Anderson impurity model in the limit $U \to \infty$

$$H = \sum_{\sigma=-M}^{M} \epsilon_d \, c_{d\sigma}^\dagger c_{d\sigma} + \sum_{\sigma=-M}^{M} \sum_k \epsilon_k \, c_{k\sigma}^\dagger c_{k\sigma} + t \sum_{\sigma=-M}^{M} \sum_k \left(c_{d\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d\sigma} \right) + U \sum_{\sigma,\sigma'=-M}^{M} c_{d\sigma}^\dagger c_{d\sigma} c_{d\sigma'}^\dagger c_{d\sigma'}$$

We assume a flat density of states for the conduction band that extends from $-W$ to W. Numerical values of some parameters entering the model:

```
Begin["data`"];
W = 1; t = 1 / 4; ϵd = -1 / 2; M = 1 / 2;
End[];
```

Application of a magnetic field B means adding an extra term to the hamiltonian

$$H_B = \sum_{\sigma=-M}^{M} B \, \sigma \, c_{d\sigma}^\dagger c_{d\sigma} + \sum_{\sigma=-M}^{M} \sum_k B \, \sigma \, c_{k\sigma}^\dagger c_{k\sigma}$$

■ Total energy

The Fermi energy E_F is at zero when no magnetic field is applied. When a magnetic field B is present, it enters only the spin-resolved Fermi energy $E_{F\sigma} = B\,\sigma$.

$$\Delta E = t^2 \frac{1}{N} \sum_{\sigma=-M}^{M} \sum_{k<k_{F\sigma}} \frac{1}{\Delta E - \epsilon_d + \epsilon_k}$$

$$a_k = \sqrt{\frac{1}{N}} \frac{t}{\Delta E - \epsilon_d + \epsilon_k}$$

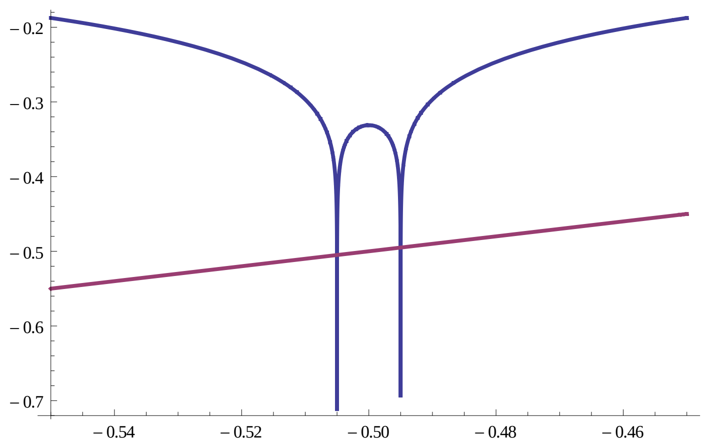
See C. M. Varma and Y. Yafet, Phys. Rev. B **13**, 2950 (1976) [http://dx.doi.org/10.1103/PhysRevB.13.2950].

Right-hand side of the equation for the energy difference ΔE

```
RHS[W_, t_, ϵd_, M_, B_, Δ_] = t^2/(2 W) Sum[Log[Abs[(ϵd - Δ + m B)/W]], {m, -M, M}];
```

Graphical solution for $M = 1/2$ and $B = 0.01$, the ground state is the lowest intersection. Left-hand side of the equation for ΔE is just a straight line.

```
Plot[{RHS[data`W, data`t, data`ϵd, 1/2, 0.01, Δ], Δ},
 {Δ, -.55, -.45}, MaxRecursion → 15, PlotStyle → Thick]
```



Numerical solution

```
ΔGS[W_, t_, ϵd_, M_, B_] := Δ /. FindRoot[RHS[W, t, ϵd, M, B, Δ] == Δ, {Δ, ϵd - M B - .000001}]
```

