Characterization of the critical magnetic field in the Dirac – Coulomb equation

Jean Dolbeault, Maria Esteban and Michael Loss

LANDAU LEVELS IN THE z VARIABLE

Definitions

```
Off[NDSolve::"ndnum"]
Off[ReplaceAll::"reps"]
Off[General::"spell"]
Off[NDSolve::"ndnl"]
```

$\alpha = \frac{1}{137.037}$;

```
units = 4.414015614986747`*^9;
```

$a[z\_] := e^{\frac{z^2}{2}} \sqrt{\frac{\pi}{2}}\ \mathrm{Erfc}\left[\frac{\sqrt{z^2}}{\sqrt{2}}\right]$

$b[z\_] := \sqrt{z^2} + e^{\frac{z^2}{2}} \sqrt{\frac{\pi}{2}}\ \mathrm{Erfc}\left[\frac{\sqrt{z^2}}{\sqrt{2}}\right]$

```
aa[z_] := a'[z]
```

$c[z\_] := 1 - \frac{1}{2} e^{\frac{z^2}{2}} z^2 \left(\mathrm{Gamma}\left[0, \frac{z^2}{2}\right] + \mathrm{Log}\left[\frac{1}{z^2}\right] + \mathrm{Log}[z^2]\right)$

- **The first eigenvalue is searched in the interval (λmin, λmax) using a step λstep**

```
λmin = -0.5;
λmax = 0.1;
λstep = 0.02;
```

- **The method uses a dichotomy. The criterion to stop is that the relative change is less than ϵ**

$\epsilon = 10^{-10}$;

- **To find a consistent way of determining zmax, we require that the value of z is at least equal to zmaxinit, and increase it by deltaz until the difference becomes less than criterionz. Note that the criterion is on an absolute erros so that it is looser for small values of ν**

```
zmaxinit = 100;
deltaz = 10;
criterionz = 10^-4;
```

- **Table of the values of ν for which we compute the first eigenvalue**

```
TableNu = Table[0.5 + 0.025 i, {i, 0, 20}]

{0.5, 0.525, 0.55, 0.575, 0.6, 0.625, 0.65, 0.675, 0.7, 0.725,
 0.75, 0.775, 0.8, 0.825, 0.85, 0.875, 0.9, 0.925, 0.95, 0.975, 1.}
```

Estimate of the error and definition of the interval

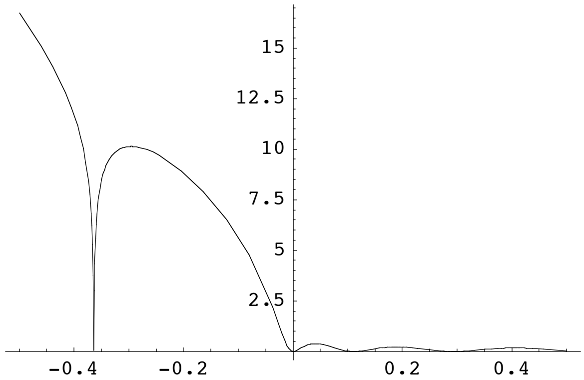
```
Hfinal[ν_, λ_, zmax_] := Evaluate[f[zmax]^2 /. EQN]

MnH[ν_, λ_, h_, V_, zmax_] :=
 Module[{v = N[Hfinal[ν, λ + h, zmax][[1]]]}, If[Abs[(v - V)/V] < ϵ, {λ, h, v},
   If[v > V, MnH[ν, λ + h, -h/2, v, zmax], MnH[ν, λ + h, h, v, zmax]]]]
MinH[ν_, λ_, h_, zmax_] := MnH[ν, λ, h, N[Hfinal[ν, λ, zmax][[1]]], zmax]

RRb[ν_, zmax_] := MinH[ν, λmin, λstep, zmax][[1]]

IterSearchZmax[ν_, z_, h_, δ_, v_] :=
 Module[{vv = RRb[ν, z + h]}, If[Abs[vv - v] < δ, z, IterSearchZmax[ν, z + h, h, δ, vv]]]
SearchZmax[ν_, z_, h_, δ_] := IterSearchZmax[ν, z, h, δ, RRb[ν, z]]
```

