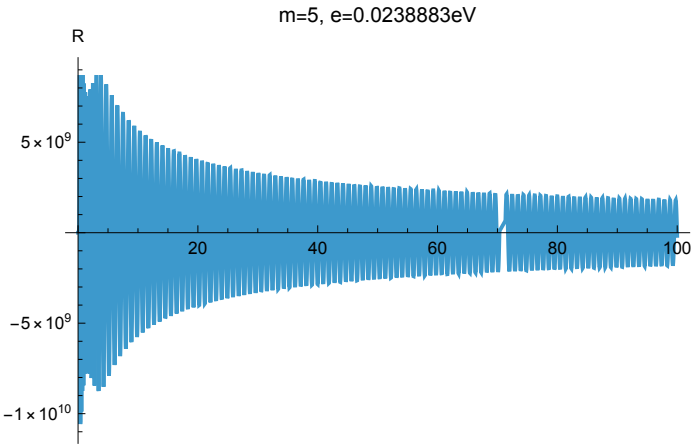

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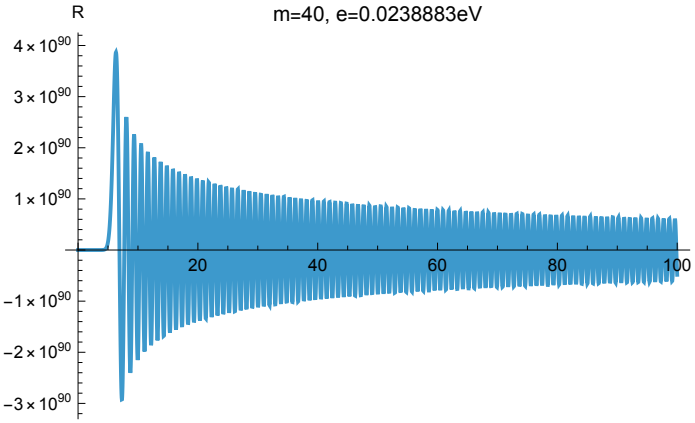

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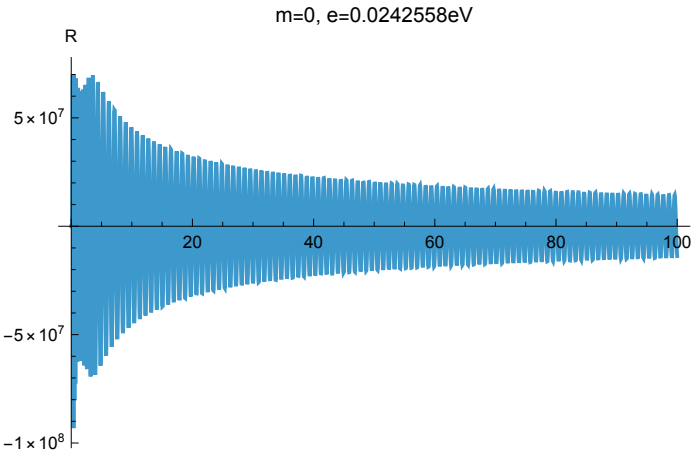

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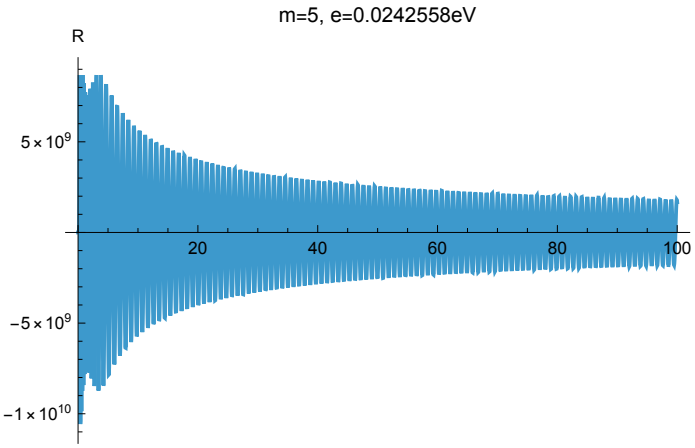

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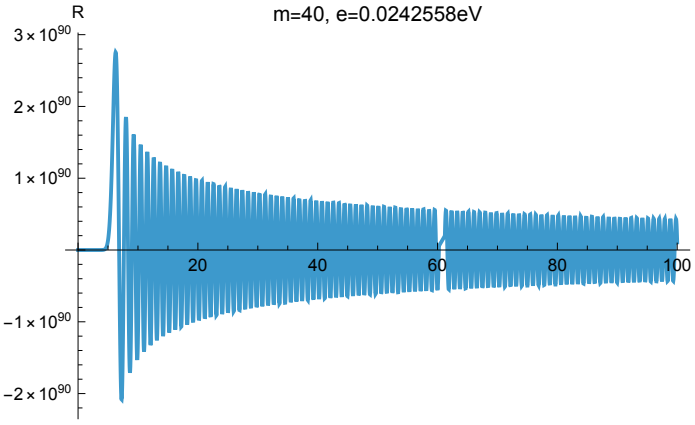

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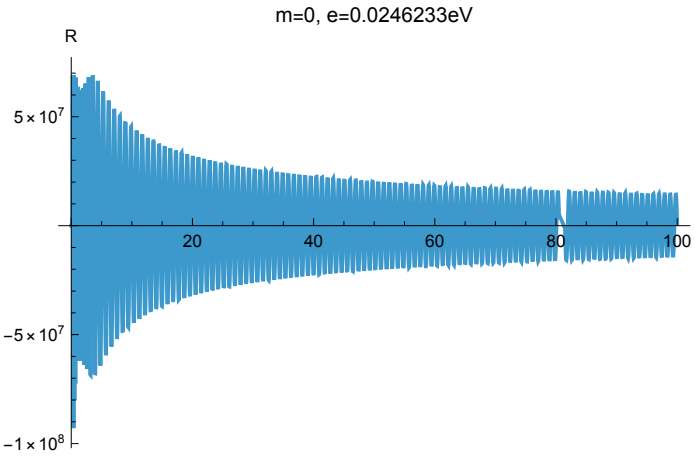

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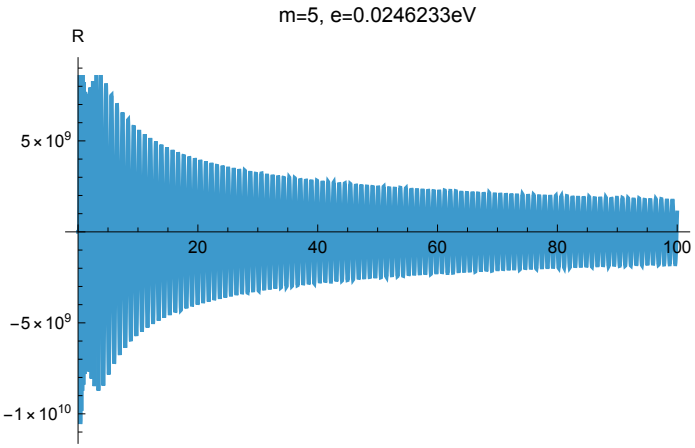

