

Research Notes

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September 11, 2024

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Chapter 1

Majorana fermions in a tunable semiconductor device

1.1 Applying an on axis Magnetic Field

A method for making a Majorana fermion tunable device has been shown in two forms, one by D. Sau (REFERENCE) and J. Alicea (REFERENCE). A zinc-blende semiconductor quantum well grown along the (100) direction is considered. We start with the relevant noninteracting Hamiltonian

$$\mathcal{H}_0 = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger \left[\frac{k^2}{2m} - \mu + \alpha(\sigma^x k_y - \sigma^y k_x) \right] c_{\mathbf{k}} \quad (1.1)$$

where m is the effective mass, μ is the chemical potential, α is the Rashba spin-orbit(REFERENCED in Alicea's paper as ref 23) coupling strength, and σ^i are the Pauli matrices that act on the spin degrees of freedom in $c_{\mathbf{k}}$. We have set $\hbar = 1$ throughout.

We next introduce a ferromagnetic insulator and a magnetic field. The ferromagnetic insulator has magnetization pointing perpendicular to the 2D semiconductor. While the magnetic field will point parallel to the 2D semiconductor. We assume this will induce a Zeeman interaction

$$\mathcal{H}_Z = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger [V_x \sigma^x + V_y \sigma^y + V_z \sigma^z] c_{\mathbf{k}} \quad (1.2)$$

but negligible orbital coupling. If we look at the combined Hamiltonian it becomes obvious there is a constant energy plus the energy eigenvalues of the Pauli matrices terms. We can easily solve the eigenvalue problem of

$$\begin{bmatrix} V_z & V_x + \alpha k_y - i(V_y - \alpha k_x) \\ V_x + \alpha k_y + i(V_y - \alpha k_x) & -V_z \end{bmatrix} \quad (1.3)$$

or in a more compact form using $\beta(\mathbf{k}) = k_y + V_x/\alpha$ and $\gamma(\mathbf{k}) = k_x - V_y/\alpha$ and $\eta^2(\mathbf{k}) = \beta^2(\mathbf{k}) + \gamma^2(\mathbf{k})$ and we produce

$$\begin{bmatrix} V_z & \alpha(\beta(\mathbf{k}) + i\gamma(\mathbf{k})) \\ \alpha(\beta(\mathbf{k}) - i\gamma(\mathbf{k})) & -V_z \end{bmatrix} \quad (1.4)$$

giving $\epsilon'_\pm = \pm\sqrt{V_z^2 + \alpha^2\eta^2(\mathbf{k})}$ with eigenvectors

$$u_+(\mathbf{k}) = \begin{pmatrix} A_\uparrow(\mathbf{k}) \\ -A_\downarrow(\mathbf{k}) \frac{\beta(\mathbf{k}) - i\gamma(\mathbf{k})}{\eta(\mathbf{k})} \end{pmatrix} \quad (1.5)$$

$$(1.6)$$

$$u_-(\mathbf{k}) = \begin{pmatrix} B_\uparrow(\mathbf{k}) \frac{\beta(\mathbf{k}) + i\gamma(\mathbf{k})}{\eta(\mathbf{k})} \\ B_\downarrow(\mathbf{k}) \end{pmatrix} \quad (1.7)$$

One can find $A_\sigma = A_\sigma^*$ and $B_\sigma = B_\sigma^*$ and the coefficients are

$$A_\uparrow(\mathbf{k}) = \frac{-\alpha\eta(\mathbf{k})}{\sqrt{2\epsilon'_+(\mathbf{k})}} \sqrt{\frac{1}{\epsilon'_+(\mathbf{k}) - V_z}} \quad (1.8)$$

$$A_\downarrow(\mathbf{k}) = \sqrt{\frac{\epsilon'_+(\mathbf{k}) - V_z}{2\epsilon'_+(\mathbf{k})}} \quad (1.9)$$

$$B_\uparrow(\mathbf{k}) = \sqrt{\frac{\epsilon'_-(\mathbf{k}) + V_z}{2\epsilon'_-(\mathbf{k})}} \quad (1.10)$$

$$B_\downarrow(\mathbf{k}) = \frac{\alpha\eta(\mathbf{k})}{\sqrt{2\epsilon'_-(\mathbf{k})}} \sqrt{\frac{1}{\epsilon'_-(\mathbf{k}) + V_z}} \quad (1.11)$$