Computation with the functions a and b

```
EQN = NDSolve[{g'[z] == -(z a[z])/b[z] g[z] - ν/b[z] (λ + ν a[z]) f[z],
    f'[z] == g[z], f[0] == 1, g[0] == 0}, {f, g}, {z, 0, zmax}];
Hfinal[ν_, λ_, zmax_] := Evaluate[f[zmax]^2 /. EQN]
```

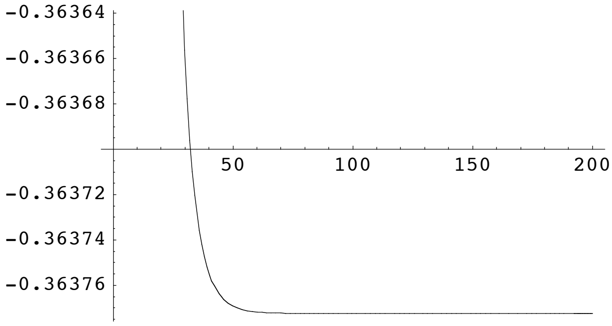
■ Recherche dur premier point critique

```
Plot[Log[1 + Hfinal[0.9, λ, 100]], {λ, -0.5, 0.5}];
```



■ Dépendance dans la taille du domaine

```
Plot[RRb[0.9, z], {z, 10, 200}];
```



■ Table de résultats numériques

```
(* TableResults=Table[ Module[{egv=RRb[TableNu[[i]],170]},
    {TableNu[[i]], TableNu[[i]]/α ,egv, 4/egv^2 ,Log[10, 4*units/egv^2 ]}],{i,1,Length[TableNu]}] *)
```

```
TableResults =
  {{0.5`, 68.5185`, -0.08874082606588977`, 507.940751363426`, 12.350646922239509`},
   {0.525`, 71.94442500000001`, -0.10214726390880739`, 383.3597515271085`,
    12.22844038007236`}, {0.55`, 75.37035000000002`, -0.11623262581568754`,
    296.0764692991197`, 12.116237758357475`}, {0.575`, 78.796275`,
    -0.1309514618267732`, 233.25947272823257`, 12.01267315477431`},
   {0.6`, 82.2222`, -0.14625975040046763`, 186.9865356695142`, 11.91664420062555`},
   {0.625`, 85.64812500000001`, -0.1621161355574667 6`, 152.19749550228582`,
    11.827241371111837`}, {0.65`, 89.07405000000001`, -0.17848240883181224`,
    125.56515990726156`, 11.743703019244037`}, {0.675`, 92.499975`,
    -0.19532342757007506`, 104.84586759561212`, 11.665385183002273`},
   {0.7`, 95.9259`, -0.21260707989145572`, 88.49210911067877`, 11.591738411335138`},
   {0.725`, 99.351825`, -0.23030403869629437`,
    75.41485204857263`, 11.522290748555614`}, {0.75`, 102.77775`,
    -0.24838753289972734`, 64.83363975736154`, 11.45663426874334`},
   {0.775`, 106.203675`, -0.26683310864518234`, 56.17984797600329 5`,
    11.394414424841093`}, {0.8`, 109.62960000000001`, -0.28561841937003146`,
    49.032898713019684`, 11.335321433688382`}, {0.825`, 113.055525`,
    -0.3047230152117298`, 43.07739944681417`, 11.279083342541092`},
   {0.8500000000000001`, 116.48145000000002`, -0.32412812846552547`,
    38.07382839736742`, 11.225460413348461`}, {0.875`, 119.907375`,
    -0.343816563409827 1`, 33.83813363520237`, 11.174240266411235`},
   {0.9`, 123.33330000000001`, -0.3637725066396342`, 30.22736192193975`,
    11.125234111180683`}, {0.925`, 126.75922500000001`,
    -0.3839814017117404`, 27.129363962739223`, 11.078273477202826`},
   {0.95`, 130.18515`, -0.404429828568962`, 24.45533591904929`, 11.033207497862213`},
   {0.9750000000000001`, 133.61107500000003`,
    -0.4251053979656569`, 22.134348933254362`, 10.989900617212461`},
   {1.`, 137.037`, -0.4459966456374332`, 20.10929321229669`, 10.948230671764234`}};
```