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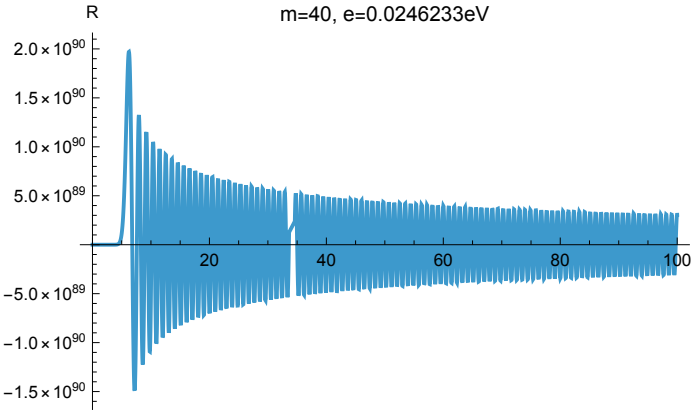

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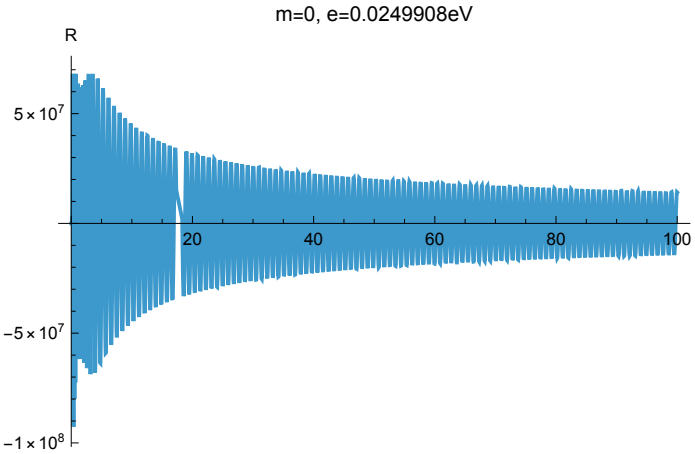

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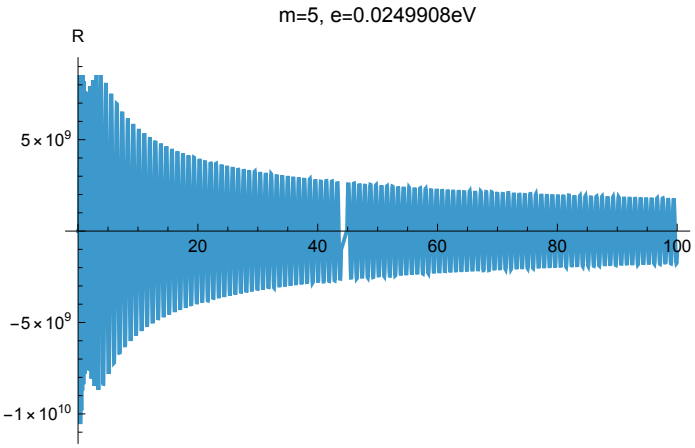

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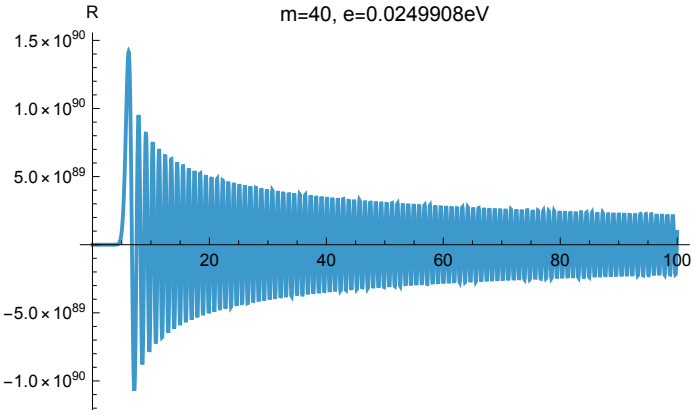

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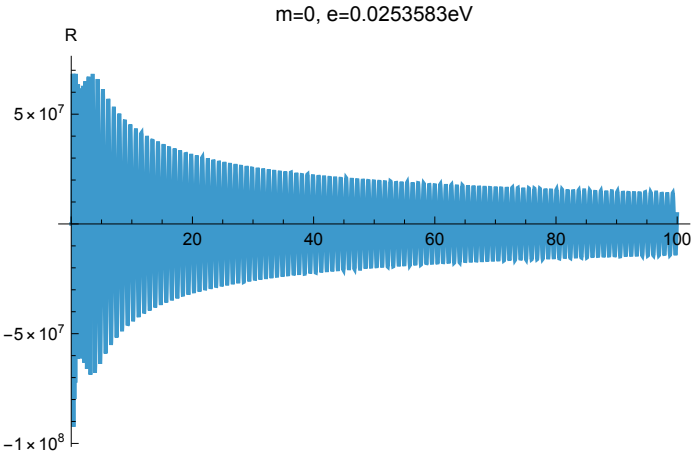

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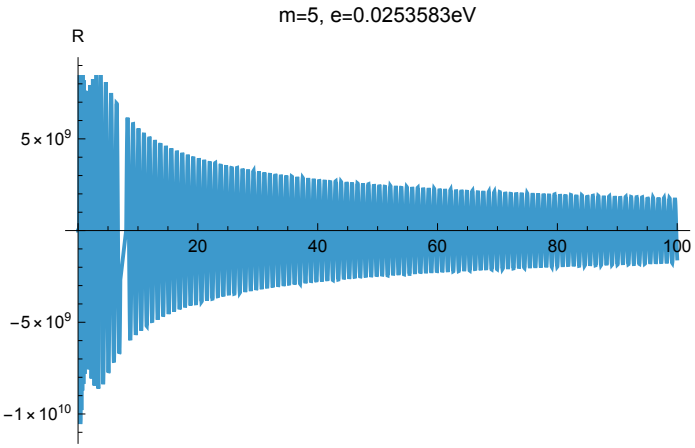

