In[14]:=

```
(* All atomic units *)
μ = 1835;
mP = 1836;  (* Proton mass *)
hbar = 1;
c = 137 ;(*SpeedOfLight, atomic units*)
(* 1 kelvin[K]=8.61732814974056E-05 electron-volt[eV]*)
(* 1 Hartree = 27.2114eV *)
R0 = 0.01; (* Min distance between nuclei, atomic units*)

(* Potential tables for the gerade and ungerade case *)
vSg1Data  =
  Import["~/Work/Physics-Thesis/thesis-2/ZelimirOverleaf/MathematicaCodeFinal/
     gerade1sV2.mx"];
vSu1Data =
  Import["~/Work/Physics-Thesis/thesis-2/ZelimirOverleaf/MathematicaCodeFinal/
     ungerade1sV2.mx"];

(* Max value of R for calculation *)
maxR = 50;


(*vSg1Data = Prepend[vSg1Data,{0,-8.0, 10^100,25.8,0,.11}];
vSu1Data=Prepend[vSu1Data,{0,-0.889,  10^100,25.81,0.041}];*)

(* Interpolatte the potential *)
vGerade := Interpolation[Transpose[{vSg1Data[[All, 1]], vSg1Data[[All, 3]]}]];
vUngerade := Interpolation[Transpose[{vSu1Data[[All, 1]], vSu1Data[[All, 3]]}]];

(* Calogero's differential equation to compute the phase shift delta *)
deltaPrime[vPotential_, r_, k_, m_, delta_] := Module[{Jm, Ym, psi},
   Jm = BesselJ[m, k * r];
   Ym = BesselY[m, k * r];
   psi = Jm * Cos[delta] - Ym * Sin[delta];
   -vPotential[r] * psi ^ 2 / k
  ];

(* Calogero's method to compute the phase shift delta *)
delta[deltaPrime_, vPotential_, k_, m_] := Module[{solDelta, deltaEq, deltaFinal},
   (* Calogero *)
   solDelta = NDSolve[
     {deltaEq'[r] == deltaPrime[vPotential, r, k - vPotential[50], m, deltaEq[r]],
      deltaEq[0.01] == 0}, deltaEq, {r, 20, 50}];
```

```
   deltaFinal = deltaEq[50] /. solDelta⟦1⟧ // N;

   deltaFinal
  ];

(* some constants for reference *)
(* 1Kelvin = 7.733675709525194`*^-7 Hartree *)
(* 1 a0 (Bohr radius = 5.29177210544*10^-11 m
     1 barn = 10^-28
      1 a^2_0=5.29177210544`*^-22 = 5.29177210544`*^6 barn
   *)
(* Scattering at around room temperature, 270-310K *)
(* kB = 3.167*10^-6  EH/T (Boltzman) *)
(* k = Sqrt[2mE/ħ] *)
(* 1 EH=3.1577464 x 10^5 K *)
(* 270K = 0.000855 EH => k = 0.0413531175145633 *)
(*300K = 0.00095 EH => k = 0.0435900132315404 *)
⋮

 (* Compute deltas for the gerade and ungerade case *)
 deltaGer[k_,m_]:= delta[deltaPrime,vGerade,k,m];
 deltaUng[k_,m_]:= delta[deltaPrime,vUngerade,k,m];

 diff[k_,m_]:=deltaGer[k,m]-deltaUng[k,m];

 Plot[diff[(k^2)*3.1577464*^5 /2, 0],{k,270,300},
  AxesLabel->{"T Temperature (K)","Phase Shift Ger, Ung"},
  PlotLabel->"Phase Shift Gerade & Ungerade vs Temperature (K)"]
```

```
eps[m_] := If[ m == 0, 1, 2];

m = 0;
(* Scattering length *)
λ[k_, m_] := 4/k Sum[eps[i] (Sin[deltaGer[k, i] - deltaUng[k, i]])^2, {i, 0, m}];

allLambda[m_] := Table[{k, λ[k, m]} , {k, 0.0413, 0.04359, 0.0001}];

(* Cross section in atomic units *)
 scatteringLength := allLambda[m] ;

(* temp in Kelvins *)
scatteringLengthK := Transpose[
   {(scatteringLength[[All, 1]] ^ 2) * 3.1577464*^5 / 2, scatteringLength[[All, 2]]}];

f = Interpolation[scatteringLengthK, InterpolationOrder → 2];

Plot[f[x],
 {x, scatteringLengthK[[1, 1]], scatteringLengthK[[Length[scatteringLength], 1]]},
 Epilog → Point[scatteringLength], AxesLabel → {"T Temperature (K)", "λ (a.u.)"},
 PlotLabel → "Scattering Length (a.u.) vs Temperature (K)"]
```