According to Schlüter, Wietschorke & Greiner (Landau levels)

According to Figure 2

$100^{\frac{7.65}{6.77}}$;

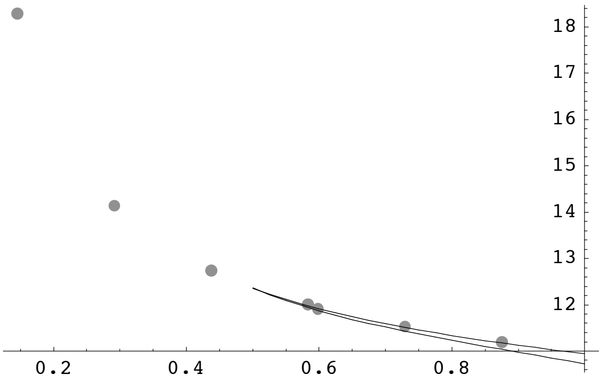
p1 = $\left\{\frac{82}{137.037}, \%\right\}$;

According to Figure 1

```
10^(8 13.84/12.82);
p2 = {20/137.037, %};
10^(8 7.19/12.82);
p3 = {40/137.037, %};
10^(8 4.94/12.82);
p4 = {60/137.037, %};
10^(8 3.78/12.82);
p5 = {80/137.037, %};
10^(8 3.01/12.82);
p6 = {100/137.037, %};
10^(8 2.47/12.82);
p7 = {120/137.037, %};
P4bis = ListPlot[{p5, p6, p7},
   PlotStyle → {PointSize[0.02], GrayLevel[0.5]}, DisplayFunction → Identity];

P1log = ListPlot[{{p1[[1]], Log[p1[[2]] * units]/Log[10]},
     {p2[[1]], Log[p2[[2]] * units]/Log[10]}, {p3[[1]], Log[p3[[2]] * units]/Log[10]},
     {p4[[1]], Log[p4[[2]] * units]/Log[10]}, {p5[[1]], Log[p5[[2]] * units]/Log[10]},
     {p6[[1]], Log[p6[[2]] * units]/Log[10]}, {p7[[1]], Log[p7[[2]] * units]/Log[10]}},
   PlotStyle → {PointSize[0.02], GrayLevel[0.5]}, DisplayFunction → Identity];
```

MARIA'S RESULTS (direct minimization)