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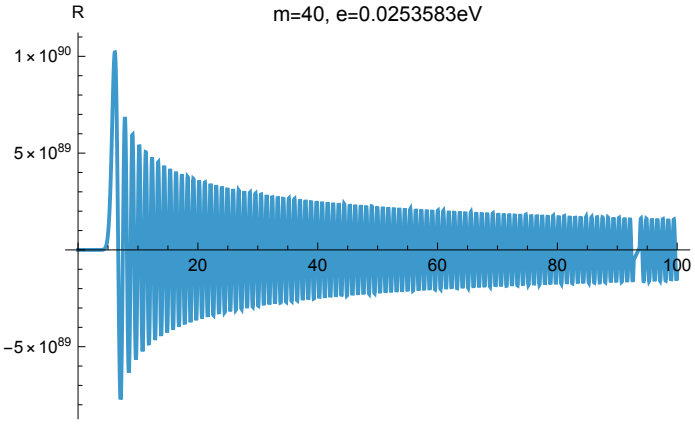

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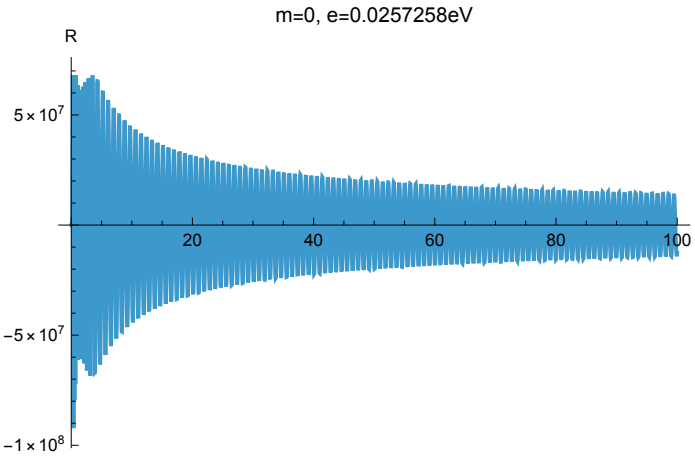

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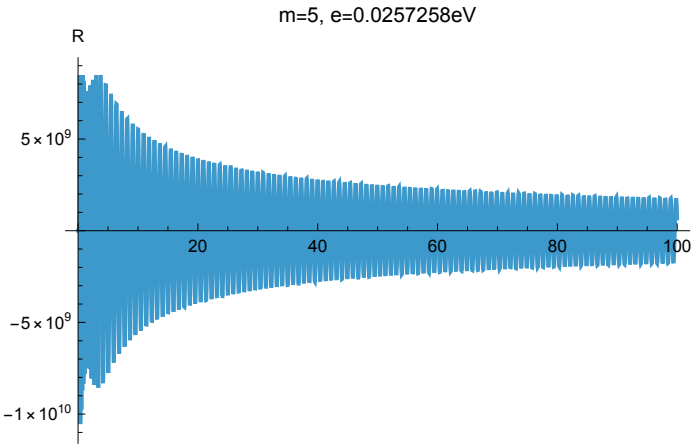

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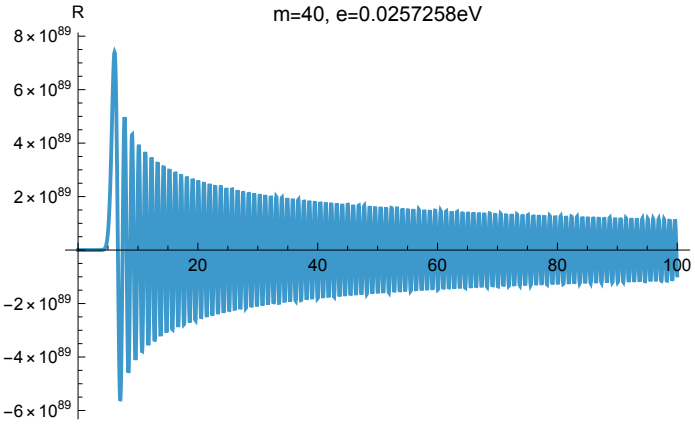

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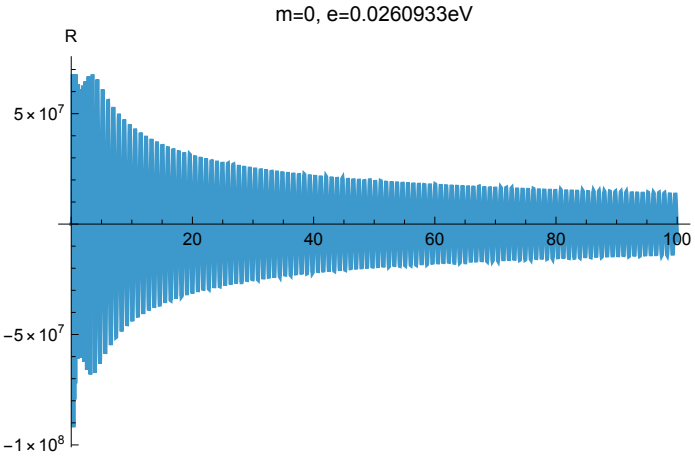

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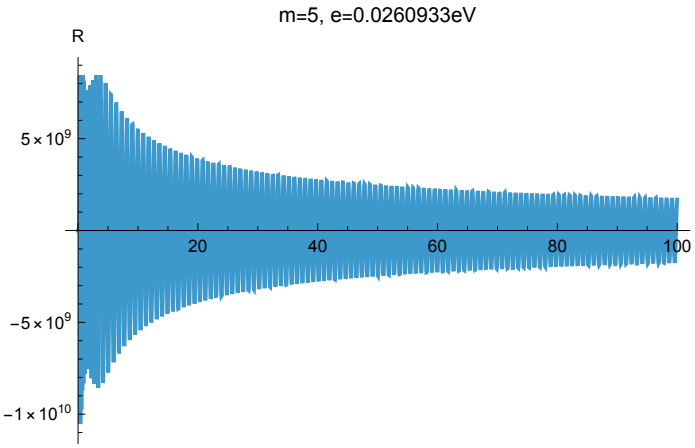

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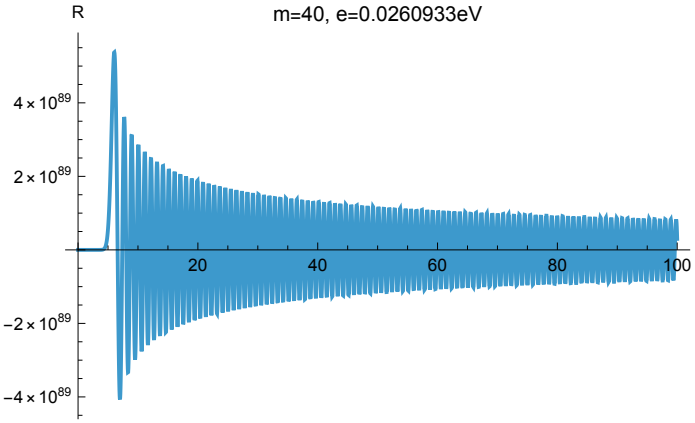

