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Condensed Matter

# Homework 2

1. a) Theorem: Let $\Lambda$ be a bravais lattice in $d$ dimensions. Assume that we have a potential $U$ s.t. for all $\vec{\pi} \in \Lambda$

$$U(\vec{r} + \vec{\pi}) = U(\vec{r}).$$

Then, a complete set of eigenvectors of $H = -\frac{\hbar^2}{2m}\Delta + U(\vec{r})$ can be taken such that for all wave functions $\psi$ in the set, there is a wave vector $\vec{k}$ s.t.

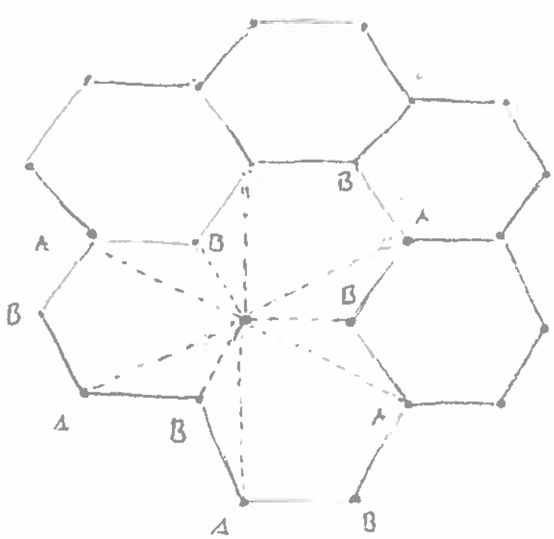
$$\psi(\vec{r} + \vec{\mathcal{R}}) = e^{i\vec{K}\cdot\vec{\mathcal{R}}}\,\psi(\vec{r})$$

for all $\vec{\mathcal{R}} \in \Lambda$.

Remarks: This version is taken entirely from reference [1]. However, in light of the discussion in [3], it is probably not correct. Namely, one must require some sort of "piecewise" continuity to $U$ to make the result stand.

b) This theorem presents a very convenient set of wave functions that take advantage of the symmetry of the crystal. Namely, they are defined completely by their associated wave vector $\vec{k}$ and their value on a primitive cell of the Bravais lattice. Moreover $\vec{k}$ may be restricte to a primitive cell of the reciprocal lattice, since for every reciprocal lattice vector $\vec{K}$ and lattice vector $\vec{R}$ we have $e^{i\vec{K}\cdot\vec{R}} = 1$. The Brillouin zone is commonly taken as this cell. Moreover, multiple energy eigenvectors may correspond to the same wave vector. This is how an electronic band structure appears, depending on which energy a state with a given wave vector is situated.

2\. a) The perturbation is also translationally invariant since $\vec{\delta}_1'$, $\vec{\delta}_2'$ and $\vec{\delta}_3'$ are lattice vectors. Moreover, one clearly sees that the swap $a \longleftrightarrow b$ is still a symmetry, i.e. the $C^2$ symmetry is still preserved. Finally the $C^3$ symmetry is also preserved. This can all be checked by noticing that the dotted line structure is invariant under translations, the




$C_2$ action and the $C_3$ action. Thus, based on the discussion in the lectures, there are two possibilities: either the cone opens or closes up, or the cone moves vertically.

b) As we already solved in the tutorial,

$$H_0 = \sum_{\vec{k}}' \Phi^{+}_{\vec{k}} h^{(0)}_{k} \Phi_{\vec{k}} ,$$

with

$$h^{(0)}_{\vec{k}} = \begin{pmatrix} 0 & -tf_{\vec{k}} \\ -tf^{*}_{\vec{k}} & 0 \end{pmatrix} .$$

On the other hand,

$$H' = -t' \sum_{\vec{n},\vec{\delta}_i',\vec{k},\vec{k}'}' \frac{1}{N}\left( e^{-i\vec{k}\cdot\vec{R}_{\vec{n}}} e^{i\vec{k}'\cdot(R_{\vec{n}}+\vec{\delta}_i')} a^{+}_{\vec{k}} a_{\vec{k}'} + c.c + a \longrightarrow b \right)$$

$$= -t' \sum_{\vec{\delta}_i,\vec{k},\vec{k}'}' \left( \frac{1}{\cancel{N}} \cancel{N} \delta_{\vec{k},\vec{k}'} e^{i\vec{k}'\cdot\vec{\delta}_i'} a^{+}_{\vec{k}} a_{\vec{k}'} + c.c. + a \longrightarrow b \right)$$

$$= -t' \sum_{\vec{\delta}_i, \vec{k}}' \left( e^{i\vec{k}\cdot\vec{\delta}_i'} a^+_{\vec{k}} a_{\vec{k}} + c.c. + a \longrightarrow b \right)$$

