In[16]:=
```
(*  2*2 nearly-free electron solution, assuming only 2
 states joined by a particular G vector;  Here u1 represents
  [1,1] and [-1,-1] components of U, cubic case.  Hamiltonian is:  *)
Clear[kx, ky, u1];
MatrixForm[{{kx^2 + ky^2, u1}, {u1, (kx - 2 * Pi)^2 + (ky - 2 * Pi)^2}}]
```

Out[16]//MatrixForm=

$$\begin{pmatrix} kx^2 + ky^2 & u1 \\ u1 & (kx - 2\pi)^2 + (ky - 2\pi)^2 \end{pmatrix}$$

In[17]:=
```
(* eigenvalues along [11] direction *)
Clear[kx, u1];
FullSimplify[Eigenvalues[{{kx^2 + kx^2, u1}, {u1, (kx - 2 * Pi)^2 + (kx - 2 * Pi)^2}}]]
```

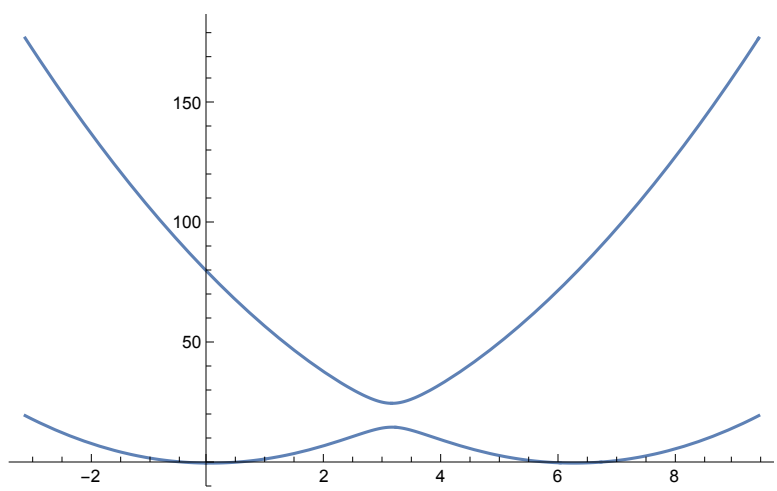
Out[17]= $\left\{2\,kx^2 - 4\,kx\,\pi + 4\,\pi^2 - \sqrt{16\,(kx - \pi)^2\,\pi^2 + u1^2},\ 2\,kx^2 - 4\,kx\,\pi + 4\,\pi^2 + \sqrt{16\,(kx - \pi)^2\,\pi^2 + u1^2}\right\}$

In[18]:=
```
(* eigenvalues specifically at zone boundary crossing, [Pi,Pi] *)
Clear[u1];
kx = Pi; Eigenvalues[{{kx^2 + kx^2, u1}, {u1, (kx - 2 * Pi)^2 + (kx - 2 * Pi)^2}}]
```

