```
In[∘]:= ClearAll[alpha1, alpha2, alpha3, alpha4]
        lösche alle
        aaa = {alpha1, alpha2, alpha3, alpha4};
        (*Well positions*)
        ClearAll[p1, p2, p3, p4];
        lösche alle
        wellPositions = {p1, p2, p3, p4};
        signWavefunctions = {sn1, sn2, sn3, sn4};
        (*Satial wavefunction*)
        phiSpatial[x_, center_] :=
          signWavefunctions[[center]] * Exp[-aaa[[center]] * (x - wellPositions[[center]]) ^ 2];
                                         Exponentialfunktion

        (*Spin wavefunction*)
        chiSpin[sigma_, spin_] := KroneckerDelta[sigma, spin];
                                  Kronecker-Delta

        (*Combined spatial and spin basis*)
        phi[x_, sigma_, center_, spin_] := phiSpatial[x, center] * chiSpin[sigma, spin];


In[∘]:=

        (*Generate all valid spin configurations*)
        validSpinConfigurations = Permutations[{"up", "up", "down", "down"}];
                                  Permutationen
        validSpinConfigurations = {{"up", "down", "up", "up"}};

        (*Total wavefunction summed over all valid spin configurations*)
         Gesamtsumme
        PsiTotal[x_, sigma_] := Sum[Det[Table[phi[x[[i]], sigma[[i]], j, spinConfig[[j]]], {i, 4}, {j, 4}]],
                                ···  D···  Tabelle
            {spinConfig, validSpinConfigurations}];


In[∘]:= DoInt2[f_] := (Integrate[f, {x3, -Infinity, Infinity}, {x4, -Infinity, Infinity},
                       integriere         Unendlic···  Unendlichkeit     Unendlic···  Unendlichkei
            Assumptions → alpha1 > 0 && alpha2 > 0 && alpha3 > 0 && alpha4 > 0 && a > 0])
            Annahmen

In[∘]:= DoInt3[f_] := (Integrate[f, {x2, -Infinity, Infinity},
                       integriere         Unendlic···  Unendlichkeit
            {x3, -Infinity, Infinity}, {x4, -Infinity, Infinity},
                 Unendlic···  Unendlichkeit     Unendlic···  Unendlichkeit
            Assumptions → alpha1 > 0 && alpha2 > 0 && alpha3 > 0 && alpha4 > 0 && a > 0])
            Annahmen
```

