10 Band Model of MA-TBG

Spenser Talkington - 15&16 August 2022
Here we implement the 10 band model of MA-TBG developed in https://arxiv.org/pdf/1808.02482.pdf .
We recreate panels (a) and (b) of Figure 2 in that paper.

Setup

```
In[●]:= (*set up*)
Remove["Global`*"];
$PrePrint = MatrixForm;
```

```
In[●]:= (*Lattice and phase accumulation*)
ξ = Exp[I 2 π / 6];
ω = ξ^2;
a0 = 1;(*sets scale of triangular lattice*)
a1 = a0 {Re[Exp[-I π / 12]], Im[Exp[-I π / 12]]};
a2 = a0 {Re[Exp[I π / 2]], Im[Exp[I π / 2]]};
φ[l_, m_, k_] := Exp[-I k.(l a1 + m a2)](*l bar = -l*)
```

```
In[●]:= (*high symmetry points*)
Γ = {0, 0};
K = π {Sqrt[3] / 2, 2 / 3};
M = π {2 - Sqrt[3], 1};
```

Model at $\delta = 0$

```
In[●]:= (*unperturbed Hamiltonian*)
hAp[k_] := {- (ω + φ[1, 1, k] ω* + φ[0, 1, k]) ξ* a, (ω* + φ[1, 1, k] ω + φ[0, 1, k]) ξ b,
   (1 + φ[1, 1, k] + φ[0, 1, k]) c, -I φ[-1, 0, k] d, -I ω d, -I φ[0, 1, k] ω* d}
hAm[k_] := {(1 + φ[1, 1, k] ω* + φ[0, 1, k] ω) ξ* a, (1 + φ[1, 1, k] + φ[0, 1, k]) c,
   (1 + φ[1, 1, k] ω + φ[0, 1, k] ω*) ξ b, -I φ[-1, 0, k] d, -I ω* d, -I φ[0, 1, k] ω d}
hBp[k_] := {(ω + φ[1, 0, k] ω* + φ[1, 1, k]) ξ a,
   (ω* + φ[1, 0, k] ω + φ[1, 1, k]) ξ* b, (1 + φ[1, 0, k] + φ[1, 1, k]) c, I d, I ω d, I ω* d}
hBm[k_] := {- (ω + φ[1, 0, k] + φ[1, 1, k] ω*) ξ a,
   (1 + φ[1, 0, k] + φ[1, 1, k]) c, (ω* + φ[1, 0, k] + φ[1, 1, k] ω) ξ* b, I d, I ω* d, I ω d}
h[k_] := t0 Transpose[{hAp[k], hAm[k], hBp[k], hBm[k]}]
H0[k_] := ArrayFlatten[{{0, h[k]}, {ConjugateTranspose[h[k]], 0}}]
```
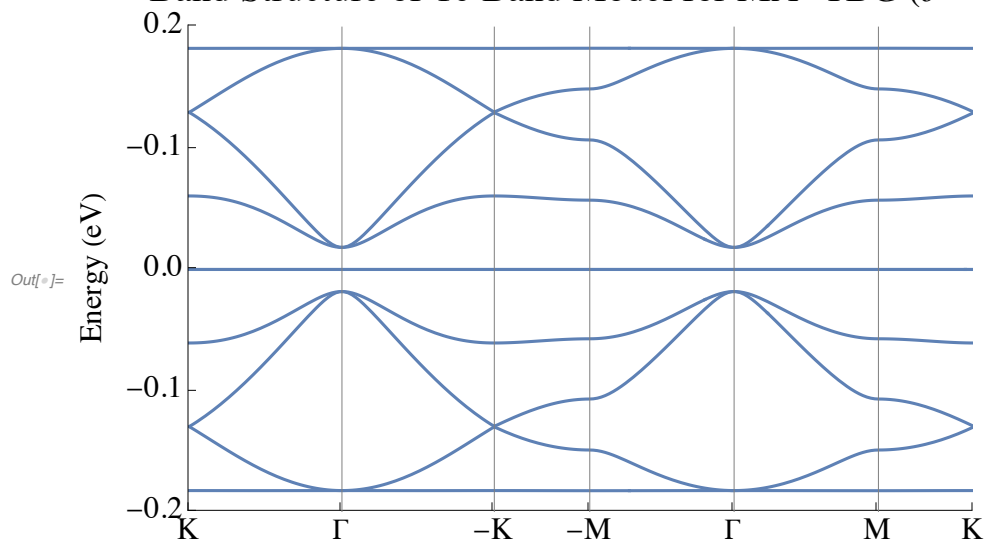
```
In[ ]:= (*model parameters*)
     a = 0.110;
     b = 0.033;
     c = 0.033;
     d = 0.573;
     t0 = 0.130;

In[ ]:= (*set up path through BZ*)
     l0 = 0;
     l1 = Norm[Γ – K];
     l2 = Norm[Γ – K] + Norm[-K – Γ];
     l3 = Norm[Γ – K] + Norm[-K – Γ] + Norm[-M + K];
     l4 = Norm[Γ – K] + Norm[-K – Γ] + Norm[-M + K] + Norm[Γ + M];
     l5 = Norm[Γ – K] + Norm[-K – Γ] + Norm[-M + K] + Norm[Γ + M] + Norm[M – Γ];
     l6 = Norm[Γ – K] + Norm[-K – Γ] + Norm[-M + K] + Norm[Γ + M] + Norm[M – Γ] + Norm[K – M];
     pathpoints = {{0, K}, {l1, Γ}, {l2, -K}, {l3, -M}, {l4, Γ}, {l5, M}, {l6, K}};
     path = Interpolation[pathpoints, InterpolationOrder → 1];
     line1 = Line[{{l1, -0.2}, {l1, 0.2}}];
     line2 = Line[{{l2, -0.2}, {l2, 0.2}}];
     line3 = Line[{{l3, -0.2}, {l3, 0.2}}];
     line4 = Line[{{l4, -0.2}, {l4, 0.2}}];
     line5 = Line[{{l5, -0.2}, {l5, 0.2}}];
```

```
(*plot*)
Plot[Sort[Eigenvalues[H0[{path[x]⟦1⟧, path[x]⟦2⟧}]]]], {x, 0, l6},
 Epilog → {{Gray, line1}, {Gray, line2}, {Gray, line3}, {Gray, line4}, {Gray, line5}},
 PlotRange → {{0, l6}, {-0.2, 0.2}}, PlotLabel →
  Style["Band Structure of 10 Band Model for MA-TBG (δ = 0)", FontSize → 20],
 Axes → False, Frame → {True, True, False, False},
 FrameLabel → {"", "Energy (eV)"}, FrameTicks →
  {{{0, "K"}, {l1, "Γ"}, {l2, "-K"}, {l3, "-M"}, {l4, "Γ"}, {l5, "M"}, {l6, "K"}},
   {{-0.2, "-0.2"}, {-0.1, "-0.1"}, {0.0, "0.0"}, {0.1, "-0.1"}, {0.2, "0.2"}}},
 LabelStyle → Directive[FontSize → 16, FontFamily → "Times"],
 ImageSize → 2 * (3 + 3 / 8) * 72, PlotPoints → 100, MaxRecursion → 1]
```

