Disclaimer

The solution at hand was written in the course of the respective class at the University of Bonn. If not stated differently on top of the first page or the following website, the solution was prepared and handed in solely by me, Marvin Zanke. Anything in a different color than the ball pen blue is usually a correction that I or a tutor made. For more information and all my material, check:
https://www.physics-and-stuff.com/

I raise no claim to correctness and completeness of the given solutions! This equally applies to the corrections mentioned above.

08.06.16 Condensed Matter Physics Exercise 4

a) $E_n(\vec{k}) = \frac{\hbar^2}{2m}(\vec{k}+\vec{G}) = \frac{\hbar^2}{2m}\left[(k_x+G_x)^2+(k_y+G_y)^2\right]$

$E_n(k+G) \hat{=} E_n(k)$

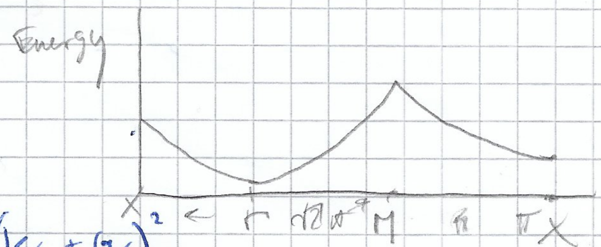
wave function are plane waves: $\psi_{\vec{k}} \sim e^{i\vec{k}\vec{r}}$

Restrict problem to first Brillouin zone because of the periodicity of the problem.

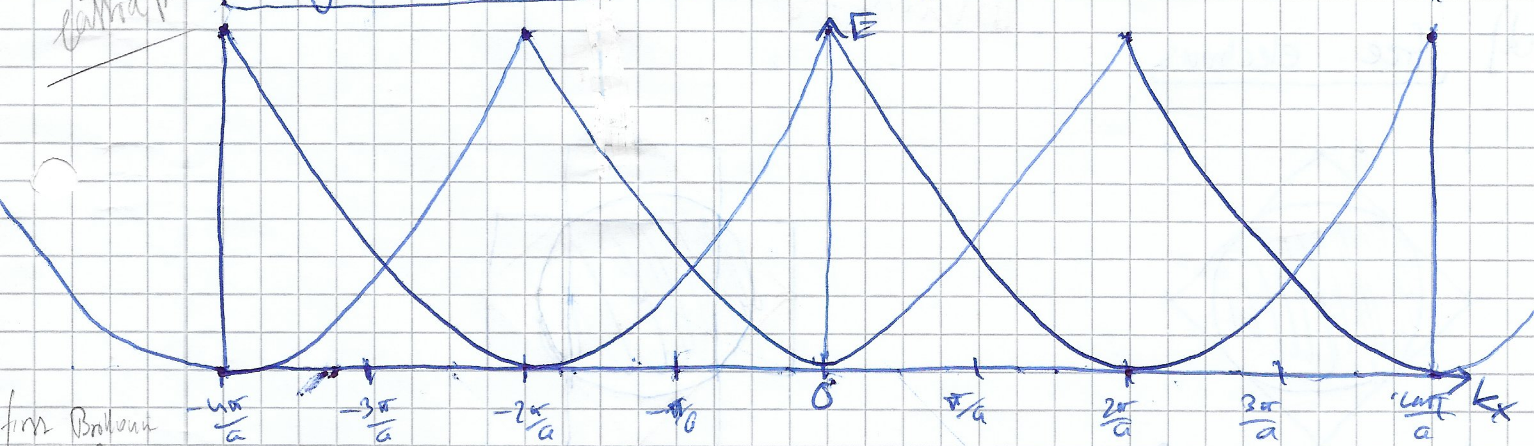
$(-\pi/a \le k \le \pi/a)$. $G_x = n_x \frac{2\pi}{a}$

$G_y = n_y \frac{2\pi}{a}$

red lines go to half of the way of next lattice point?