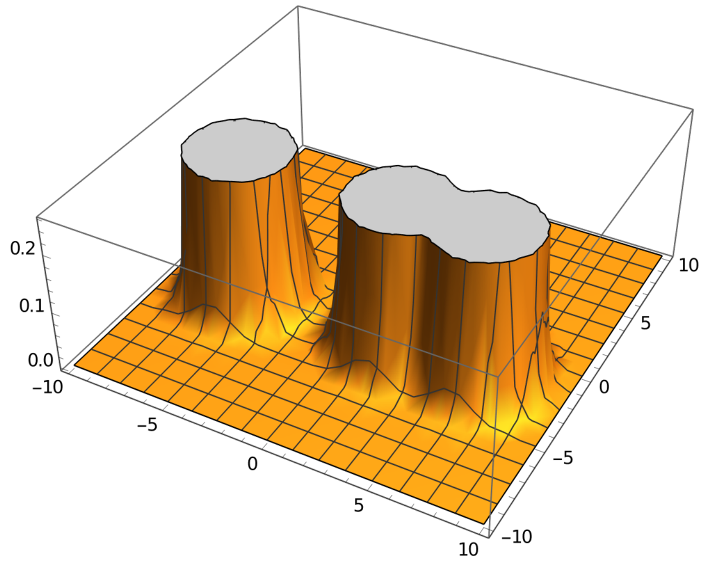
```
In[∘]:= DoInt4[f_] := (Integrate[Simplify[f], {x1, -Infinity, Infinity},
                      integriere   vereinfache        Unendlic···  Unendlichkeit
           {x2, -Infinity, Infinity}, {x3, -Infinity, Infinity}, {x4, -Infinity, Infinity},
                Unendlic···  Unendlichkeit     Unendlic···  Unendlichkeit     Unendlic···  Unendlichkei
           Assumptions → alpha1 > 0 && alpha2 > 0 && alpha3 > 0 && alpha4 > 0 && a > 0])
           Annahmen

In[∘]:= ClearAll[s1, s2, s3, s4, a, AmpPot]
        lösche alle

In[∘]:= V[x_] := Sum[-Exp[-a (x - xi) ^ 2], {xi, wellPositions}];
                 s···  Exponentialfunktion

        V[x_] := -AmpPot * Cos[2 * Pi * x * a];
                           Kosi···  Kreiszahl π

In[∘]:= KineticEnergy[{x1_, x2_, x3_, x4_}, spins_] :=
          Simplify[-1 / 2 * (D[PsiTotal[{x1, x2, x3, x4}, spins], {x1, 2}] +
          vereinfache         leite ab
              D[PsiTotal[{x1, x2, x3, x4}, spins], {x2, 2}] + D[PsiTotal[{x1, x2, x3, x4}, spins],
              leite ab                                        leite ab
               {x3, 2}] + D[PsiTotal[{x1, x2, x3, x4}, spins], {x4, 2}])];
                          leite ab

        EnergyIntegrand[{x1_, x2_, x3_, x4_}, spins_] :=
          PsiTotal[{x1, x2, x3, x4}, spins] * (KineticEnergy[{x1, x2, x3, x4}, spins] +
             (V[x1] + V[x2] + V[x3] + V[x4]) * PsiTotal[{x1, x2, x3, x4}, spins]);


In[∘]:= (*TotalEnergy=ParallelMap[DoInt4,Expand[
                      wende parallel an   multipliziere aus
            EnergyIntegrand[{x1,x2,x3,x4},{"up","down","up","down"}]],Method→"FinestGrained"];*)
                                                                         Methode

In[∘]:=

        InputList = List @@ Expand[EnergyIntegrand[{x1, x2, x3, x4}, {"up", "down", "up", "up"}]];
                    Liste    multipliziere aus

In[∘]:= (*InputList = InputList[[1;;5]];*)
        Length[InputList]
        Länge

Out[∘]= 660
```

```
In[∘]:= sublength = 40;
        TotalEnergySub[ppp_] := (CloseKernels[];
                                 schließe Kernels
            LaunchKernels[];
            starte Kernels
            ParallelEvaluate[$HistoryLength = 10];
            werte parallel aus  Verlaufslänge
            ParallelMap[DoInt4, ppp, Method → "FinestGrained"]);
            wende parallel an      Methode
        result = Map[TotalEnergySub, Partition[InputList, sublength, sublength, 1, {}]];
                 wende an               partitioniere

In[∘]:= result = Flatten[result];
                 ebne ein

In[∘]:= Length[result]
        Länge

Out[∘]= 660

In[∘]:=
        TotalEnergy = Plus @@ result;
                      addiere
        (*memory problems with longer runs in subkernels*)

In[∘]:= CloseKernels[]; LaunchKernels[]; ParallelEvaluate[$HistoryLength = 10];
        schließe Kernels  starte Kernels   werte parallel aus  Verlaufslänge

In[∘]:= Normalization = ParallelMap[DoInt4, Expand[
                        wende parallel an   multipliziere aus
            PsiTotal[{x1, x2, x3, x4}, {"up", "down", "up", "up"}]^2], Method → "FinestGrained"];
                                                                       Methode

In[∘]:= CloseKernels[]; LaunchKernels[]; ParallelEvaluate[$HistoryLength = 10];
        schließe Kernels  starte Kernels   werte parallel aus  Verlaufslänge

In[∘]:= summandCorrelation = ParallelMap[DoInt2,
                             wende parallel an
            Expand[PsiTotal[{x1, x2, x3, x4}, {"up", "down", s3, s4}]^2], Method → "FinestGrained"];
            multipliziere aus                                             Methode

In[∘]:= CloseKernels[]; LaunchKernels[]; ParallelEvaluate[$HistoryLength = 10];
        schließe Kernels  starte Kernels   werte parallel aus  Verlaufslänge

In[∘]:= TwoParticleCorrelationUpDownududn[xx1_,
            xx2_, al1_, al2_, al3_, al4_, aa_, pp1_, pp2_, pp3_, pp4_] :=
          Sum[summandCorrelation /. {x1 → xx1, x2 → xx2, s3 → sigma34[[1]], s4 → sigma34[[2]],
          summiere
              alpha1 → al1, alpha2 → al2, alpha3 → al3, alpha4 → al4, a → aa,
              p1 → pp1, p2 → pp2, p3 → pp3, p4 → pp4}, {sigma34, {{"up", "up"}}}];
```

```
In[◦]:= summandDensityU = ParallelMap[DoInt3,
                          wende parallel an
           Expand[PsiTotal[{x1, x2, x3, x4}, {"up", s2, s3, s4}]^2], Method → "FinestGrained"];
           multipliziere aus                                        Methode

In[◦]:= CloseKernels[]; LaunchKernels[]; ParallelEvaluate[$HistoryLength = 10];
        schließe Kernels  starte Kernels  werte parallel aus  Verlaufslänge

In[◦]:= OneParticleDensityUududn[xx1_, al1_, al2_, al3_, al4_, aa_, pp1_, pp2_, pp3_, pp4_] :=
          Count[validSpinConfigurations[[1]], "up"]*
          zähle
           Sum[summandDensityU / Normalization /. {x1 → xx1, s2 → sigma234[[1]], s3 → sigma234[[2]],
           summiere
              s4 → sigma234[[3]], alpha1 → al1, alpha2 → al2, alpha3 → al3, alpha4 → al4, a → aa,
              p1 → pp1, p2 → pp2, p3 → pp3, p4 → pp4}, {sigma234, {{"down", "up", "up"}}}];

In[◦]:= CloseKernels[]; LaunchKernels[]; ParallelEvaluate[$HistoryLength = 10];
        schließe Kernels  starte Kernels  werte parallel aus  Verlaufslänge

In[◦]:= summandDensityD = ParallelMap[DoInt3,
                          wende parallel an
           Expand[PsiTotal[{x2, x1, x3, x4}, {s2, "down", s3, s4}]^2], Method → "FinestGrained"];
           multipliziere aus                                          Methode

In[◦]:= OneParticleDensityDududn[xx1_, al1_, al2_, al3_, al4_, aa_, pp1_, pp2_, pp3_, pp4_] :=
          Count[validSpinConfigurations[[1]], "down"]*
          zähle
           Sum[summandDensityD / Normalization /. {x1 → xx1, s2 → sigma234[[1]], s3 → sigma234[[2]],
           summiere
              s4 → sigma234[[3]], alpha1 → al1, alpha2 → al2, alpha3 → al3, alpha4 → al4,
              a → aa, p1 → pp1, p2 → pp2, p3 → pp3, p4 → pp4}, {sigma234, {{"up", "up", "up"}}}];

In[◦]:= Energyududn[al1_, al2_, al3_, al4_, aa_, pp1_, pp2_, pp3_, pp4_] :=
         Evaluate[(TotalEnergy / Normalization) /. {alpha1 → al1, alpha2 → al2,
         werte aus
            alpha3 → al3, alpha4 → al4, a → aa, p1 → pp1, p2 → pp2, p3 → pp3, p4 → pp4}]

In[◦]:= sn1 = sn2 = sn3 = sn4 = 1;
```