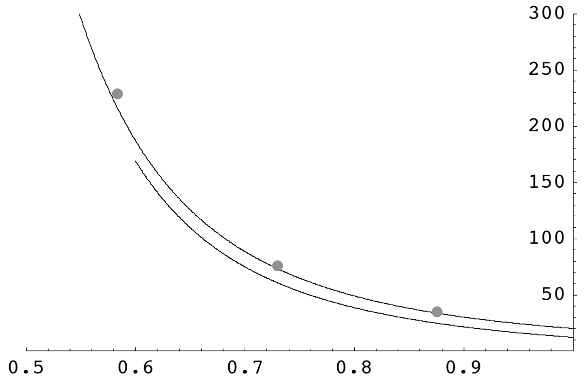
```
NuM = {0.500000000000000, 0.525000000000000, 0.550000000000000, 0.575000000000000,
   0.600000000000000, 0.625000000000000, 0.650000000000000, 0.675000000000000,
   0.700000000000000, 0.725000000000000, 0.750000000000000, 0.775000000000000,
   0.800000000000000, 0.825000000000000, 0.850000000000000, 0.875000000000000,
   0.900000000000000, 0.925000000000000, 0.950000000000000, 0.975000000000000, 1};

R1M ={ 0.929344234232870, 0.910473951505417 , 0.891536857069414, 0.872428108311625,
   0.853053584174947,  0.833327312976449, 0.813169175173238,  0.792502675526893,
   0.771252605008707,  0.749342416680782,  0.726691119390697,  0.703209438722700,
   0.678794890162816,  0.653325225411398,  0.626649396604712 ,   0.59857463};

R2M = {0.914928681409598,  0.898568379200249,
   0.881787353015900, 0.864512884216253,  0.846682534005467,  0.828241859548291,
   0.809141976880482,  0.789336919797267,  0.768780768945880, 0.747424511969375,
   0.725212544831218,  0.702078637027087,  0.677941052894770,  0.652696329046734,
   0.626210911808866, 0.598309377484827,  0.568757137328418,  0.537234069586941,
   0.503292828179034,  0.466290425311812,  0.425271469815194};

R3M = { 0.912578581410501,  0.896831548015472,
   0.880542131234248,  0.863654583736963,  0.846118433777931,
   0.827899977870430 ,  0.808963241250332,  0.789275503482810,  0.768802376999166,
   0.747504620305323,  0.725334781065251,  0.702233459554815,  0.678124858829652 ,
   0.652911121587164 ,  0.626464703474517,  0.598617626711661 ,  0.569145767393729,
   0.537745116668589,  0.503994761127126,  0.467297238410979,  0.426779130376463};

P2log = ListPlot[Table[{TableResults[[i]][[1]], TableResults[[i]][[5]]},
    {i, 1, Length[TableResults]}], PlotJoined → True, DisplayFunction → Identity];
P3log = ListPlot[Table[{NuM[[i]], Log[10, 4 units/(R3M[[i]] - 1)^2]}, {i, 1, Length[NuM]}],
   PlotJoined → True, DisplayFunction → Identity];
Show[P1log, P3log, P2log, DisplayFunction → $DisplayFunction, PlotRange → All];
```



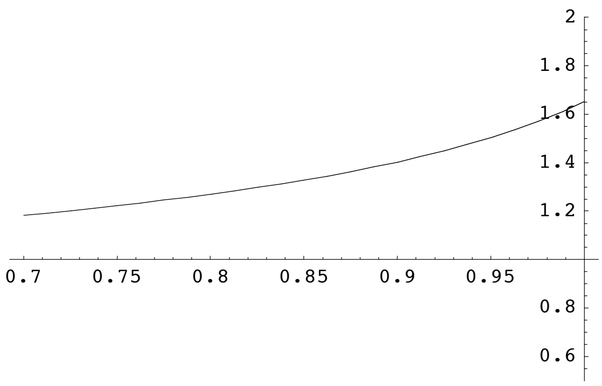
Interpolating functions

```
TM = Table[{NuM[[i]], 4/(R3M[[i]] - 1)^2}, {i, 1, Length[NuM]}];
recMaria = Interpolation[TM];
TJ = Table[{NuM[[i]], TableResults[[i]][[4]]}, {i, 1, Length[NuM]}];
recJean = Interpolation[TJ];
Nbre = 1000;
```

```
PR = {{0.5, 1}, {0, 300}};
LMaria = ListPlot[Table[{x, recMaria[x]}, {x, 0.6, 1, 0.5/Nbre}],
   PlotJoined → True, DisplayFunction → Identity];
LJean = ListPlot[Table[{x, recJean[x]}, {x, 0.5, 1, 0.5/Nbre}],
   PlotJoined → True, DisplayFunction → Identity];
Show[LMaria, LJean, P4bis, DisplayFunction → $DisplayFunction, PlotRange → PR];
```




```
P9 = Plot[recJean[x]/recMaria[x], {x, 0.7, 1}, PlotRange → {All, {0.5, 2}}];
```