■ Magnetic moment at the impurity

...calculated from the coefficients in the wave function.

```
(*md[W_,t_,∊d_,M_,B_,Δ_]:=Module[{s1,s2},
  s1=t^2 Sum[m/(Δ-∊d-m B) - m/(Δ-∊d+W),{m,-M,M}];
  s2=t^2 Sum[1/(Δ-∊d-m B),{m,-M,M}] - t^2(2M+1)/(Δ-∊d+W);
  -s1/(1+s2)]*)
```

```
md[W_, t_, ∊d_, M_, B_, Δ_] := Module[{s1, s2},
  s1 = t^2 Sum[m/(Δ - ∊d - m B), {m, -M, M}];
  s2 = t^2 Sum[1/(Δ - ∊d - m B), {m, -M, M}];
  -s1/(1 + s2)]
```

- **Illustration for spin 1/2**

```
Begin["spinonehalf`"];
```

Approximate solution for $M = 1/2$, it is very accurate when $\delta 0$ is small.

```
Δapprox[W_, t_, ∊d_, B_] = ∊d - Sqrt[δ0^2 + B^2/4] /. δ0 → W Exp[W ∊d / t^2];
```

Magnetic moment as a derivativative of the total energy. It is linear in B for small B.

```
mdapprox[W_, t_, ∊d_, B_] = -∂_B Δapprox[W, t, ∊d, B]
```

$$\frac{B}{4\sqrt{\frac{B^2}{4}+e^{\frac{2\,W\,\epsilon d}{t^2}}\,W^2}}$$

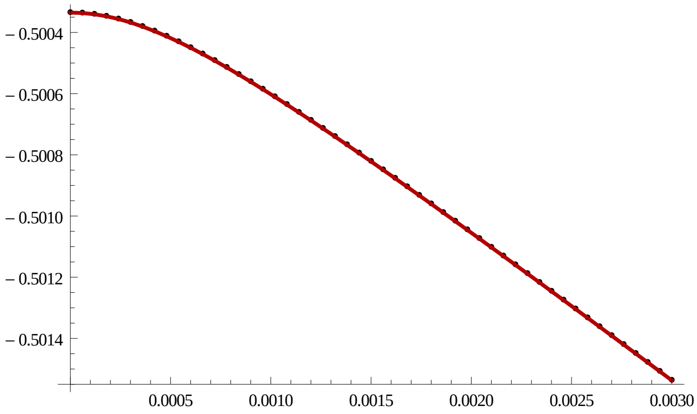
Arrays for plotting

```
BMax = 0.003;
iMax = 50;
```

```
ΔvsB = Table[{i BMax / iMax, ΔGS[data`W, data`t, data`∊d, data`M, i BMax / iMax]}, {i, 0, iMax}]
```

```
{{0., -0.500334}, {0.00006, -0.500335}, {0.00012, -0.500339},
 {0.00018, -0.500346}, {0.00024, -0.500354}, {0.0003, -0.500366}, {0.00036, -0.500379},
 {0.00042, -0.500394}, {0.00048, -0.500411}, {0.00054, -0.500429}, {0.0006, -0.500448},
 {0.00066, -0.500469}, {0.00072, -0.50049}, {0.00078, -0.500513}, {0.00084, -0.500536},
 {0.0009, -0.500559}, {0.00096, -0.500584}, {0.00102, -0.500609}, {0.00108, -0.500634},
 {0.00114, -0.50066}, {0.0012, -0.500686}, {0.00126, -0.500712}, {0.00132, -0.500739},
 {0.00138, -0.500765}, {0.00144, -0.500793}, {0.0015, -0.50082}, {0.00156, -0.500847},
 {0.00162, -0.500875}, {0.00168, -0.500903}, {0.00174, -0.500931}, {0.0018, -0.500959},
 {0.00186, -0.500987}, {0.00192, -0.501015}, {0.00198, -0.501044}, {0.00204, -0.501072},
 {0.0021, -0.501101}, {0.00216, -0.501129}, {0.00222, -0.501158}, {0.00228, -0.501187},
 {0.00234, -0.501215}, {0.0024, -0.501244}, {0.00246, -0.501273}, {0.00252, -0.501302},
 {0.00258, -0.501331}, {0.00264, -0.50136}, {0.0027, -0.501389}, {0.00276, -0.501418},
 {0.00282, -0.501448}, {0.00288, -0.501477}, {0.00294, -0.501506}, {0.003, -0.501535}}
```