Out[●]=

Band Structure of 10 Band Model for MA−TBG ($\delta = 0$)
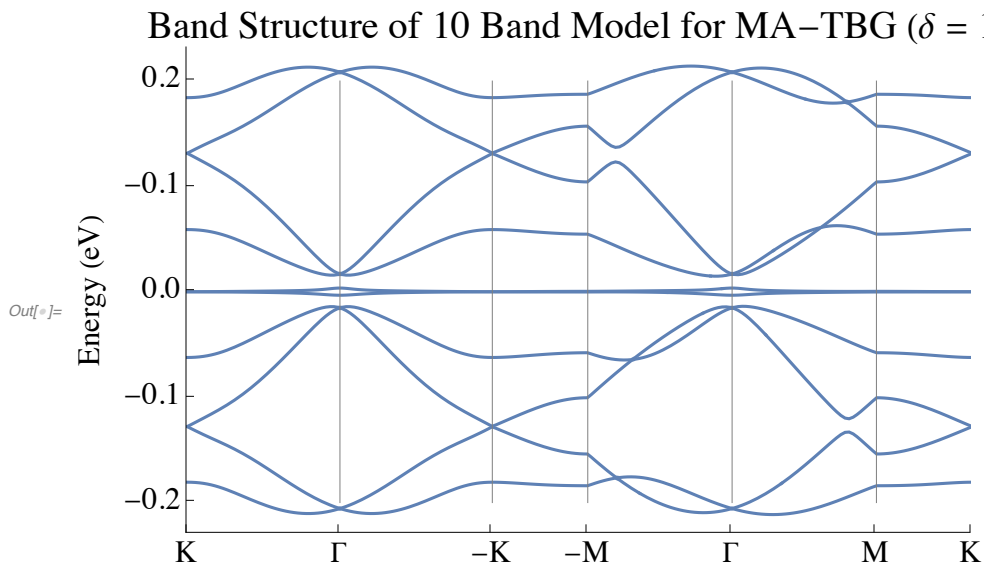
Model at $\delta = 1$

```
In[∘]:= (*perturbation*)
     μz = -6 tz + δz;
     μpm = 3 tpm + δpm;
     μκ = -4 (tκ + tκprime) + δκ;
     Cpmz[k_] := I tpmzp {{ϕ[0, 1, k] + ϕ[-1, -1, k] ω + ϕ[1, 0, k] ω*},
          {-(ϕ[0, -1, k] + ϕ[1, 1, k] ω* + ϕ[-1, 0, k] ω)}} -
        I tpmzm {{ϕ[0, -1, k] + ϕ[1, 1, k] ω + ϕ[-1, 0, k] ω*},
          {-(ϕ[0, 1, k] + ϕ[-1, -1, k] ω* + ϕ[1, 0, k] ω)}}
     Cκpm[k_] :=
      tkpmp {{ϕ[-1, 0, k], ϕ[-1, -1, k]}, {ϕ[-1, -1, k] ω*, ω}, {ω, ϕ[-1, 0, k] ω*}} -
        tkpmm {{ϕ[-1, -1, k], ϕ[-1, 0, k]}, {ω*, ϕ[-1, -1, k] ω}, {ϕ[-1, 0, k] ω, ω*}}
     Cpmpm[k_] := tpmpmp (ϕ[0, 1, k] + ϕ[-1, -1, k] ω + ϕ[1, 0, k] ω*) +
        tpmpmm (ϕ[0, -1, k] + ϕ[1, 1, k] ω + ϕ[-1, 0, k] ω*)
     Hz[k_] :=
      tz (ϕ[0, 1, k] + ϕ[1, 1, k] + ϕ[1, 0, k] + Conjugate[ϕ[0, 1, k] + ϕ[1, 1, k] + ϕ[1, 0, k]])
     Hpm[k_] :=
      tpm (ϕ[0, 1, k] + ϕ[1, 1, k] + ϕ[1, 0, k] + Conjugate[ϕ[0, 1, k] + ϕ[1, 1, k] + ϕ[1, 0, k]])
         {{1, 0}, {0, 1}} + {{0, Conjugate[Cpmpm[k]]}, {Cpmpm[k], 0}}
     Hκ[k_] := tκ {{0, ϕ[-1, 0, k], 1}, {1, 0, ϕ[0, -1, k]}, {ϕ[1, 1, k], 1, 0}} +
        tκprime {{0, ϕ[-1, -1, k], ϕ[-1, 0, k]},
          {ϕ[0, -1, k], 0, ϕ[1, 0, k]}, {ϕ[0, 1, k], ϕ[1, 1, k], 0}} +
        ConjugateTranspose[tκ {{0, ϕ[-1, 0, k], 1}, {1, 0, ϕ[0, -1, k]}, {ϕ[1, 1, k], 1, 0}} +
          tκprime {{0, ϕ[-1, -1, k], ϕ[-1, 0, k]},
            {ϕ[0, -1, k], 0, ϕ[1, 0, k]}, {ϕ[0, 1, k], ϕ[1, 1, k], 0}}]
     Hη[k_] := KroneckerProduct[{{0, Exp[I ϕη] (1 + ϕ[0, -1, k] + ϕ[1, 0, k])},