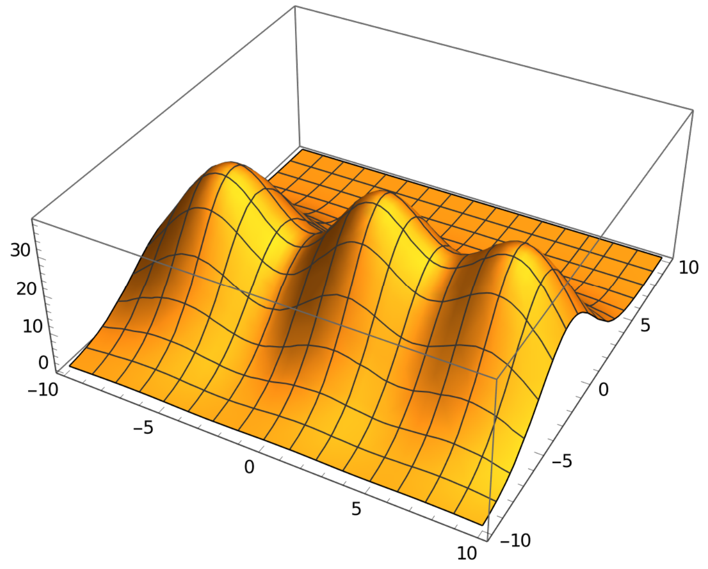
```
In[∘]:= Plot3D[TwoParticleCorrelationUpDownududn[x, y, 0.3, 0.3, 0.3, 0.3, 0.3, -6, -2, 6, 2],
        stelle Funktion graphisch in 3D dar
         {x, -10, 10}, {y, -10, 10}]
```