LEVEL LINES (Landau levels)

Level lines of the eigenfunction in the Landau levels approximation

Definitions

```
PtLL = TableResults[[17]]
Off[Plot3D::"plnc"]
zmaxconst = 165;
eps = 0.00001;
{0.9`, 123.33330000000001`, -0.3637725066396342`,
 30.22736192193975`, 11.125234111180683`}
HzPltbList[ν_, λ_, z1_] :=
 Table[{zz, Evaluate[f[zz] /. NDSolve[{g'[z] == -(z a[z])/(b[z]) f'[z] - ν/(b[z]) (λ + ν a[z]) f[z],
      g[z] == f'[z], f[0] == 1, g[0] == 0}, {f, g}, {z, 0, z1}]][[1]]}, {zz, 0, z1, 0.1}]
```

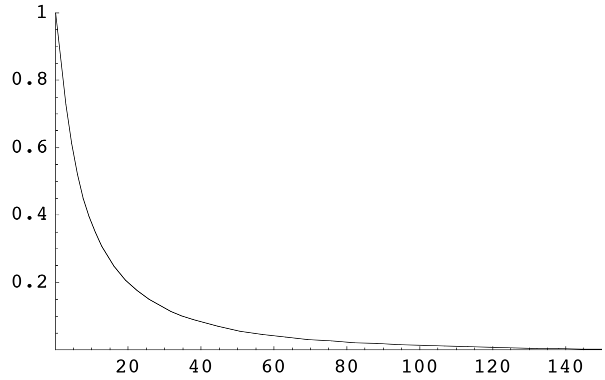
```
{0.9, 123.333, -0.363773, 30.2274, 11.1252}

{0.9, 123.333, -0.363773, 30.2274, 11.1252}

{0.9, 123.333, -0.363773, 30.2274, 11.1252}

{0.9, 123.333, -0.363773, 30.2274, 11.1252}
```

Plots corresponding to ν=0.5

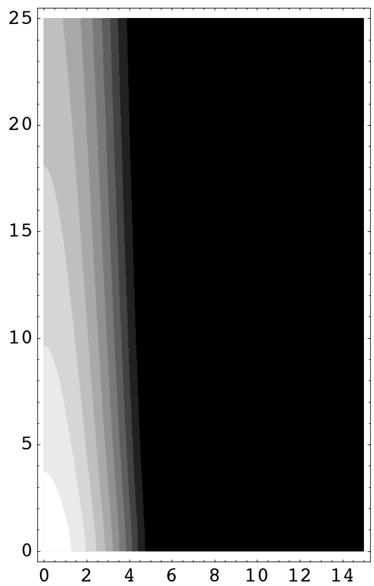
```
PtLL = TableResults[[1]]
HzPltbList[ν_, λ_, z1_] :=
 Table[{zz, Evaluate[f[zz] /. NDSolve[{g'[z] == -(z a[z])/(b[z]) f'[z] - ν/(b[z]) (λ + ν a[z]) f[z],
      g[z] == f'[z], f[0] == 1, g[0] == 0}, {f, g}, {z, 0, z1}]][[1]]}, {zz, 0, z1, 1}]
HzPltbList[0.5, -0.08874083854258046`, 150];
```

```
{0.5, 68.5185, -0.0887408, 507.941, 12.3506}
```

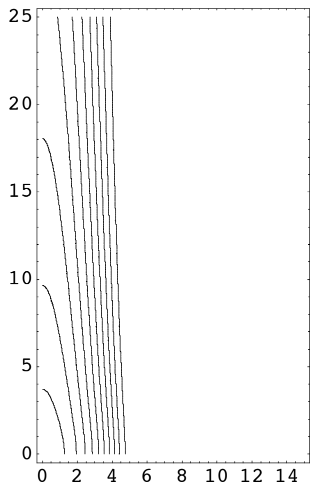
```
recLandau = Interpolation[%];
Plot[recLandau[zz], {zz, 0, 150}, PlotRange → {{0, 150}, {0, 1}}];
```



