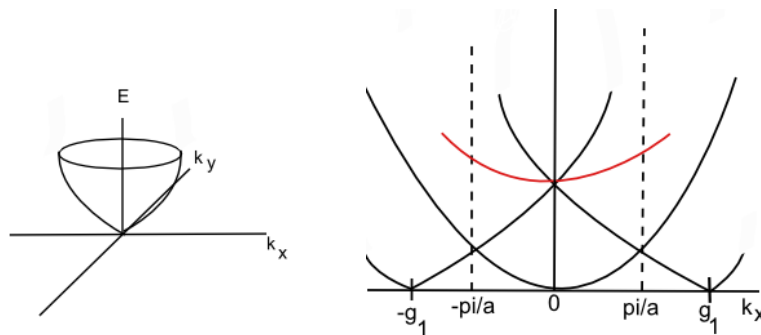


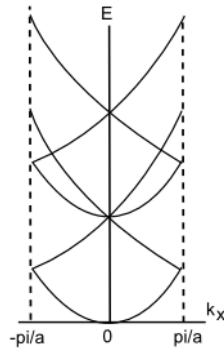
Topic 9-2: Vanishing Potential and Brillouin Zones  
Kittel Pages: 176,177

**Summary:** Our goal here is to extend Bloch's theorem to 2D, building on vanishing potential idea from last video. In doing this we develop a way to label points within the first Brillouin zone. We also develop spaghetti diagrams to capture all the electronic properties of a solid.

- Assumptions
  - Keep using the free electron model and the resulting parabolic dispersion
  - Periodic lattice with potential from atoms very small (basically heavily screened metal) so the parabola is undistorted
  - Square lattice
- Recall since  $\psi_n(\vec{k}) = \psi_n(\vec{k} + \vec{G})$  and  $E_n(\vec{k}) = E_n(\vec{k} + \vec{G})$  so we get dispersions of repeating parabolas
  - One parabola centered at  $k_x=0$
  - One parabola centered at  $g_1$  and one at  $-g_1$  that also extend into the first Brillouin zone
  - Also find parabolas centered at  $\pm 1g_2$  and so on
- In 2D we have a bowl

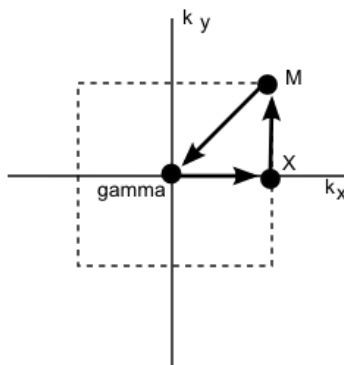


- Top red parabola is what happens when we add the parabola with an origin at  $1g_2$ 
  - Same curve will be created for the parabola at  $-1g_2$
- The  $g_2$  top curve has the same curvature as the one at the origin
- Can continue to add higher and higher bands by turning on parabolas further and further away from the origin
- Today we will call it good with the following parabolas along  $k_x$



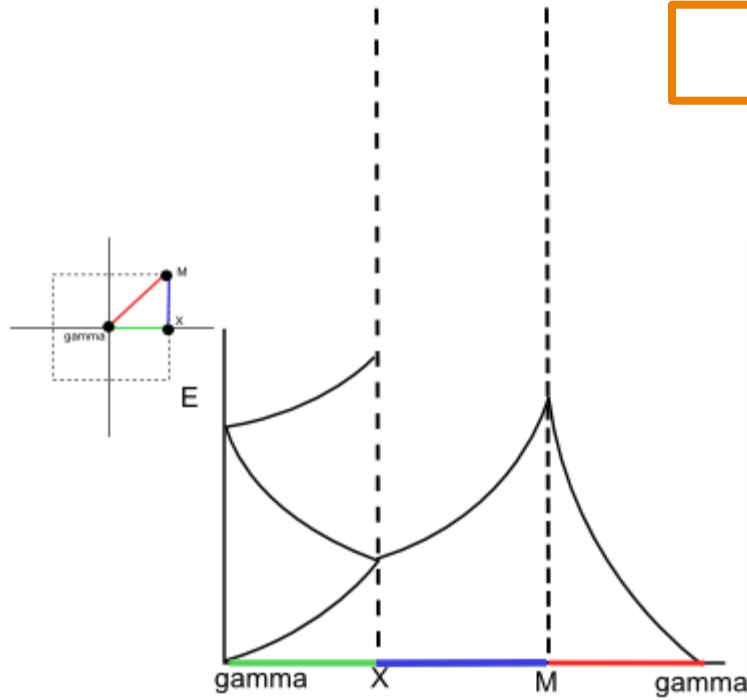
### Describing the energy surface *across* the Brillouin zone

- Using Mathematica to plot many parabolas in 2D isn't very helpful visually, unfortunately.
- Instead, we'll plot the energy along the high symmetry lines. This should give a good approximation of the dispersion



- Above is how we label a square lattice
- For a square X and Y are the same point due to symmetry so we don't bother labeling Y at the top
- In other Brillouin zone shapes the Y would be important
- Can now manipulate plot cross sections
- Call the above triangular path a spaghetti diagram
  - Path should cover all electronic properties
- From gamma to X is what we already did
  - Bottom curve is the original parabola, then the next one up is shifted by  $1g_1$  and then  $1g_2$  is on top

Sketch the other bands



- Trace the path through the first Brillouin zone and estimate if the distance from the parabolas origin increases (as in the bottom parabola above) or decreases

Questions to Ponder

1. Prove mathematically why the parabola at  $1g_2$  is equivalent to the origin. By equivalent we mean that the  $1g_2$  parabola has the same curvature as the one at the origin even though it is at a higher energy.
2. Within the vanishing periodic potential limit, there are only so many unique band structures. How many are there in 2D? How many in 3D? Sketch one.
3. What real materials will have band structures similar to the ones we have been calculating from the vanishing potential assumption?
4. How do you choose which path to trace along the first Brillouin zone to build a spaghetti diagram?