Out[∘]=



```
In[∘]:= Plot3D[TwoParticleCorrelationUpDownududn[x, y, 0.03,
        stelle Funktion graphisch in 3D dar
          0.03, 0.03, 0.03, 0.03, -6, -2, 6, 2], {x, -10, 10}, {y, -10, 10}]
```

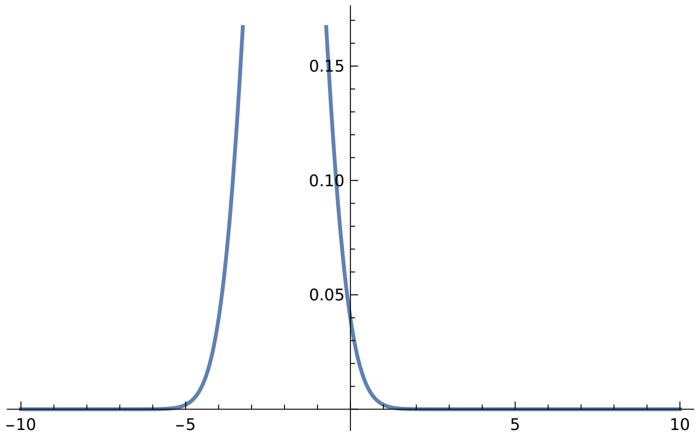
Out[∘]=



In[∘]:=

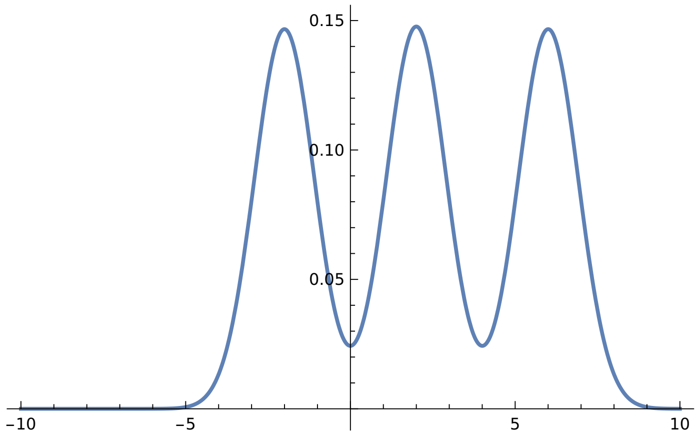
In[∘]:=

In[•]:=
```
Plot[OneParticleDensityDududn[x,
stelle Funktion graphisch dar
   Sequence @@ {0.3, 0.3, 0.3, 0.3, 0.3, -6, -2, 2, 6}], {x, -10, 10}]
   Sequenz
```

Out[•]=


In[•]:=
```
alpha1 = alpha2 = alpha3 = alpha4 = 0.3
Plot[OneParticleDensityUududn[x,
stelle Funktion graphisch dar
   Sequence @@ {0.3, 0.3, 0.3, 0.3, 0.3, -2, -2, 2, 6}], {x, -10, 10}]
   Sequenz
```

Out[•]=
```
0.3
```

Out[•]=


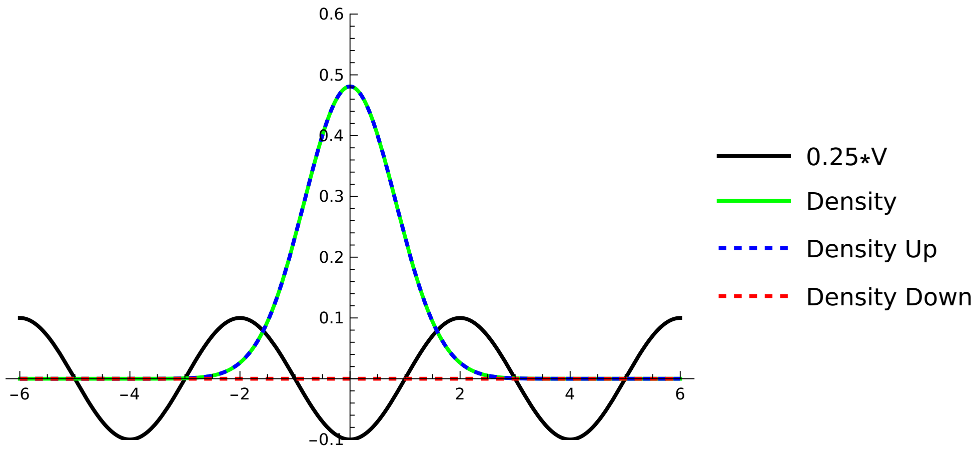
In[•]:=
```
ClearAll[ alpha1, alpha2, alpha3, alpha4, a, p1, p2, p3, p4];
lösche alle
```