          {Exp[-I ϕη] (1 + ϕ[0, 1, k] + ϕ[-1, 0, k]), 0}}, {{1, 0}, {0, 1}}]
     V[k_] :=
      tη ArrayFlatten[{{Hz[k] + μz IdentityMatrix[1], ConjugateTranspose[Cpmz[k]], 0, 0},
          {Cpmz[k], Hpm[k] + μpm IdentityMatrix[2], ConjugateTranspose[Cκpm[k]], 0},
          {0, Cκpm[k], Hκ[k] + μκ IdentityMatrix[3], 0}, {0, 0, 0, Hη[k]}}];
       (*tη sets energy scale here--in other functions above they
       are just ratios of this overall scale*)
```

```
In[ ]:= (*perturbation parameters*)
    ϕη = -Pi / 2; (*guess--if Pi/2 it flips the perturbation upside-down*)
    tη = 0.0325;
    δz = -0.100;
    δpm = 0;
    δκ = 0.110;
    tz = 0;
    tpm = 0.003;
    tpmpmm = 0.004;
    tκ = 0;
    tκprime = 0;
    tpmzp = 0.016;
    tκpmp = 0.016;
    tκpmm = -0.016;
    tpmzm = 0;
    tkpmp = 0;
    tkpmm = 0;
    tpmpmp = 0;
```

```
(*plot*)
Plot[Sort[Eigenvalues[H0[{path[x]〚1〛, path[x]〚2〛}] + V[{path[x]〚1〛, path[x]〚2〛}]]],
 {x, 0, l6},
 Epilog → {{Gray, line1}, {Gray, line2}, {Gray, line3}, {Gray, line4}, {Gray, line5}},
 PlotRange → {{0, l6}, {-0.23, 0.23}}, PlotLabel →
  Style["Band Structure of 10 Band Model for MA-TBG (δ = 1)", FontSize → 20],
 Axes → False, Frame → {True, True, False, False},
 FrameLabel → {"", "Energy (eV)"}, FrameTicks →
  {{{0, "K"}, {l1, "Γ"}, {l2, "-K"}, {l3, "-M"}, {l4, "Γ"}, {l5, "M"}, {l6, "K"}},
   {{-0.2, "-0.2"}, {-0.1, "-0.1"}, {0.0, "0.0"}, {0.1, "-0.1"}, {0.2, "0.2"}}},
 LabelStyle → Directive[FontSize → 16, FontFamily → "Times"],
 ImageSize → 2 * (3 + 3 / 8) * 72, PlotPoints → 100, MaxRecursion → 1]
```