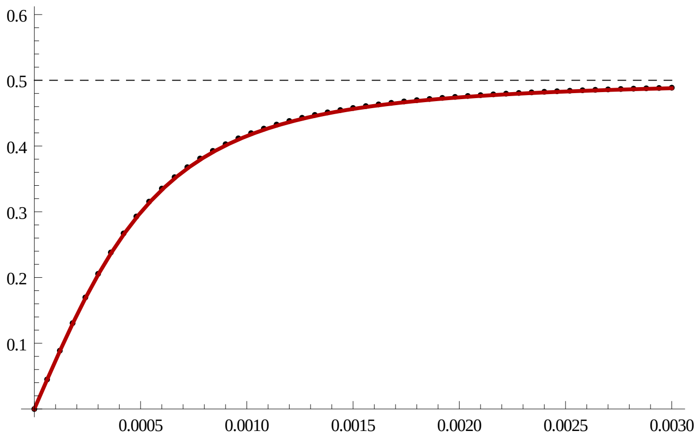
```
plotΔvsBexact = ListPlot[ΔvsB, PlotStyle → Black];
plotΔvsBapprox = Plot[Δapprox[data`W, data`t, data`εd, B],
   {B, 0, BMax}, PlotStyle → {RGBColor[0.7, 0, 0], Thick}];
Show[plotΔvsBexact, plotΔvsBapprox]
```




```
mdvsB = Table[
  {ΔvsB[[i, 1]], md[data`W, data`t, data`εd, data`M, ΔvsB[[i, 1]], ΔvsB[[i, 2]]]}, {i, 1, iMax + 1}]
```

```
{{0., 0.}, {0.00006, 0.0448934}, {0.00012, 0.0887287},
 {0.00018, 0.130567}, {0.00024, 0.169682}, {0.0003, 0.205594}, {0.00036, 0.238077},
 {0.00042, 0.267109}, {0.00048, 0.292825}, {0.00054, 0.315458}, {0.0006, 0.335295},
 {0.00066, 0.352641}, {0.00072, 0.367795}, {0.00078, 0.381039}, {0.00084, 0.392626},
 {0.0009, 0.402783}, {0.00096, 0.411705}, {0.00102, 0.419563}, {0.00108, 0.426504},
 {0.00114, 0.432652}, {0.0012, 0.438114}, {0.00126, 0.442982}, {0.00132, 0.447333},
 {0.00138, 0.451234}, {0.00144, 0.45474}, {0.0015, 0.457902}, {0.00156, 0.46076},
 {0.00162, 0.46335}, {0.00168, 0.465704}, {0.00174, 0.467848}, {0.0018, 0.469806},
 {0.00186, 0.471598}, {0.00192, 0.473241}, {0.00198, 0.474751}, {0.00204, 0.476142},
 {0.0021, 0.477425}, {0.00216, 0.478611}, {0.00222, 0.479709}, {0.00228, 0.480728},
 {0.00234, 0.481675}, {0.0024, 0.482556}, {0.00246, 0.483377}, {0.00252, 0.484144},
 {0.00258, 0.48486}, {0.00264, 0.485531}, {0.0027, 0.486159}, {0.00276, 0.486749},
 {0.00282, 0.487303}, {0.00288, 0.487824}, {0.00294, 0.488315}, {0.003, 0.488777}}
```

```
plotmdvsBexact = ListPlot[mdvsB, PlotStyle → Black];
plotmdvsBapprox = Plot[{mdapprox[data`W, data`t, data`εd, B], 1 / 2}, {B, 0, BMax},
   PlotStyle → {{RGBColor[0.7, 0, 0], Thick}, {Black, Dashed}}, PlotRange → {0, .6}];
Show[plotmdvsBexact, plotmdvsBapprox, PlotRange → {0, .6}]
```




```
End[];
```

- **Illustration for large local moment**

```
Begin["largeM`"];
```

Let's say we have an f level split by spin-orbital coupling to $j = 5/2$ and $j = 7/2$ multiplets occupied by a single electron (Ce) or hole (Yb). The hopping t has to be reduced in order to stay within the accuracy limits of the simple analytical approximations when the spin multiplicity is increased.

```
data`M = 7 / 2; data`t = 0.13;
```