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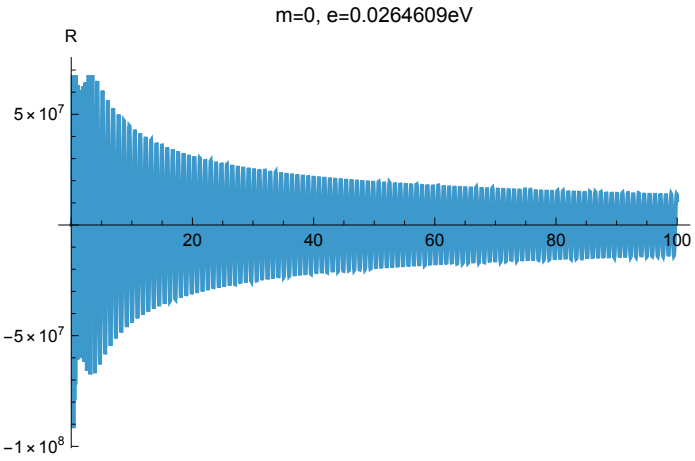

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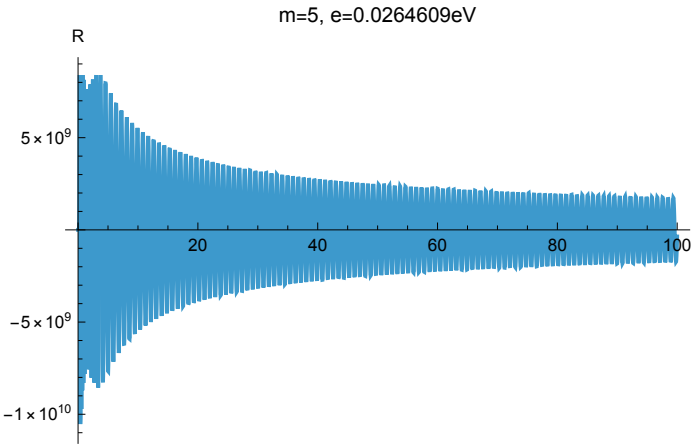

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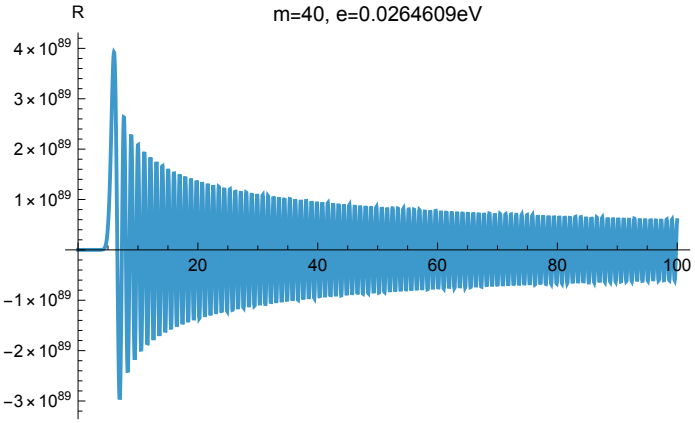

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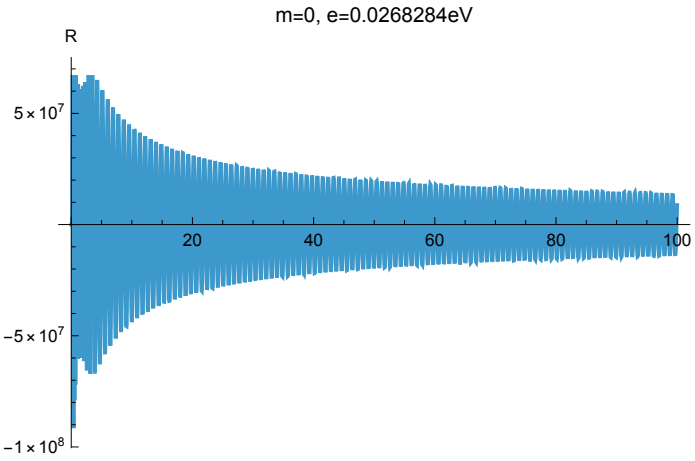

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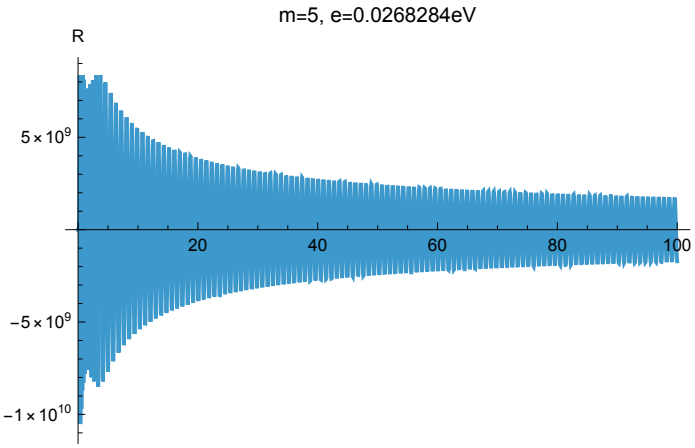

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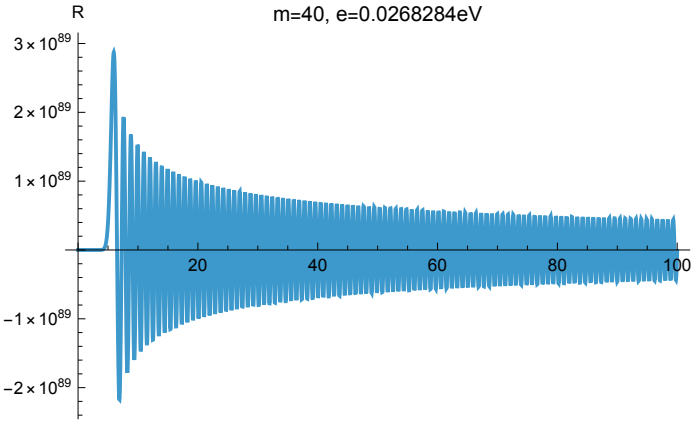