Out[•]=

Band Structure of 10 Band Model for MA−TBG ($\delta = 1$)

```
(*plot*)
Plot[
 {Sort[Eigenvalues[H0[{path[x]〚1〛, path[x]〚2〛}] + V[{path[x]〚1〛, path[x]〚2〛}]]]〚5〛,
  Sort[Eigenvalues[H0[{path[x]〚1〛, path[x]〚2〛}] + V[{path[x]〚1〛, path[x]〚2〛}]]]〚6〛},
 {x, 0, l6}, Epilog → {{Gray, line1}, {Gray, line2}, {Gray, line3},
   {Gray, line4}, {Gray, line5}}, PlotRange → {{0, l6}, {-0.004, 0.004}},
 PlotLabel → Style["Flat Bands of 10 Band Model for MA-TBG (δ = 1)", FontSize → 20],
 Axes → False, Frame → {True, True, False, False},
 FrameLabel → {"", "Energy (meV)"}, FrameTicks →
  {{{0, "K"}, {l1, "Γ"}, {l2, "-K"}, {l3, "-M"}, {l4, "Γ"}, {l5, "M"}, {l6, "K"}},
   {{-0.004, "-4"}, {-0.002, "-2"}, {0.0, "0"}, {0.002, "2"}, {0.004, "4"}}},
 LabelStyle → Directive[FontSize → 16, FontFamily → "Times"],
 PlotStyle → RGBColor[0.368417, 0.506779, 0.709798],
 ImageSize → 2 * (3 + 3 / 8) * 72, PlotPoints → 100, MaxRecursion → 1]
```

Out[∘]=

Flat Bands of 10 Band Model for MA−TBG ($\delta = 1$)