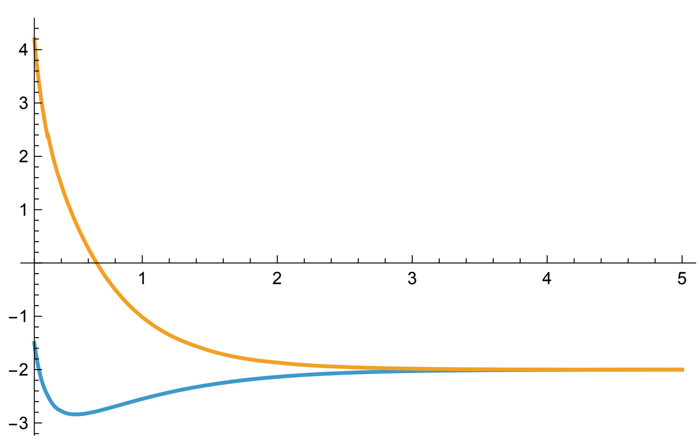
```
In[2]:= (* this routine needs to run Vpots.nb *)

In[3]:= 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 → 200000]];
    solsU = Flatten[NDSolve[
       {equU == 0, yu[r0] == 0, yu'[r0] == 1}, yu, {r, r0, rend}, MaxSteps → 200000]];
    fg[r_] = yg[r] /. solsG;
    fu[r_] = yu[r] /. solsU;
    (*If[(e > 0.002 && e < 0.004) && (m==40  || m==0),
     Print["k=",k];
     Print[Plot[fg[r],{r,r0,rend},PlotLabel→
        StringJoin["m=",ToString[m],", e=",ToString[e],"eV"],AxesLabel→"R"]]];
    Print[Plot[fg[r]-fu[r],{r,r0,rend}]]*)
    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[19]=



Out[21]=

```
0.695
```

In[26]:=

```
(* 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 = Sqrt[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}];
(*crossSection // TableForm*)
```

In[∘]:=

```
crossSectionGraphSC =
 Interpolation[{crossSection[[All, 1]], crossSection[[All, 2]][[All, 1]]} // Transpose]
crossSectionGraphCT =
  Interpolation[{crossSection[[All, 1]], crossSection[[All, 2]][[All, 2]]} // Transpose];
```

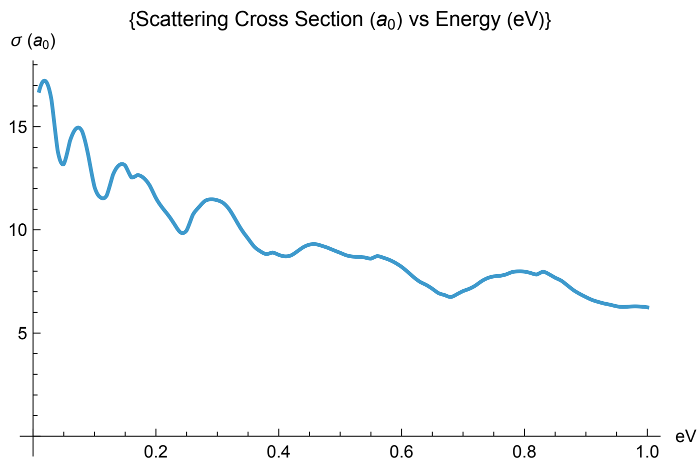
Out[∘]=

```
InterpolatingFunction[ Domain: {{0.01, 1. }} Output: scalar ]
```

In[∘]:=

```
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)"}]
```

Out[∘]=



Out[∘]=