In[•]:=
```
ClearAll[alpha1, alpha2, alpha3, alpha4]
lösche alle
```

```
In[∘]:= DoResults[parameters_, ww_] := (
          ppp = {alpha1, alpha2, alpha3, alpha4, Sequence @@ parameters};
                                                 Sequenz

          res =
           NMinimize[{Re[Energyududn[ alpha1, alpha2, alpha3, alpha4, Sequence @@ parameters]],
           minimiere···  Realteil                                   Sequenz

              alpha1 > 0 && alpha2 > 0 && alpha3 > 0 && alpha4 > 0},
            { alpha1, alpha2, alpha3, alpha4}, Method → "DifferentialEvolution"];
                                               Methode

          ppp = ppp /. res[[2]];
          Print[res];
          gib aus
          ppp1 = Plot[{0.2 * V[x] /. Thread[{a, p1, p2, p3, p4} → parameters],
                 stelle Funktion g···  fädle auf

              OneParticleDensityUududn[x, Sequence @@ ppp] +
                                          Sequenz

               OneParticleDensityDududn[x, Sequence @@ ppp], OneParticleDensityUududn[

               x, Sequence @@ ppp], OneParticleDensityDududn[x, Sequence @@ ppp]},
                  Sequenz                                   Sequenz

            {x, -ww, ww}, PlotStyle → {Black, Green, {Blue, Dashed}, {Red, Dashed}},
                          Darstellungss·· schw···  grün  blau  gestrichelt rot  gestrichelt

            PlotLegends → {"0.25*V", "Density", "Density Up", "Density Down"},
            Legenden der Graphik                                     nach unten

            PlotRange → {Automatic, {-0.1, 0.6}}]
            Koordinaten···  automatisch

         )

In[∘]:= pw = 1 / 4
        AmpPot = 0.5

Out[∘]= 1
        —
        4

Out[∘]= 0.5
```

4 electrons in seperated minima of a cosin potential. Potential, Up and Down spatial density is plottet for different configurations. Afterwords the energy per particle of the discussed particles is calculated

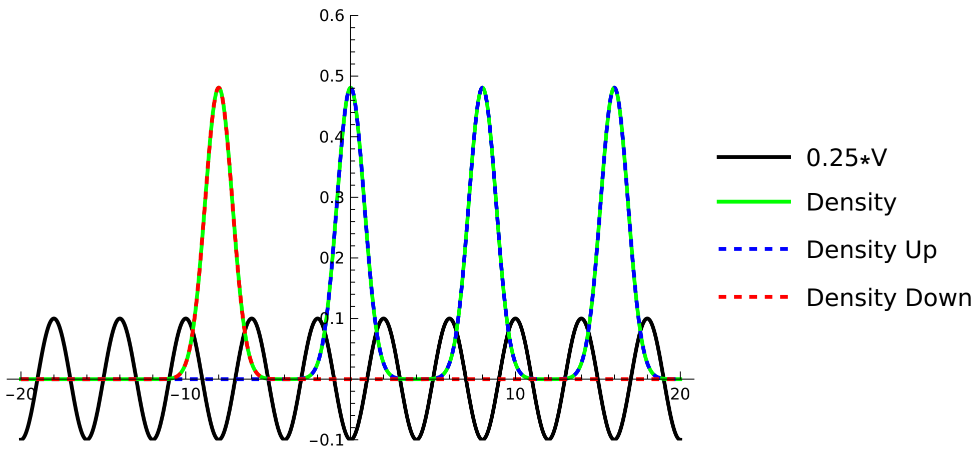
```
In[∘]:= DoResults[{pw, 0, -40, 40, 80}, 6]
        {-0.129124, {alpha1 → 0.363244, alpha2 → 0.363244, alpha3 → 0.363244, alpha4 → 0.363244}}
        ··· General: Exp[-2324.76] is too small to represent as a normalized machine number; precision may be lost.
        ··· General: Exp[-1743.57] is too small to represent as a normalized machine number; precision may be lost.
        ··· General: Exp[-3861.99] is too small to represent as a normalized machine number; precision may be lost.
        ··· General: Further output of General::munfl will be suppressed during this calculation.
Out[∘]=
```



```
In[∘]:= eP = res[[1]] / 4
Out[∘]= -0.032281
```