$$= -t' \sum_{\vec{k}}' \left( \left( e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2} + e^{i\vec{k}\cdot(\vec{a}_1 - \vec{a}_2)} \right) a^+_{\vec{k}} a_{\vec{k}} + c.c. \right.$$

$$\left. + a \longrightarrow b \right)$$

$$= -t' \sum_{\vec{k}}' \left( \left( e^{i\frac{3}{2}k_x a} e^{i\sqrt{3}/2\, k_y a} + e^{i\,3/2\, k_x a} e^{-i\sqrt{3}/2\, k_y a} \right.\right.$$

$$\left.\left. + e^{i\sqrt{3}\, k_y a} \right) a^+_{\vec{k}} a_{\vec{k}} + c.c. + a \longrightarrow b \right)$$

$$= -t' \sum_{\vec{k}}' \left( \left( 2 e^{i\frac{3}{2}k_x a} \cos\left( \frac{\sqrt{3}}{2} k_y a \right) + c.c. + 2\cos\left( \sqrt{3}\, k_y a \right) \right) a^+_{\vec{k}} a_{\vec{k}} \right.$$

$$\left. + a \longrightarrow b \right)$$

$$= -t' \sum_{\vec{k}}' \left( \left( 4\cos\left( 3/2\, k_x a \right) \cos\left( \sqrt{3}/2\, k_y a \right) + 2\cos\left( \sqrt{3}\, k_y a \right) \right) a^+_{\vec{k}} a_{\vec{k}} \right.$$

$$\left. + a \longrightarrow b \right)$$

$$= \sum_{\vec{k}}' (-t') g_{\vec{k}}\, a^+_{\vec{k}} a_{\vec{k}} + a \longrightarrow b = \sum_{\vec{k}}' \Phi^+_{\vec{k}} \begin{pmatrix} -t' g_{\vec{k}} & 0 \\ 0 & -t' g_{\vec{k}} \end{pmatrix}.$$

Thus,

$$H_{nnn} = \sum_{\vec{k}}{}' \, \Phi^{\dagger}_{\vec{k}} \, h_{\vec{k}} \, \Phi_{\vec{k}} \, .$$

c) The characteristic polinomial of $h_{\vec{k}}$ is

$$p(\lambda) = \left(-t' g_{\vec{k}} - \lambda\right)\left(-t' g_{\vec{k}} - \lambda\right) - \left(-t f_{\vec{k}}\right)\left(-t f^{*}_{\vec{k}}\right)$$

$$= \left(t' g_{\vec{k}}\right)^2 + 2\lambda t' g_{\vec{k}} + \lambda^2 - \left(t\,|f_{\vec{k}}|\right)^2 ,$$

whose zeros are at

$$\varepsilon_{\pm}(\vec{k}) = \frac{-\cancel{2} t' g_{\vec{k}} \pm \sqrt{\cancel{4} t'^2 g^2_{\vec{k}} - \cancel{4}\left(\left(t' g_{\vec{k}}\right)^2 - \left(t|f_{\vec{k}}|\right)^2\right)}}{\cancel{2}}$$

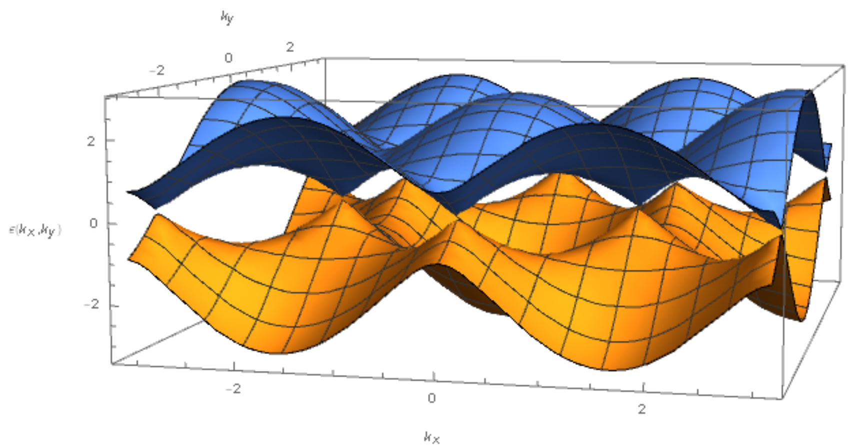
$$= -t' g_{\vec{k}} \pm |t f_{\vec{k}}| .$$

Comparing with the energy spectrum we had before $\varepsilon_{\pm}(\vec{k})\Big|_{t'=0} = \pm |t f_{\vec{k}}|$, we see that in both cases the bands touch at the same points, namely, the solutions of