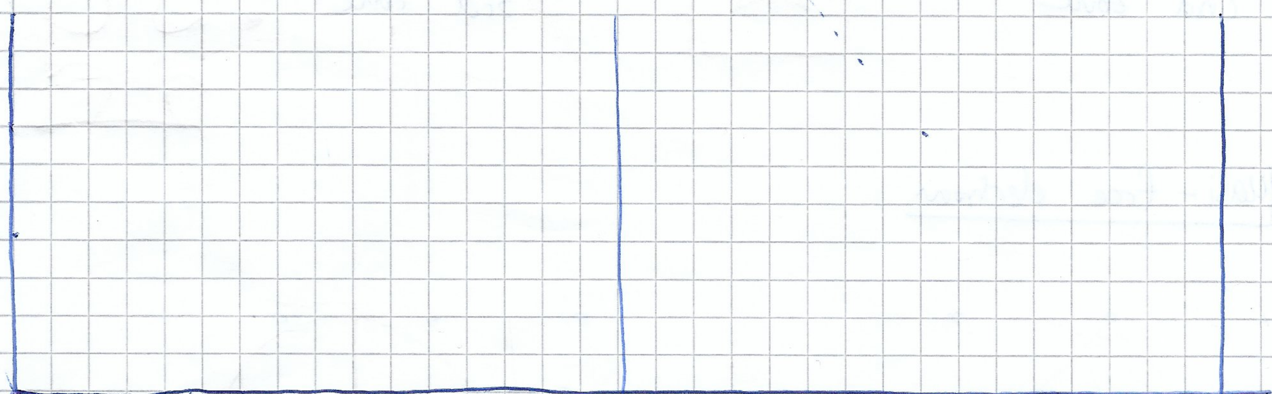


$k_y | k_x$ - Symmetric Direction: $E_n(\vec{k}) = \frac{\hbar^2}{2m}(k_x+G_x)^2$



first Brillouin Zone $\hat{=}$ Wigner-Seitz-Cell. Also second

Wigner Seitz Cell: same distance to what

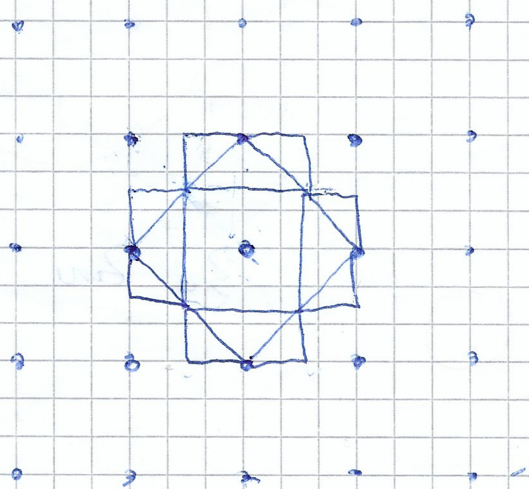


↑Combination?

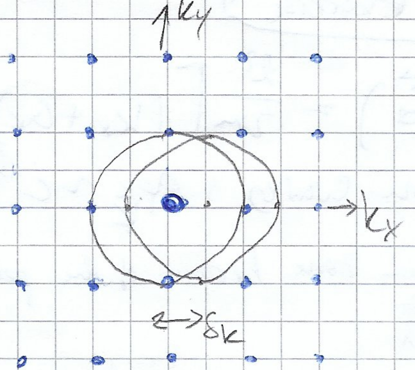
b)

Why 3rd? taken ... into account other BZ

How to change k or $\frac{2\pi}{a}$

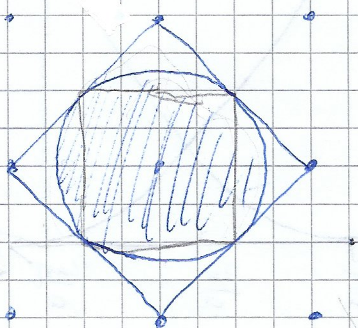


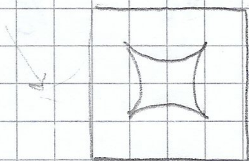
c)

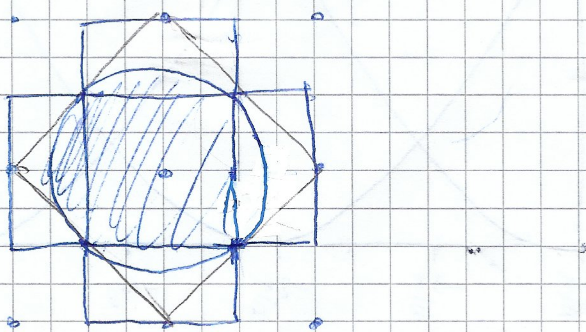


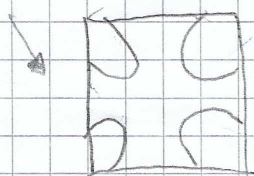
No Fermi surface in 1^{st} BZ

d) free electrons :