Test with other positions

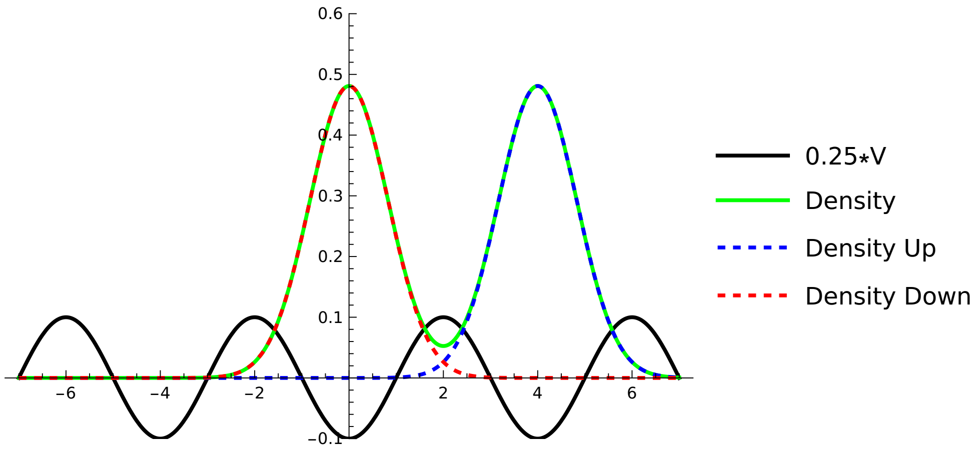
```
In[∘]:= DoResults[{pw, 0, -8, 8, 16}, 20]
        {-0.129124, {alpha1 → 0.363244, alpha2 → 0.363244, alpha3 → 0.363244, alpha4 → 0.363244}}
        ··· General: Exp[-964.733] is too small to represent as a normalized machine number; precision may be lost.
        ··· General: Exp[-941.485] is too small to represent as a normalized machine number; precision may be lost.
        ··· General: Exp[-767.133] is too small to represent as a normalized machine number; precision may be lost.
        ··· General: Further output of General::munfl will be suppressed during this calculation.
Out[∘]=
```



```
In[•]:= res⟦1⟧ - 3 * eP
Out[•]= -0.032281
```

Now two neighboring with oposite spin, others far away

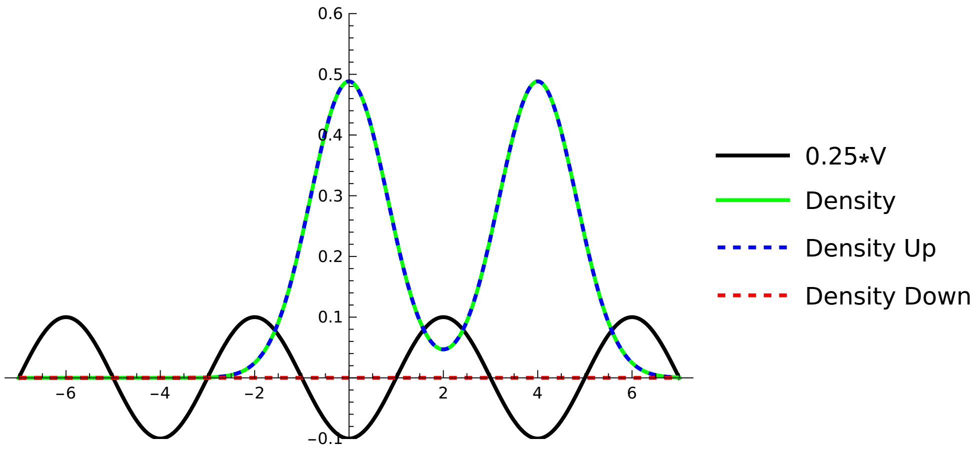
```
In[•]:= DoResults[{pw, -20, 0, 4, 20}, 7]
{-0.129124, {alpha1 → 0.363244, alpha2 → 0.363244, alpha3 → 0.363244, alpha4 → 0.363244}}
```