Out[18]= $\left\{2\,\pi^2 - u1,\ 2\,\pi^2 + u1\right\}$

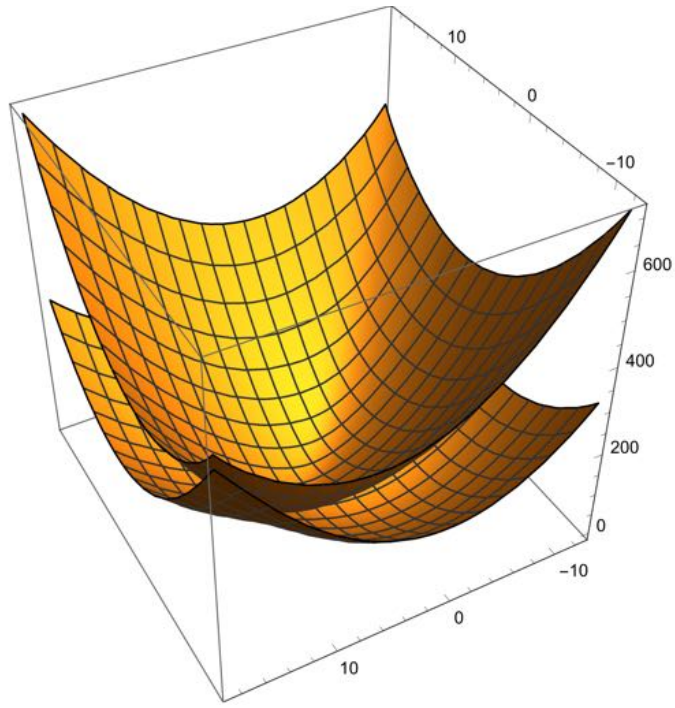
In[19]:=
```
(*  1D plot along [1,1] direction  *)
u1 = 5; Plot[Eigenvalues[{{kx^2 + kx^2, u1},
   {u1, (kx - 2 * Pi)^2 + (kx - 2 * Pi)^2}}], {kx, -1 * Pi, 3 * Pi}]
```

Out[19]=



In[20]:=
```
(*  2D plot of energies *)
Clear[kx, ky, u1]; u1 = 15;
Plot3D[Eigenvalues[{{kx^2 + ky^2, u1}, {u1, (kx - 2 * Pi)^2 + (ky - 2 * Pi)^2}}],
 {kx, -4 * Pi, 6 * Pi}, {ky, -4 * Pi, 6 * Pi}, BoxRatios → {1, 1, 1}]
```

Out[21]=



In[22]:=
```
(*  With k limited to the first quadrant, a 4*4 Hamiltonian suffices
  to solve out to kx=3Pi/2a and ky=3Pi/2a, a region that includes
 the entire (1st quadrant of) 1st BZ, and parts of 2nd-4th zones.
   Here u1 represents [1,0] and [0,1] components of U,
and u3 represents the [1,1] component.  Hamiltonian is:  *)
Clear[kx, ky, u1, u3];
MatrixForm[{{kx^2 + ky^2, u1, u1, u3}, {u1, (kx - 2 * Pi)^2 + ky^2, u3, u1},
  {u1, u3, kx^2 + (ky - 2 * Pi)^2, u1}, {u3, u1, u1, (kx - 2 * Pi)^2 + (ky - 2 * Pi)^2}}]
```