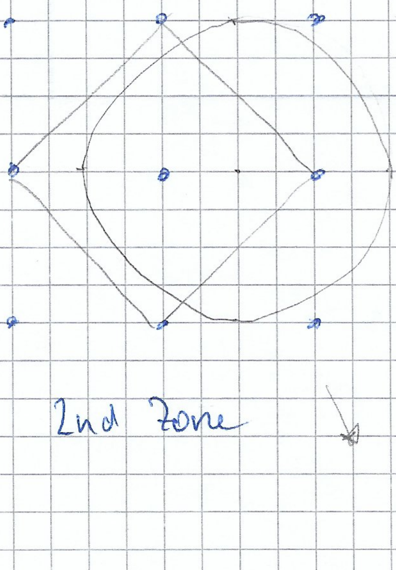


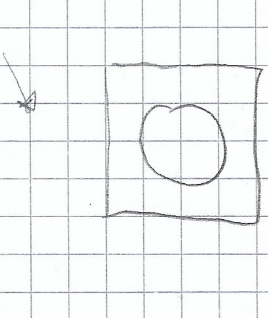


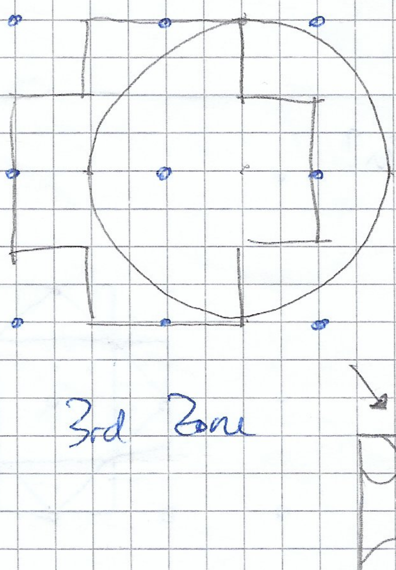
2nd Zone

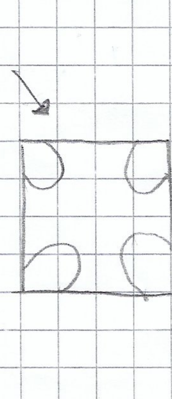
3rd Zone

quasi-free electrons









2nd Zone

3rd Zone

2)

$$U(x,y) = -4U \cos\left(\frac{2\pi}{a}x\right) \cos\left(\frac{2\pi}{a}y\right)$$

$$U_G = \frac{1}{a^2} \int_{-a/2}^{a/2} dx \int_{-a/2}^{a/2} dy \; U(x,y)\, e^{i\left(\frac{2\pi}{a}x + \frac{2\pi}{a}y\right)}$$

$$= \frac{4}{a^2} \int_0^{a/2} dx \int_0^{a/2} dy \; U(x,y) \cos(Gx)\cos(G'y)$$

$$\left(\int_0^c dx \cos\frac{2n\pi x}{a} \cos\frac{2m\pi x}{a} = \frac{c}{2} G_{mn} \right)$$

$$= \frac{1}{a^2} \int dx \int dy \left(-4U \cos\left(\frac{2\pi}{a}x\right) \cos\left(\frac{2\pi}{a}y\right)\right) e^{i\left(\frac{2\pi x}{a} + \frac{2\pi y}{a}\right)}$$

$$= -\frac{4U}{a^2} \cdot 2 \int_0^{a/2} dx \cos\left(\frac{2\pi x}{a}\right)\left(\cos\left(\frac{2\pi x}{a}\right) + i\sin\left(\frac{2\pi x}{a}\right)\right) \cdot 2 \int_0^{a/2} dy \cos\left(\frac{2\pi}{a}y\right)\left(\cos\left(\frac{2\pi y}{a}\right) + i\sin\left(\frac{2\pi y}{a}\right)\right)$$

$$= -\frac{4U}{a^2} \cdot 4 \left[\int_0^{a/2} \frac{1 + 2\cos\left(\frac{2\pi x}{a}\right)}{2} dx + i \int_0^{a/2} \cancel{\sin\frac{2\pi x}{a} \cos\frac{2\pi x}{a}}_{0} \cdot \int_0^{a/2} \frac{1 + 2\cos\left(\frac{2\pi y}{a}\right)}{2} dy \right] = -\frac{4U}{a^2} \cdot 4 \left(\frac{a}{4}\right)\left(\frac{a}{4}\right) = -U$$

$$\Rightarrow \Delta E = 2|U_G| = 2U$$

See last pages

3) a) $E(\vec{k}) \approx E_i - A_i - \sum_{m \neq n} e^{ik(R_n - R_m)} B_{i,m}$

$$A_i = -\int \phi_i^*(r-R_m)\, V(r-R_n)\, \phi_i(r-R_n)\, dr$$

$$= -\int \phi_i^*(r-R_n) \left[H(r-R_n) - H_A(r-R_n) \right] \phi_i(r-R_n)\, dr$$

$$= -(E_0 - E_i) = E_i - E_0$$

$$B_{i,m} = -\int \phi_i^*(r-R_m)\, v(r-R_n)\, \phi_i(r-R_m)\, dr$$

$$= -\int \phi_i^*(r-R_m) \left[H(r-R_n) - H_A(r-R_n) \right] \phi_i(r-R_n)\, dr$$