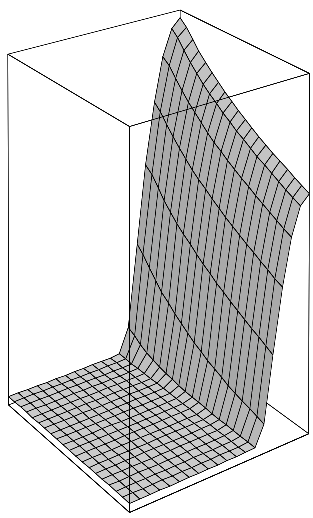

```
HzPltbContour[s1_, z1_, z2_] :=
 ContourPlot[Log[10, eps + recLandau[Abs[zz]]^2 e^(-s^2/2)], {s, 0, s1}, {zz, z2, z1},
  PlotRange → All, ContourLines → False, PlotPoints → 500, AspectRatio → (z2 - z1)/s1]
HzPltbContour[15, 0, 25];
```



```
HzPltbContour[s1_, z1_, z2_] := ContourPlot[Log[10, eps + recLandau[Abs[zz]]^2 e^(-s^2/2)],
  {s, 0, s1}, {zz, z2, z1}, PlotRange → All, ContourLines → True,
  PlotPoints → 500, ContourShading → False, AspectRatio → (z2 - z1)/s1, Ticks → None]
HzPltbContour[15, 0, 25];
```



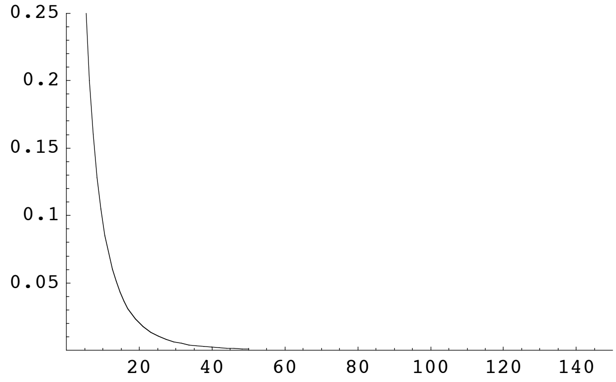

```
HzPltb[s1_, z1_, z2_] := Plot3D[Log[10, eps + recLandau[Abs[zz]]^2 e^(-s^2/2)], {s, 0, s1},
  {zz, z2, z1}, PlotRange → All, PlotPoints → 20, AspectRatio → (z2 - z1)/s1,
  ViewPoint → {5, 7, 1}, ColorOutput → GrayLevel, Ticks → None]
HzPltb[15, 0, 25];
```



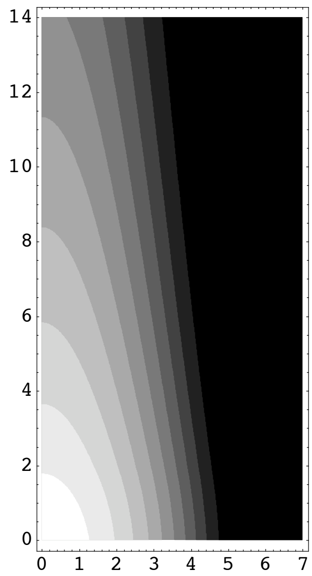
Plots corresponding to ν=0.9

```
PtLL = TableResults[[17]]
HzPltbList[0.9, -0.36377250663963057`, 50];
recLandau = Interpolation[%];
Plot[recLandau[zz], {zz, 0, 50}, PlotRange → {{0, 150}, {0, 0.25}}];
```

