

# Introduction to graphene and 2D materials

## Homework problem set 3

17.06.2024

### 1 Graphene with SOC

Atomic spin orbit coupling (SOC) strength ( $\lambda_{ASOC}$ ) generally scales as  $\sim Z^4$  vertically down the periodic table. [\*This should be taken with a grain of salt since we know the spin orbit interaction for Au ( $Z = 79$ ) is negligible compared to Te ( $Z = 52$ )]. Therefore, in the tight binding calculations of graphene (allotrope of C,  $Z = 6$ ,  $\lambda_{ASOC} \approx 0$ ), the SOC term is often omitted.

- Search literature for controlling spin orbit interaction (not just atomic SOC). Are any of these methods applicable to graphene? Devise an experiment to study the effect of spin orbit interaction in graphene.
- As a thought experiment, let's assume that there is a new 2D material with the same crystal structure as graphene but with significantly higher SOC. Perform the tight binding calculation for this new 2D material with  $\lambda_{ASOC} \gg 0$ . How does the band structure change with SOC?

### 2 Parallel Magnetic Field

When dealing with the classical Hall effect and the quantum Hall effect, the magnetic field  $B_{\perp}$ , is often pointed along the  $z$  direction perpendicular to the sample plane. Now consider that the magnetic field points towards the  $x$  direction, parallel to the electron flow in the 2DEG (i.e.  $B_{\parallel}$ ). The 2DEG is confined with a quantum well potential of  $V(z) = \frac{1}{2}m^*\omega_0^2z^2$

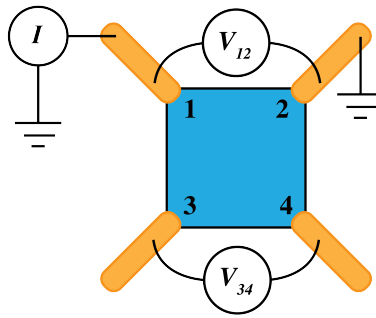
- Write the Schrödinger equation for this system using the vector potential  $\vec{A} = (0, -zB_{\parallel}, 0)$ , plane wave ansatz  $\Psi(\vec{r}) = e^{ik_x x} e^{ik_y y} \Phi(z)$  and  $\omega_c = \frac{qB}{m^*}$ .  
(\* remember that  $H = \frac{1}{2m}(\vec{p} - q\vec{A})^2 + V(z)$ )
- Show that the Schrödinger equation can be expressed in the following form

$$\left[ \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} \frac{\omega_0^2}{\omega^2(B)} + \frac{1}{2}m^*\omega^2(B)(z + \zeta)^2 \right] \Psi = E\Psi \quad (1)$$

where  $\zeta \equiv \left( \frac{\hbar k_y \omega_c}{m^* \omega^2(B)} \right)$  and  $\omega^2(B) \equiv \omega_0^2 + \omega_c^2$ .

- Sketch the confining potential along the  $z$  direction (i.e.  $E$  vs  $z(k_y)$ ) for  $B_{\parallel} = 0$  and  $B_{\parallel} \neq 0$
- What can be said about the effective masses for  $x$  and  $y$  at  $B_{\parallel} \neq 0$ ?
- What can be said about the energy levels of the new system?

### 3 Quantum Transport



The figure above shows a four terminal, van der Pauw device made from a topological insulator.  $I$  is the applied current,  $V_{12} = V_1 - V_2$  the 2-probe voltage,  $V_{34} = V_3 - V_4$  the 4-probe voltage. As we explored in HW 11, the transport properties of a topological insulator can be explained in the Landauer-Büttiker (LB) formalism:

$$I_i = \frac{e^2}{h} \sum_j (T_{ji}V_i - T_{ij}V_j), \quad (2)$$

where  $I_i$  is the current flowing from the  $i$ th electrode and  $V_i$  is the voltage on the  $i$ th electrode, and  $T_{ji}$  is the transmission probability from the  $i$ th to the  $j$ th electrode. Remember that  $I_1 = I = -I_2$ .

- (e) Discuss the differences between classical Hall, integer quantum Hall, fractional quantum Hall, quantum anomalous Hall, and quantum spin Hall effects. (i.e. What makes them - except the classical Hall - “Quantum”?)
- (f) Write down the criterium for the transmission probability  $T$  of a Quantum Anomalous Hall (QAH) system.
- (g) Write down the criterium for the transmission probability  $T$  of a Quantum Spin Hall (QSH) system.
- (h) Write down the Landauer-Büttiker system of equations for the van der Pauw geometry shown above, assuming that it is a QAH system.
- (i) Calculate the expected 2-probe resistance,  $R_{12,12} = \frac{V_{12}}{I_{12}}$  (i.e. measuring the voltage drop across leads 1 and 2 while flowing current between leads 1 and 2) of the QAH system.
- (j) Calculate the expected 4-probe resistance,  $R_{12,34} = \frac{V_{34}}{I_{12}}$  (i.e. measuring the voltage drop across leads 3 and 4 while flowing current between leads 1 and 2) of the QAH system.