$$= +V + \underbrace{\ldots}_{0}$$

$$E(\vec{k}) = E_i - (E_i - E_0) - V(e^{ika} + e^{-ika}) = E_0 - 2V\cos(ka)$$

b) $D(E)\, dE = \frac{L}{\pi} dk = \frac{L}{\pi} \frac{dk}{dE} dE$

$$\leadsto D(E) = \frac{L}{\pi} \frac{1}{\frac{dE}{dk}} = \frac{L}{2\pi a V \sin(ka)}$$

c) $\left(\frac{1}{m^*}\right) = \frac{1}{\hbar^2} \frac{\partial^2 E_n(\vec{k})}{\partial k^2}$

$$\leadsto m^* = \hbar^2 \frac{1}{\frac{\partial^2 E}{\partial k^2}} = \frac{1}{a^2 V \cos(ka)}$$

4) 1. $k_h = -k_n$ just momentum conservation

2. $|S\rangle_h = -|S\rangle_n$ Same argument: Spin should be zero in sum in System where one band is fully filled.

3. $E_h(k_h) = -E_n(k_n)$

$$E_n(k_n) \underset{r \to -r}{=} E_n(-k_n) = -E_h(-k_n) = -E_h(k_h)$$

4. $v_h(k_h) = v_n(k_n)$

$$v_n = \frac{1}{\hbar} \nabla_{k_n} E_n(k_n) \quad , \nabla_{k_n} E_n(k_n) = \nabla_{k_n} E_n(-k_h) = \nabla_{k_n}(-E_h(k_h))$$
$$= \nabla_{k_h}(E_h(k_h)) = v_h$$

5. $m_h^* = -m_n^*$

$$\frac{1}{m_n^*} \propto \frac{d^2 E_n(k_n)}{dk_n^2} = -\frac{d^2 E_h(k_h)}{dk_h^2}$$

$$2)\quad U(x,y) = -4U \cos\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right)$$

$$\rightarrow \quad = -4U\left(e^{\frac{iGx}{2}} + e^{-\frac{iGx}{2}}\right)\left(e^{\frac{iGy}{2}} + e^{-\frac{iGy}{2}}\right)$$

$$U(x,y) = \sum_G \sum_{G'} U_{GG'} e^{iGx} e^{iG'y}$$

$$= -4U \sum_G \sum_{G'} U_{GG'} \cos(Gx)\cos(G'y)$$

We find $U_{GG'}$ through a fourier-transformation:

$$U_{GG'} = \int dx \int dy \; U(x,y)\, e^{i(Gx + G'y)}$$

$$\Rightarrow \quad U_G = \frac{1}{a^2} \int_{-a/2}^{a/2} dx \int_{-a/2}^{a/2} dy \; U(x,y)\, e^{i(Gx+G'y)}$$

$$= -\frac{4U}{a^2} \int_{-a/2}^{a/2} dx \int_{-a/2}^{a/2} dy \; \cos(Gx)\cos(G'y)\, e^{i(Gx+G'y)}$$

$$= -U$$

Central equation:

$$\left(\frac{\hbar^2 k^2}{2m} - E\right) C(k_x, k_y) + \sum_{G,G'} U_{GG'} C(k_x - G, k_y - G') = 0$$

result from fourier trafo $\rightarrow$

$$\left(\frac{\hbar^2 k^2}{2m} - E\right) C(k_x, k_y) - U\, C(k_x - G, k_y - G') = 0$$

$$k = \pm\frac{\pi}{a} \Leftrightarrow k = \pm\frac{1}{2}G$$

$$\Rightarrow \left(\frac{\hbar^2 k^2}{2m} - E\right) C\left(\tfrac{1}{2}G\right) - U\, C\left(-\tfrac{1}{2}G\right) = 0$$

$$\left(\frac{\hbar^2 k^2}{2m} - E\right) C\left(-\tfrac{1}{2}G\right) - U\, C\left(\tfrac{1}{2}G\right) = 0$$

For a nontrivial solution for C, the following equation must be fullfilled:

$$\det\begin{pmatrix} \frac{\hbar^2 k^2}{2m} - E & -U \\ -U & \frac{\hbar^2 k^2}{2m} - E \end{pmatrix} = 0$$

$$\Rightarrow \left(\frac{\hbar^4 k^4}{4m^2} - 2\frac{\hbar^2 k^2}{2m^2} E + E^2\right) - U^2 = 0 \,, \quad \frac{\hbar^2 k^2}{2m} := \alpha$$

$$\left(\alpha^2 - 2\alpha E + E^2\right) - U^2 = 0 \Rightarrow E_{1/2} = \alpha \pm U$$

$$\Rightarrow \Delta E = E_1 - E_2 = 2U$$