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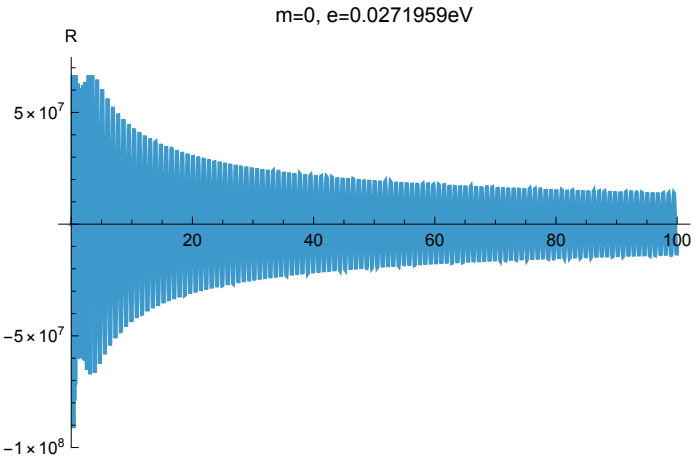

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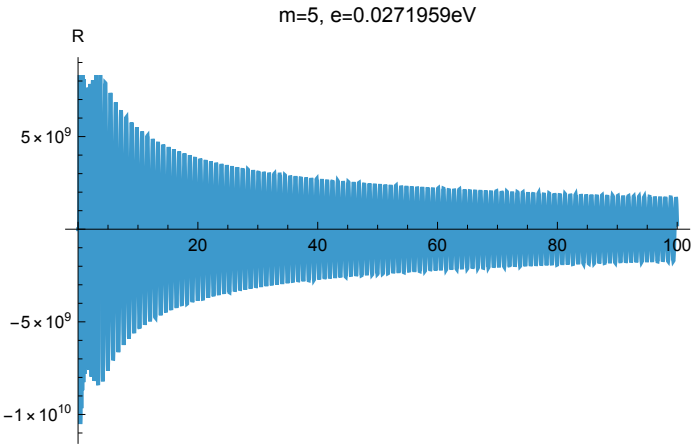

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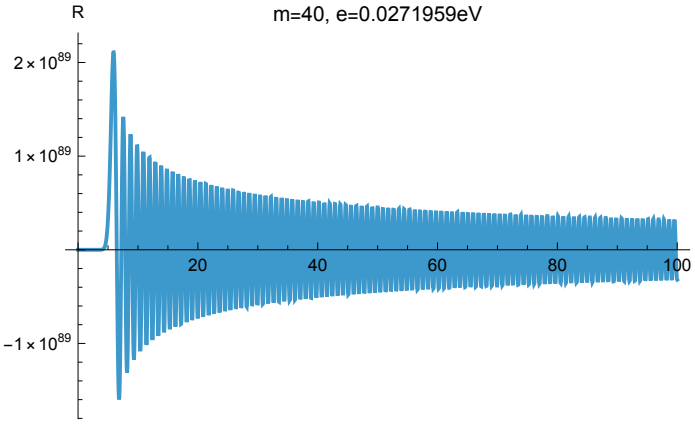

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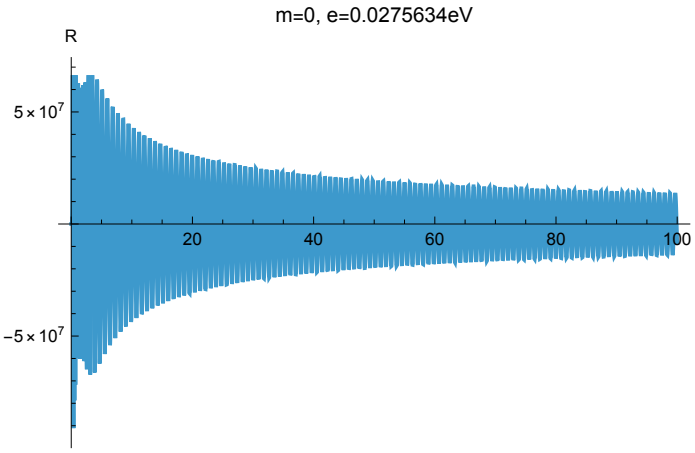

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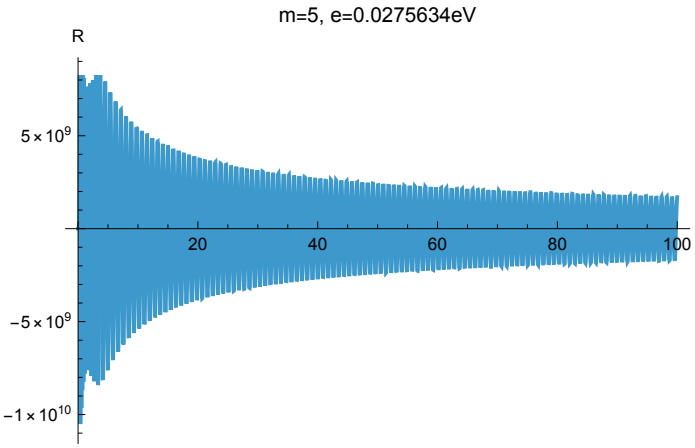

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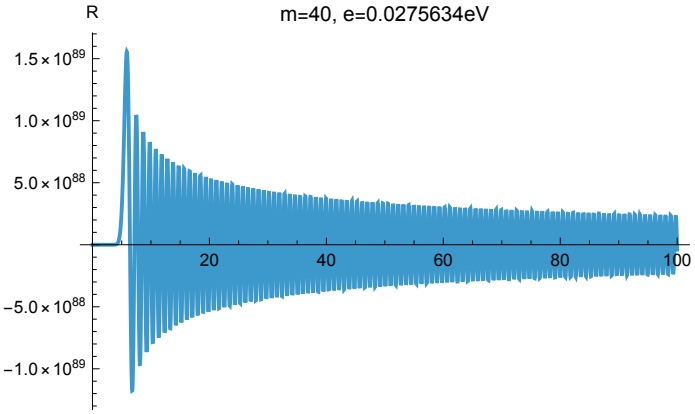

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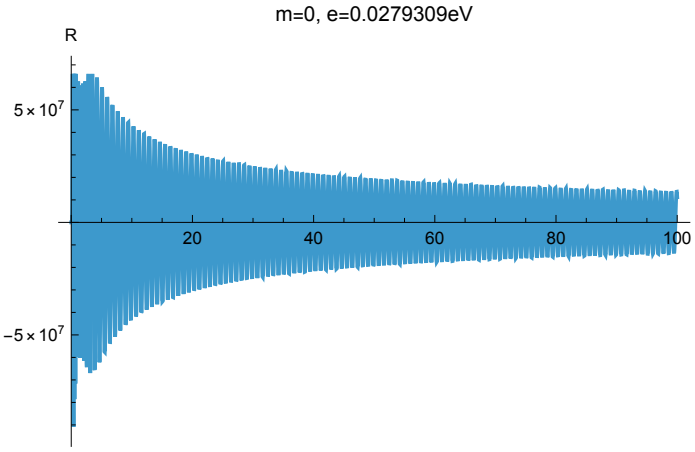