Approximate expressions valid at small magnetic fields *B*. An analytical expression for any *B* would require finding roots of an high-order polynomial.

$$\frac{1}{4}\,\text{Sum}\left[(2\,q-1)^2,\ \{q,\ 1,\ (2\,M+1)/2\}\right]$$

$$\frac{1}{6}\left(M+3\,M^2+2\,M^3\right)$$

$$\Delta\text{smallB}[W\_,\ t\_,\ \epsilon d\_,\ M\_,\ B\_] = \epsilon d - W\,\text{Exp}\left[\frac{2}{2\,M+1}\ \frac{W\,\epsilon d}{t^2}\right] - \frac{B^2}{6\,W}\ \frac{M+3\,M^2+2\,M^3}{2\,M+1}\ \text{Exp}\left[-\frac{2}{2\,M+1}\ \frac{W\,\epsilon d}{t^2}\right];$$

$$\text{mdsmallB}[W\_,\ t\_,\ \epsilon d\_,\ M\_,\ B\_] = -\partial_B\,\Delta\text{smallB}[W,\ t,\ \epsilon d,\ M,\ B];$$

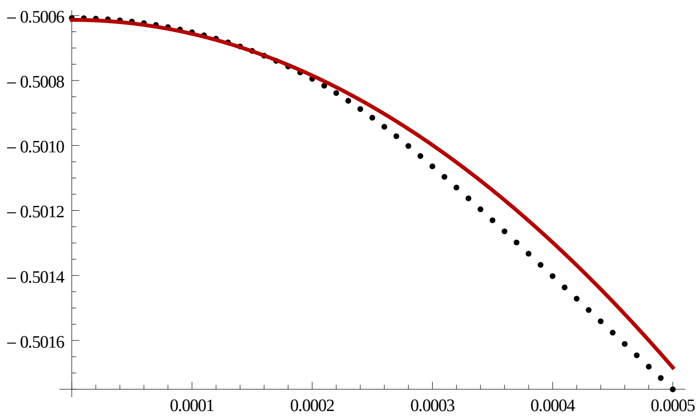
Arrays for plotting

```
BMax = 0.0005;
iMax = 50;
```

```
ΔvsB = Table[{i BMax / iMax, ΔGS[data`W, data`t, data`ϵd, data`M, i BMax / iMax]}, {i, 0, iMax}]
```

```
{{0., -0.500608}, {0.00001, -0.500608}, {0.00002, -0.50061},
 {0.00003, -0.500612}, {0.00004, -0.500615}, {0.00005, -0.500619}, {0.00006, -0.500623},
 {0.00007, -0.500629}, {0.00008, -0.500636}, {0.00009, -0.500643}, {0.0001, -0.500652},
 {0.00011, -0.500661}, {0.00012, -0.500671}, {0.00013, -0.500683}, {0.00014, -0.500695},
 {0.00015, -0.500709}, {0.00016, -0.500724}, {0.00017, -0.50074}, {0.00018, -0.500757},
 {0.00019, -0.500775}, {0.0002, -0.500795}, {0.00021, -0.500816}, {0.00022, -0.500839},
 {0.00023, -0.500863}, {0.00024, -0.500888}, {0.00025, -0.500915}, {0.00026, -0.500942},
 {0.00027, -0.500971}, {0.00028, -0.501002}, {0.00029, -0.501032}, {0.0003, -0.501064},
 {0.00031, -0.501097}, {0.00032, -0.501129}, {0.00033, -0.501163}, {0.00034, -0.501196},
 {0.00035, -0.50123}, {0.00036, -0.501264}, {0.00037, -0.501299}, {0.00038, -0.501333},
 {0.00039, -0.501367}, {0.0004, -0.501402}, {0.00041, -0.501437}, {0.00042, -0.501471},
 {0.00043, -0.501506}, {0.00044, -0.501541}, {0.00045, -0.501576}, {0.00046, -0.501611},
 {0.00047, -0.501646}, {0.00048, -0.501681}, {0.00049, -0.501715}, {0.0005, -0.50175}}
```