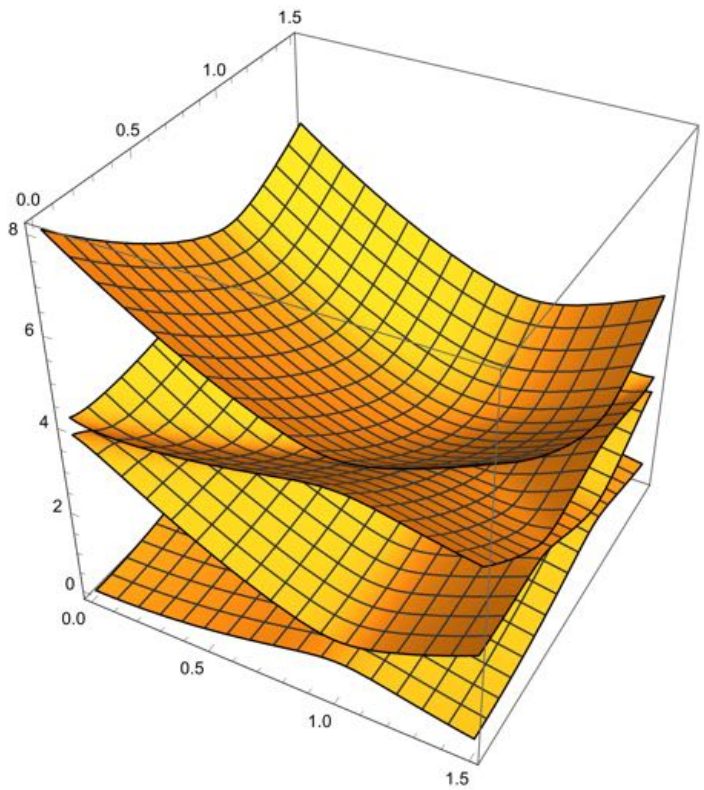
Out[22]//MatrixForm=

$$\begin{pmatrix} kx^2 + ky^2 & u1 & u1 & u3 \\ u1 & ky^2 + (kx - 2\pi)^2 & u3 & u1 \\ u1 & u3 & kx^2 + (ky - 2\pi)^2 & u1 \\ u3 & u1 & u1 & (kx - 2\pi)^2 + (ky - 2\pi)^2 \end{pmatrix}$$

In[23]:=
```
(* Here I diagonalized the 4*4 matrix representing the Hamiltonian,
in the first quadrant in (kx,ky), extending to parts of 2nd - 4th zones.
   Note k changed to units of (Pi/a), and energy units are ((Pi/a)^2/2m).
   Plotting all 4 eigenvalues yields 4 overlapping sheets in extended +
 reduced scheme.  *)
```

In[24]:=
```
u1 = .3; u3 = .2;
Plot3D[Eigenvalues[{{kx^2 + ky^2, u1, u1, u3},
    {u1, (kx - 2)^2 + ky^2, u3, u1},
    {u1, u3, kx^2 + (ky - 2)^2, u1},
    {u3, u1, u1, (kx - 2)^2 + (ky - 2)^2}}],
 {kx, 0, 1.5}, {ky, 0, 1.5}, BoxRatios → {1, 1, 1}]
```

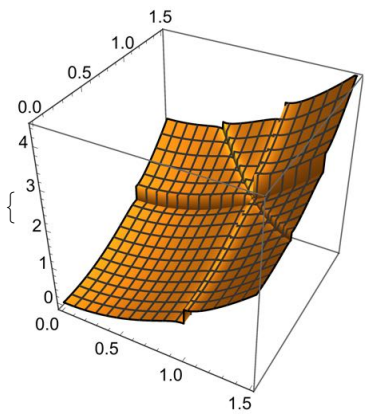
Out[25]=



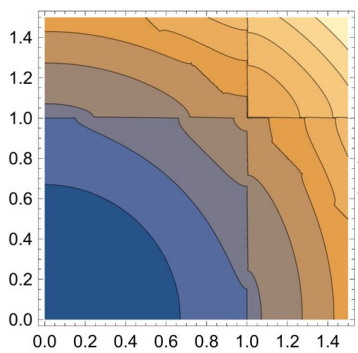
In[26]:=
```
(* Eigenvalues from Mathematica in numerically descending order;
Here I used a somewhat convoluted
 method to pick out Nth band in the Nth zone. *)
```

In[27]:=
```
u1 = .2; u3 = .1; eF = 4.5;
{Plot3D[Eigenvalues[{{kx^2 + ky^2, u1, u1, u3},
      {u1, (kx - 2)^2 + ky^2, u3, u1},
      {u1, u3, kx^2 + (ky - 2)^2, u1},
      {u3, u1, u1, (kx - 2)^2 + (ky - 2)^2}}][[
    4 - Floor[kx] - Floor[ky] - Floor[(kx + ky) / 2]]],
   {kx, 0, 1.5}, {ky, 0, 1.5}, BoxRatios → {1, 1, eF / 4.5},
   PlotPoints → 100, PlotRange → {0 - .2, eF}],
  ContourPlot[Eigenvalues[{{kx^2 + ky^2, u1, u1, u3},
      {u1, (kx - 2)^2 + ky^2, u3, u1},
      {u1, u3, kx^2 + (ky - 2)^2, u1},
      {u3, u1, u1, (kx - 2)^2 + (ky - 2)^2}}][[
    4 - Floor[kx] - Floor[ky] - Floor[(kx + ky) / 2]]],
   {kx, 0, 1.5}, {ky, 0, 1.5}, Contours → 10, PlotPoints → 40]}
```

Out[28]=



,



}