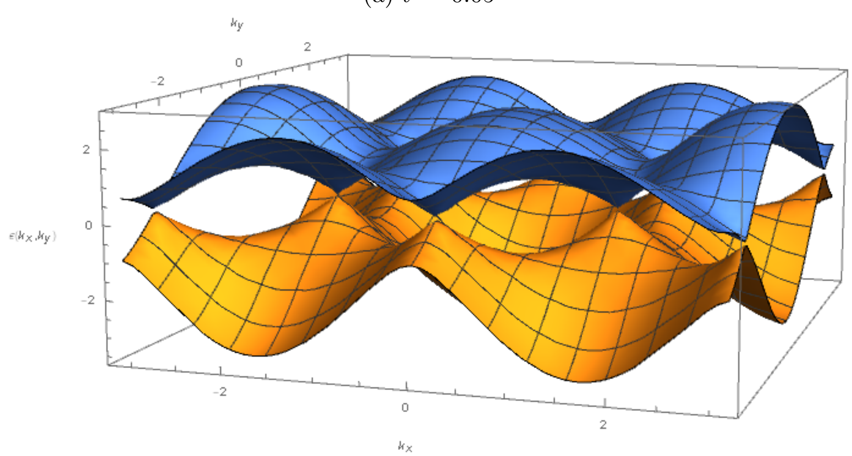
$$f_{\vec{k}} = 0 .$$

From the previous tutorial we know these are the points K and K'.

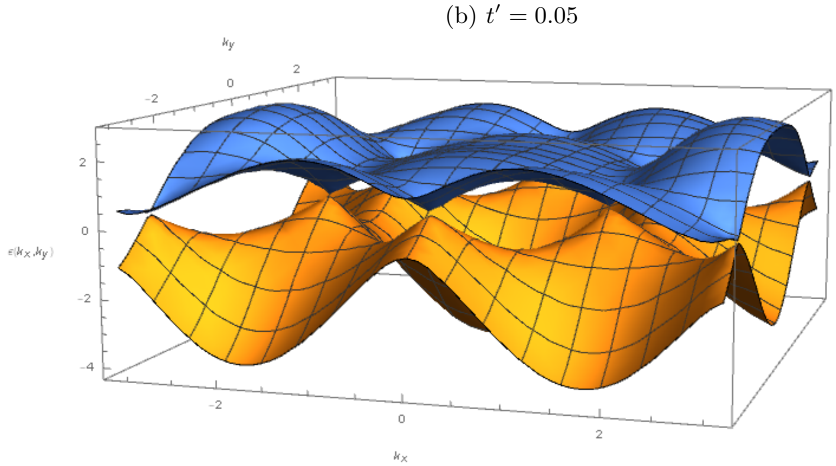
d) With the plots encountered in next page, we see that the predictions from part a) were correct. Indeed, as $t'$ gets bigger we notice that the cones rise and become flatter. They, however, do not move horizontally or separate.




(a) $t' = 0.05$




(b) $t' = 0.05$




(c) $t' = 0.05$

c) Translation symmetry by the primitive vectors is still preserved. The $C_3$ symmetry is preserved as well, since A points continue to be equivalent (and the same for B points) under $120°$ degree rotations. However, since A and B points are no longer equivalent, the $C_2$ symmetry is broken. In particular, we expect a gap to open at the Dirac cones.

f) We have

$$H'' = \frac{\Delta}{N} \sum_{\vec{n},\vec{k},\vec{k}'} \left( e^{-i\vec{k}\cdot\vec{n}} e^{i\vec{k}'\cdot\vec{n}} a^+_{\vec{k}} a_{\vec{k}'} - e^{-i\vec{k}\cdot\vec{n}} e^{i\vec{k}'\cdot\vec{n}} b^+_{\vec{k}} b_{\vec{k}'} \right)$$

$$= \Delta \sum_{\vec{k}} \left( a^+_{\vec{k}} a_{\vec{k}} - b^+_{\vec{k}} b_{\vec{k}} \right) = \sum_{\vec{k}} \Phi^+_{\vec{k}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Phi_{\vec{k}} .$$

We conclude (9) with

$$h_{\vec{k}} = \begin{pmatrix} \Delta & -tf_{\vec{k}} \\ -tf_{\vec{k}}^{*} & -\Delta \end{pmatrix}.$$