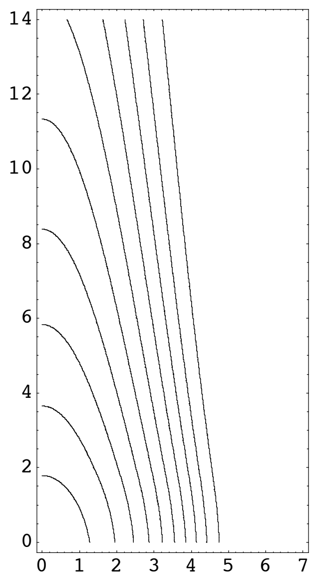
```
{0.9, 123.333, -0.363773, 30.2274, 11.1252}
```



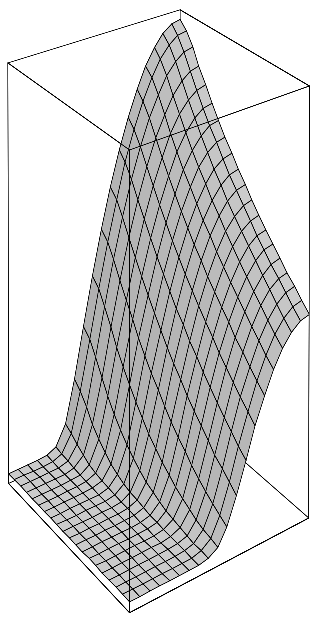

```
HzPltbContour[s1_, z1_, z2_] :=
  ContourPlot[Log[10, eps + recLandau[Abs[zz]]^2 e^(-s^2/2)], {s, 0, s1}, {zz, z2, z1},
   PlotRange → All, ContourLines → False, PlotPoints → 500, AspectRatio → (z2 - z1)/s1]
HzPltbContour[7, 0, 14];
```



```
HzPltbContour[s1_, z1_, z2_] := ContourPlot[Log[10, eps + recLandau[Abs[zz]]^2 e^(-s^2/2)],
  {s, 0, s1}, {zz, z2, z1}, PlotRange → All, ContourLines → True,
  PlotPoints → 500, ContourShading → False, AspectRatio → (z2 - z1)/s1, Ticks → None]
HzPltbContour[7, 0, 14];
```




```
HzPltb[s1_, z1_, z2_] := Plot3D[Log[10, eps + recLandau[Abs[zz]]^2 e^(-s^2/2)], {s, 0, s1},
  {zz, z2, z1}, PlotRange → All, PlotPoints → 20, AspectRatio → (z2 - z1)/s1,
  ViewPoint → {5, 7, 1}, ColorOutput → GrayLevel, Ticks → None]
HzPltb[7, 0, 14];
```