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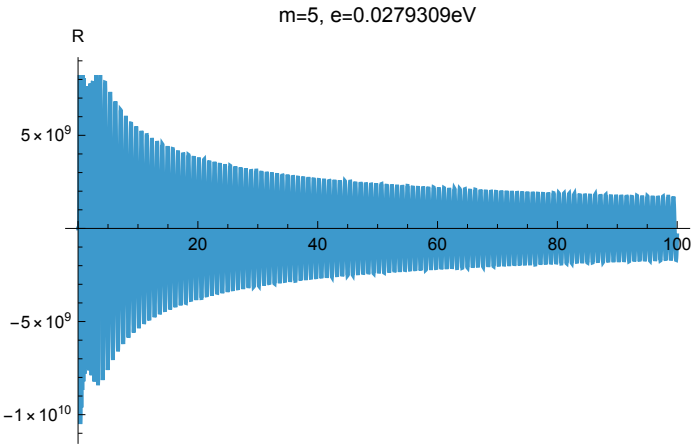

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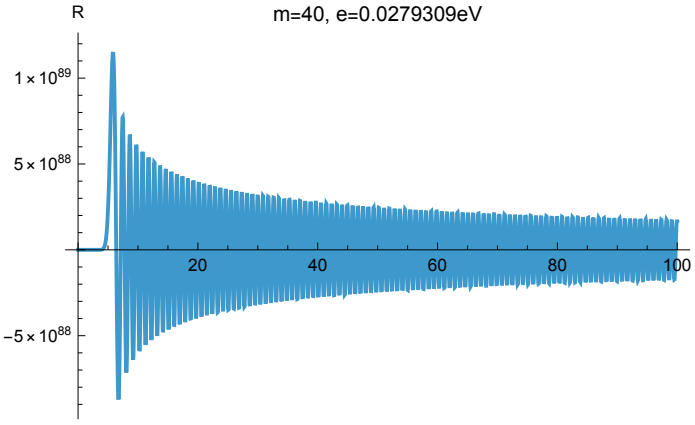

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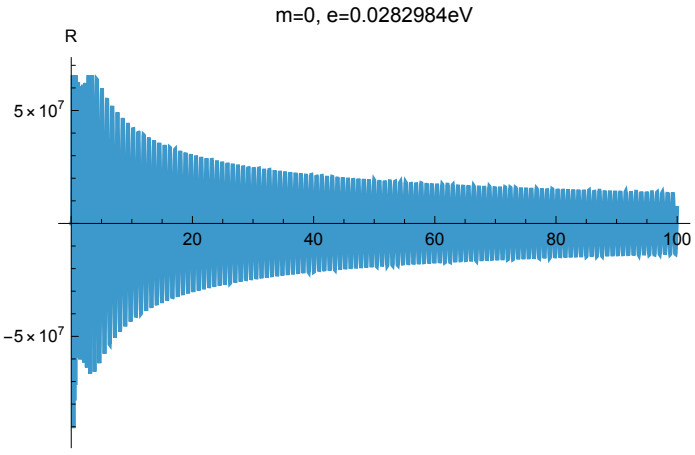

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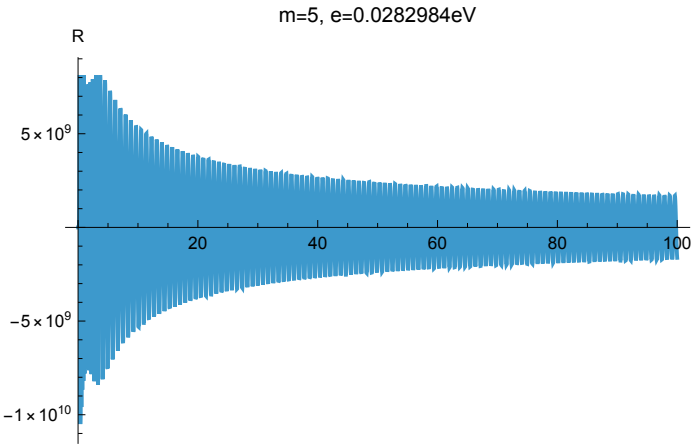

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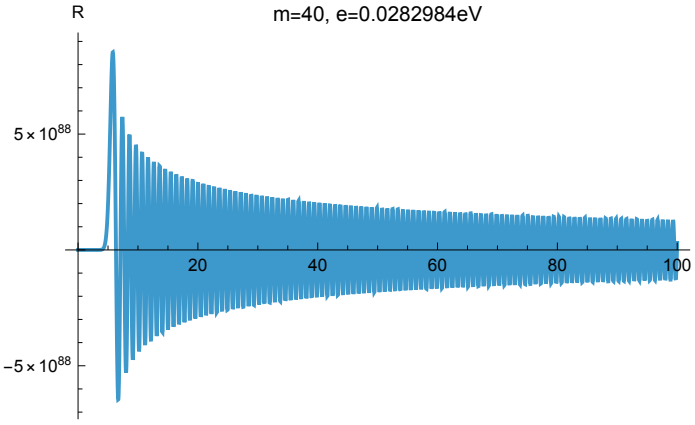

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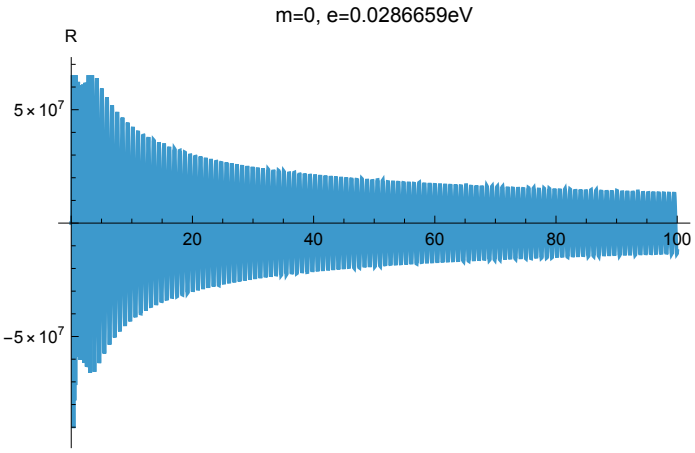