The characteristic polynomial is

$$p(\lambda) = (\Delta - \lambda)(-\Delta - \lambda) - |tf_{\vec{k}}|^2$$

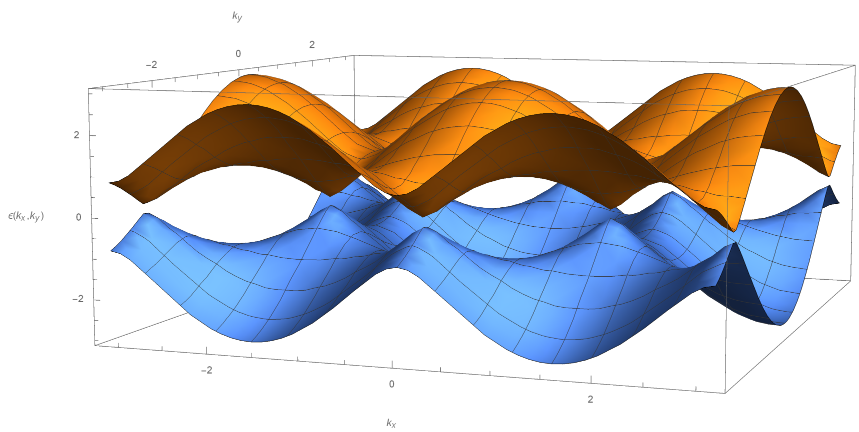
$$= \lambda^2 - \Delta^2 - |tf_{\vec{k}}|^2.$$

Its zeros are at

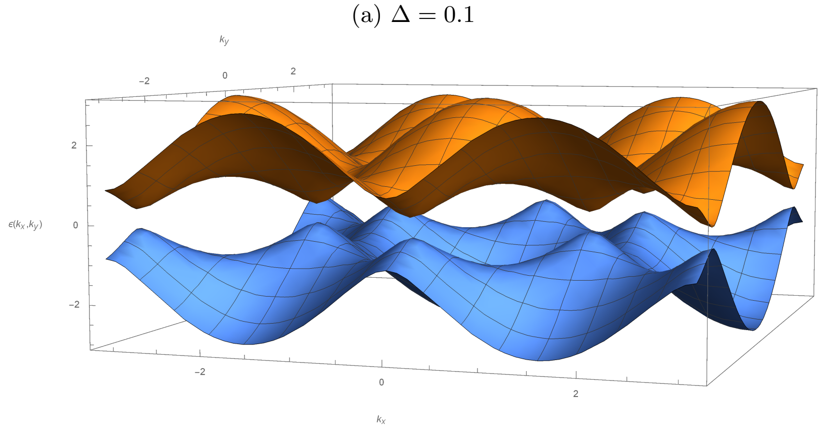
$$\varepsilon_{\pm}(\vec{k}) = \pm \frac{\sqrt{\cancel{4}(\cancel{4}\Delta^2 \cancel{4}|tf_{\vec{k}}|^2)}}{\cancel{2}}$$

$$= \pm \sqrt{\Delta^2 + |tf_{\vec{k}}|^2}$$

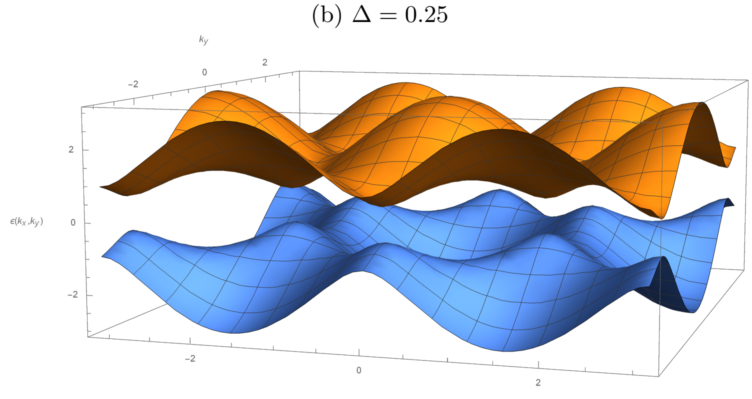
g) Indeed, as we predicted, as $\Delta$ increases the band gap opens. It becomes bigger with $\Delta$. The plots are found on the next page.




(a) $\Delta = 0.1$




(b) $\Delta = 0.25$




(c) $\Delta = 0.5$

# References

[1] Neil W. Ashcroft and N. David Mermin. *Solid State Physics*. Harcourt College Publishers, 1976. ISBN: 0-03-083993-9.

[2] Gerald D. Mahan. *Condensed Matter in a Nutshell*. Princeton University Press, 2011. ISBN: 978-0-691-14016-2.

[3] Frederic Schuller. *Lectures on Quantum Theory*. 2016. URL: https://www.youtube.com/playlist?list=PLPH7f%7B%5C_%7D7ZlzxQVx5jRjbfRGEzWY%7B%5C_%7DupS5K6.