Out[•]=


```
In[•]:= (res⟦1⟧ - 2 * eP) / 2
Out[•]= -0.032281
```

Two neighboring with same spin

```
In[•]:= DoResults[{pw, -0, -20, 4, 20}, 7]
```

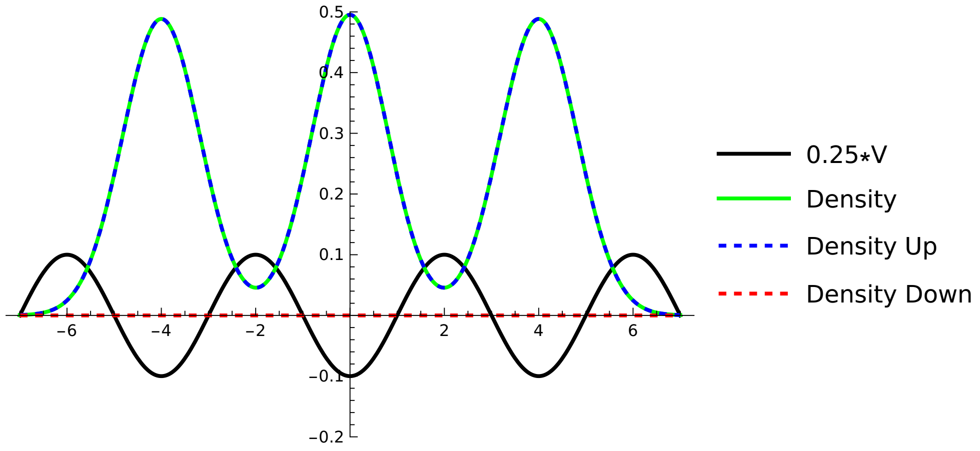
Out[•]=


```
In[•]:= (res⟦1⟧ - 2 * eP) / 2
Out[•]= -0.030473
```

Three neighbours with same spin

```
In[◦]:= DoResults[{pw, -4, -20, 4, 0}, 7]

{-0.122015, {alpha1 → 0.372996, alpha2 → 0.363244, alpha3 → 0.372996, alpha4 → 0.381919}}
```

Out[◦]=

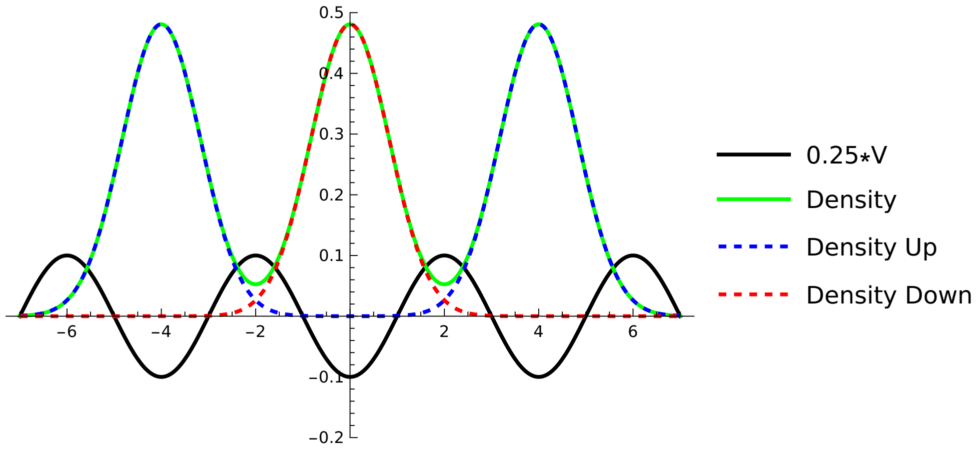


```
In[◦]:= (res[[1]] - eP) / 3

Out[◦]= -0.0299114
```

Three neighbors with opposite spin

```
In[◦]:= DoResults[{pw, -4, 0, 4, -20}, 7]

{-0.129124, {alpha1 → 0.363244, alpha2 → 0.363244, alpha3 → 0.363244, alpha4 → 0.363244}}
```

Out[◦]=



```
In[◦]:= (res[[1]] - eP) / 3

Out[◦]= -0.032281
```