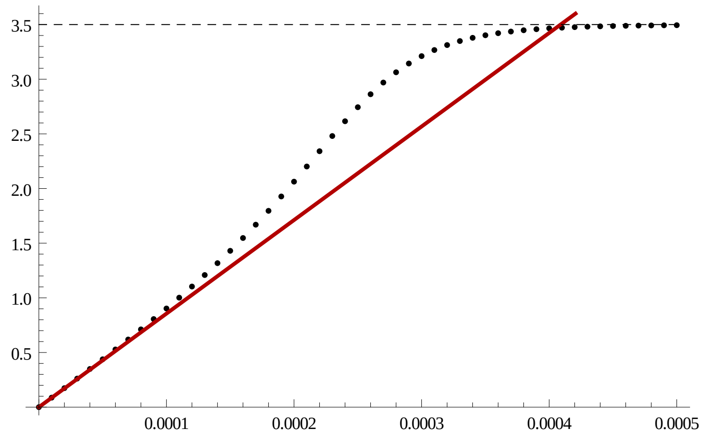
```
plotΔvsBexact = ListPlot[ΔvsB, PlotStyle → Black];
plotΔvsBapprox = Plot[ΔsmallB[data`W, data`t, data`ϵd, data`M, B],
   {B, 0, BMax}, PlotStyle → {RGBColor[0.7, 0, 0], Thick}];
Show[plotΔvsBexact, plotΔvsBapprox]
```



```
mdvsB = Table[
  {ΔvsB[[i, 1]], md[data`W, data`t, data`ϵd, data`M, ΔvsB[[i, 1]], ΔvsB[[i, 2]]]}, {i, 1, iMax + 1}]
```

```
{{0., 0.}, {0.00001, 0.0867806}, {0.00002, 0.173757}, {0.00003, 0.261129}, {0.00004, 0.3491},
 {0.00005, 0.437884}, {0.00006, 0.527708}, {0.00007, 0.618813}, {0.00008, 0.711459},
 {0.00009, 0.805929}, {0.0001, 0.902533}, {0.00011, 1.00161}, {0.00012, 1.10351},
 {0.00013, 1.20864}, {0.00014, 1.3174}, {0.00015, 1.4302}, {0.00016, 1.5474}, {0.00017, 1.6693},
 {0.00018, 1.79601}, {0.00019, 1.92739}, {0.0002, 2.06291}, {0.00021, 2.20149},
 {0.00022, 2.34143}, {0.00023, 2.48041}, {0.00024, 2.61559}, {0.00025, 2.74396},
 {0.00026, 2.86269}, {0.00027, 2.96961}, {0.00028, 3.06343}, {0.00029, 3.14383},
 {0.0003, 3.21135}, {0.00031, 3.26712}, {0.00032, 3.31259}, {0.00033, 3.34932},
 {0.00034, 3.37879}, {0.00035, 3.40236}, {0.00036, 3.42116}, {0.00037, 3.43616},
 {0.00038, 3.44814}, {0.00039, 3.45773}, {0.0004, 3.46541}, {0.00041, 3.47159},
 {0.00042, 3.47658}, {0.00043, 3.48062}, {0.00044, 3.48391}, {0.00045, 3.48659},
 {0.00046, 3.48878}, {0.00047, 3.49058}, {0.00048, 3.49207}, {0.00049, 3.4933}, {0.0005, 3.49432}}
```

```
plotmdvsBexact = ListPlot[mdvsB, PlotStyle → Black];
plotmdvsBsmallB = Plot[{mdsmallB[data`W, data`t, data`ϵd, data`M, B], 7 / 2}, {B, 0, BMax},
   PlotStyle → {{RGBColor[0.7, 0, 0], Thick}, {Black, Dashed}}, PlotRange → {0, 3.6}];
Show[plotmdvsBexact, plotmdvsBsmallB, PlotRange → {0, 3.6}]
```



Such a curve with inflection point is indeed observed in $YbAgCu_4$, T. Graf *et al.*, Phys. Rev. B **51**, 15053 (1995) [http://dx.doi.org/10.1103/PhysRevB.51.15053].

```
End[];
```