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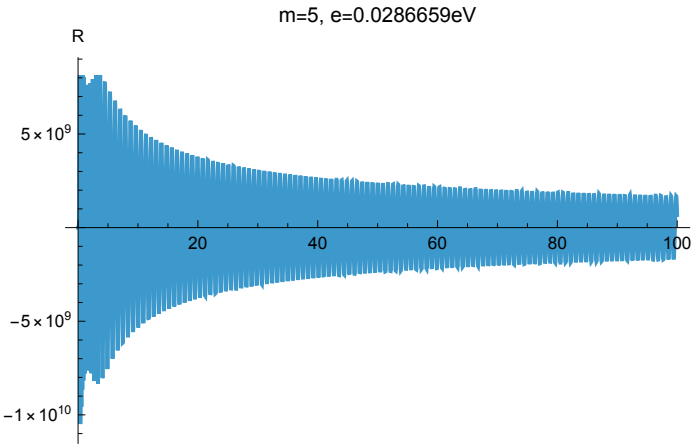

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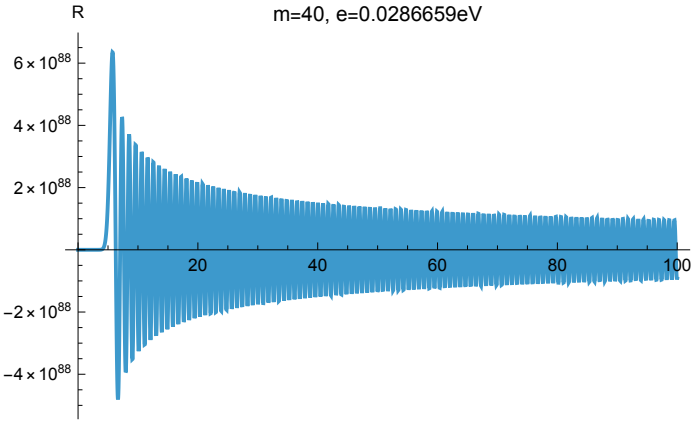

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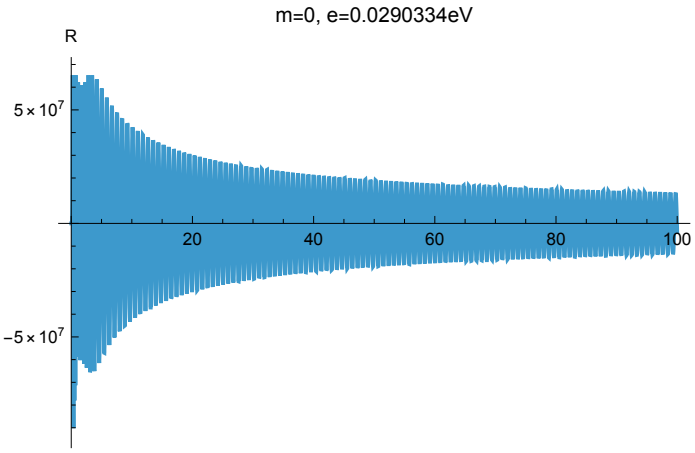

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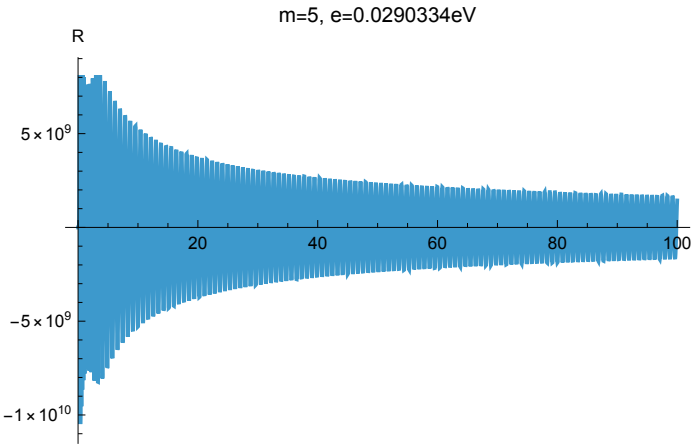

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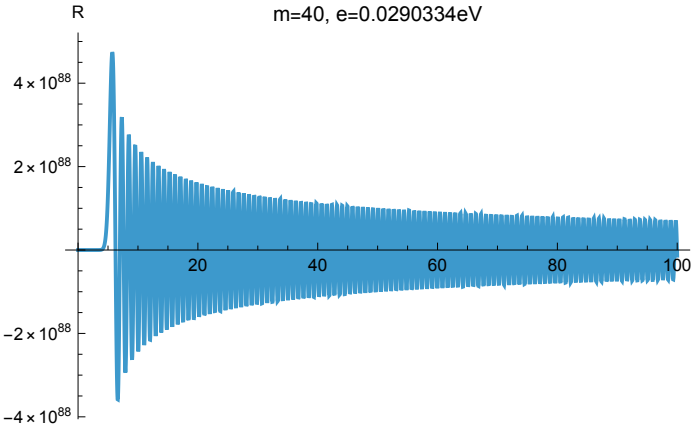

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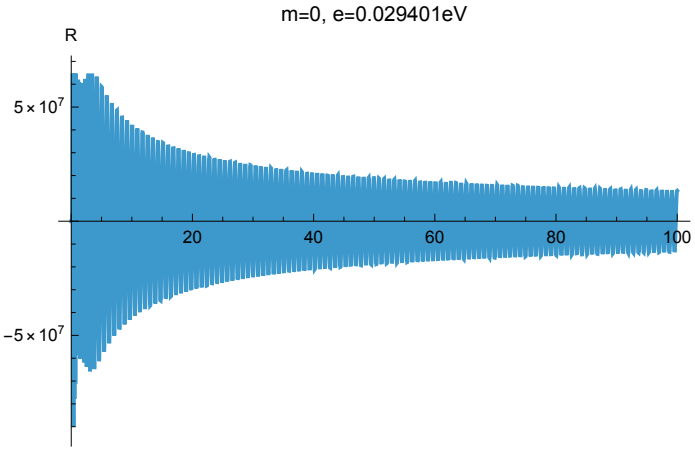

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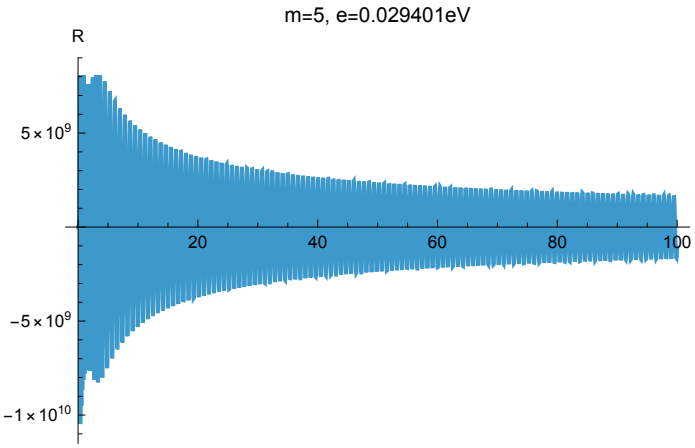