DATA TAKEN FROM MATLAB (ν=0.9) - DIRECT MINIMIZATION

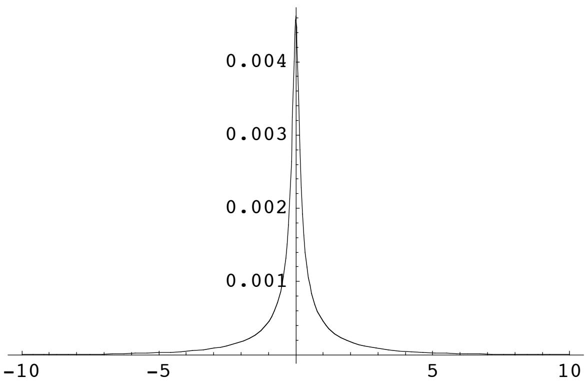
Level lines of the eigenfunction

```
η = 0.001;
eps = 0.00001;

Ns = Length[s] - 1;
smax = s[[Ns + 1]];
fns[s_] := IntegerPart[Ns Log[s + 1]/Log[smax + 1] + 0.000001] + 1

Nz = IntegerPart[(Length[z] - 1) / 2 + 0.000001];

zmax = z[[2 Nz + 1]];
fnz[z_] := If[z ≥ 0, IntegerPart[Nz Log[z + 1]/Log[zmax + 1] + 0.000001] + 1 + Nz,
  Nz - IntegerPart[Nz Log[-z + 1]/Log[zmax + 1] + 0.000001]]

Coefs[s_] := Module[{ii = fns[s]}, (s - sgrille[[ii]])/(sgrille[[ii + 1]] - sgrille[[ii]])]
Coefz[z_] := Module[{jj = fnz[z]}, (z - zgrille[[jj]])/(zgrille[[jj + 1]] - zgrille[[jj]])]

fnd[s_, z_] := Module[{m = {fns[s], fnz[z], Coefs[s], Coefz[z]}},
  (1 - m[[3]]) (1 - m[[4]]) dgrille[[m[[1]]]][[m[[2]]]] +
   m[[3]] (1 - m[[4]]) dgrille[[m[[1]] + 1]][[m[[2]]]] + (1 - m[[3]]) m[[4]]
    dgrille[[m[[1]]]][[m[[2]] + 1]] + m[[3]] m[[4]] dgrille[[m[[1]] + 1]][[m[[2]] + 1]]]

fnd[0.1, 10]
```

2.55055×10^{-6}

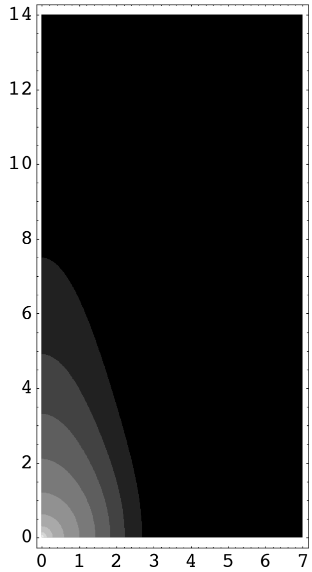
2.55055×10^{-6}

```
Plot[fnd[0.1, zz], {zz, -10, 10}];
```

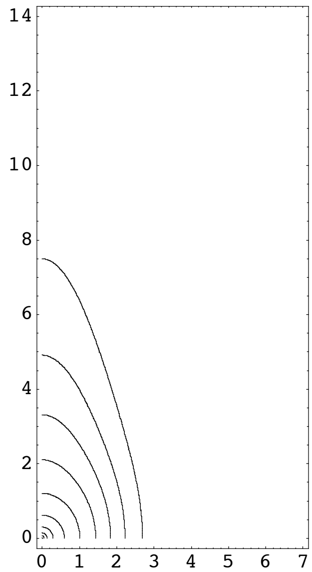



```
HzPltbContourFin[s1_, z1_, z2_] :=
 ContourPlot[Log[10, eps + fnd[ss, zz]], {ss, η, s1 - η}, {zz, z1 + η, z2 - η},
  PlotRange → All, ContourLines → False, PlotPoints → 500, AspectRatio → (z2 - z1)/s1]
```

```
HzPltbContourFin[7, 0, 14];
```




```
HzPltbContourFin[s1_, z1_, z2_] := ContourPlot[Log[10, eps + fnd[ss, zz]],
  {ss, η, s1 - η}, {zz, z1 + η, z2 - η}, PlotRange → All, PlotPoints → 500,
  ContourShading → False, AspectRatio → (z2 - z1)/s1, Ticks → None]
HzPltbContourFin[7, 0, 14];
```



```
HzPltb[s1_, z1_, z2_] := Plot3D[Log[10, eps + fnd[ss, zz]], {ss, η, s1 - η},
  {zz, z1 + η, z2 - η}, PlotRange → All, PlotPoints → 20, AspectRatio → (z2 - z1)/s1,
  ViewPoint → {5, 7, 1}, ColorOutput → GrayLevel, Ticks → None]
HzPltb[7, 0, 14];
```