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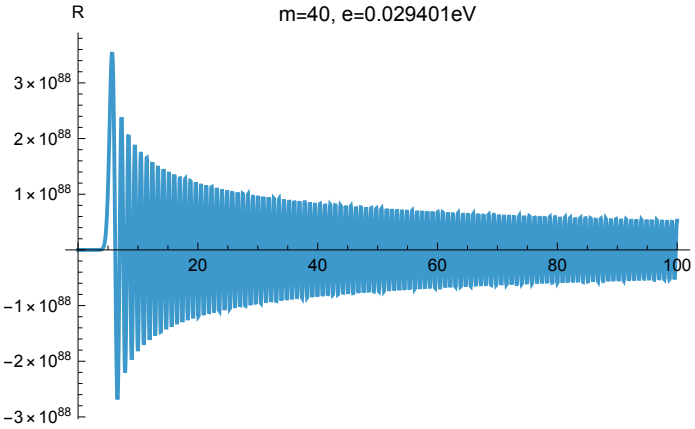

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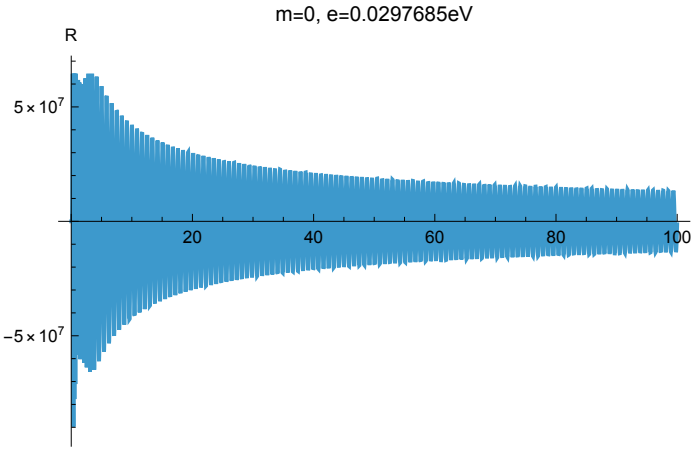

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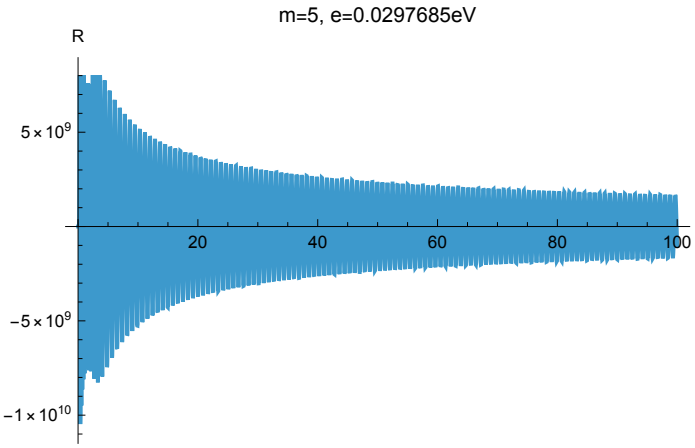

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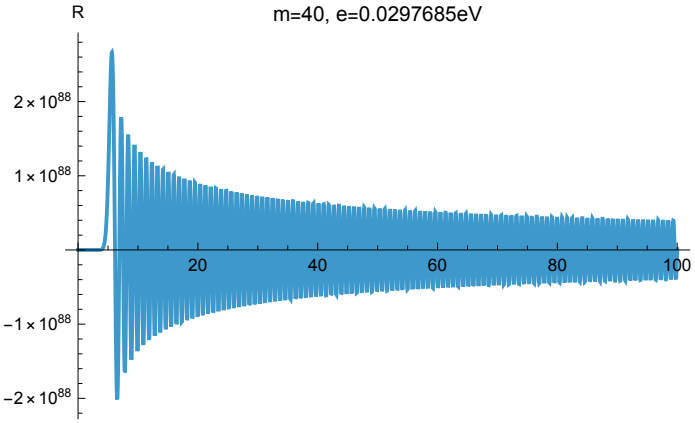

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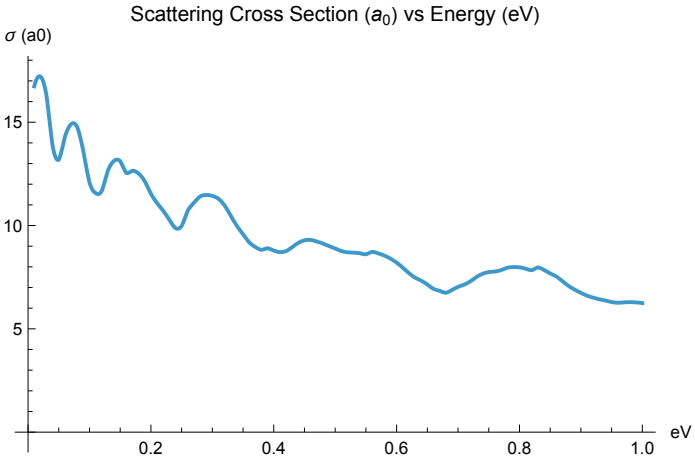

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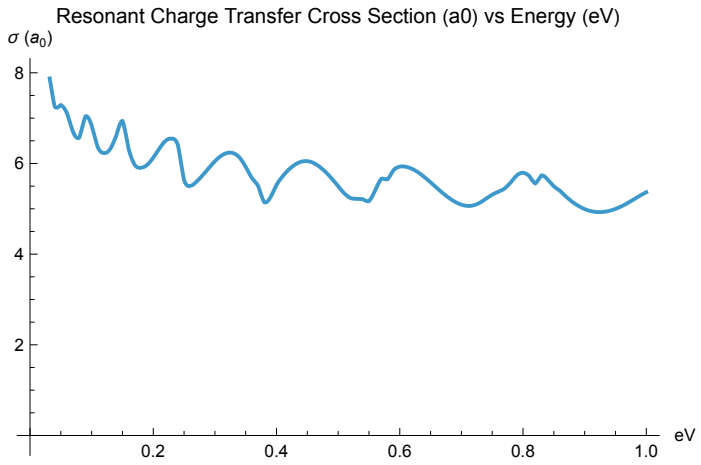
Resonant Charge Transfer Cross Section (a0) vs Energy (eV)
σ (a0)
8
6
4
2
0.2
0.4
0.6
0.8
1.0
eV