If in the case of $V_x = V_y = 0$ we arrive back at solution Sau *et al.* calculate for eigenvalues, vectors, and coefficients. The expressions for $A_{\uparrow,\downarrow}$ and $B_{\uparrow,\downarrow}$ can be written in convenient terms as

$$f_p(\mathbf{k}) = A_\uparrow(\mathbf{k})A_\downarrow(-\mathbf{k}) = B_\uparrow(-\mathbf{k})B_\downarrow(\mathbf{k}) \quad (1.12)$$

$$= \frac{-\alpha\eta(\mathbf{k})}{2\sqrt{\epsilon'_+(\mathbf{k})\epsilon'_+(-\mathbf{k})}} \sqrt{\frac{\epsilon'_+(-\mathbf{k}) - V_z}{\epsilon'_+(\mathbf{k}) - V_z}} \quad (1.13)$$

When putting the semiconductor in contact with an s -wave superconductor a pairing term is generated by the proximity effect. The full Hamiltonian becomes $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_Z + \mathcal{H}_{SC}$ with

$$\mathcal{H}_{SC} = \sum_{\mathbf{k}} \Delta c_{\uparrow,\mathbf{k}}^\dagger c_{\downarrow,-\mathbf{k}}^\dagger + H.c. \quad (1.14)$$

We now want to write the pairing potential in terms of c_\pm using a basis transformation.

$$c_{\uparrow,\mathbf{k}} = \langle \uparrow | u_+(\mathbf{k}) \rangle c_{\mathbf{k},+} + \langle \uparrow | u_-(\mathbf{k}) \rangle c_{\mathbf{k},-} \quad (1.15)$$

$$= A_\uparrow(\mathbf{k}) c_{\mathbf{k},+} + B_\uparrow(\mathbf{k}) \frac{\beta(\mathbf{k}) + i\gamma(\mathbf{k})}{\eta(\mathbf{k})} c_{\mathbf{k},-} \quad (1.16)$$

$$c_{\downarrow,-\mathbf{k}} = \langle \downarrow | u_+(-\mathbf{k}) \rangle c_{-\mathbf{k},+} + \langle \downarrow | u_-(-\mathbf{k}) \rangle c_{-\mathbf{k},-} \quad (1.17)$$

$$= -A_\downarrow(-\mathbf{k}) \frac{\beta(-\mathbf{k}) - i\gamma(-\mathbf{k})}{\eta(-\mathbf{k})} c_{-\mathbf{k},+} + B_\downarrow(-\mathbf{k}) c_{-\mathbf{k},-} \quad (1.18)$$

with the adjoints being

$$c_{\uparrow,\mathbf{k}}^\dagger = A_\uparrow(\mathbf{k}) c_{\mathbf{k},+}^\dagger + B_\uparrow(\mathbf{k}) \frac{\beta(\mathbf{k}) - i\gamma(\mathbf{k})}{\eta(\mathbf{k})} c_{\mathbf{k},-}^\dagger \quad (1.19)$$

$$c_{\downarrow,-\mathbf{k}}^\dagger = -A_\downarrow(-\mathbf{k}) \frac{\beta(-\mathbf{k}) + i\gamma(-\mathbf{k})}{\eta(-\mathbf{k})} c_{-\mathbf{k},+}^\dagger + B_\downarrow(-\mathbf{k}) c_{-\mathbf{k},-}^\dagger \quad (1.20)$$

Continue reducing the pairing potential which becomes

$$\begin{aligned} \Delta c_{\uparrow,\mathbf{k}}^\dagger c_{\downarrow,-\mathbf{k}}^\dagger &= \Delta [-A_\uparrow(\mathbf{k}) A_\downarrow(-\mathbf{k}) \frac{\beta(-\mathbf{k}) + i\gamma(-\mathbf{k})}{\eta(-\mathbf{k})} c_{\mathbf{k},+}^\dagger c_{-\mathbf{k},+}^\dagger \\ &\quad + B_\uparrow(\mathbf{k}) B_\downarrow(-\mathbf{k}) \frac{\beta(\mathbf{k}) - i\gamma(\mathbf{k})}{\eta(\mathbf{k})} c_{\mathbf{k},-}^\dagger c_{-\mathbf{k},-}^\dagger \\ &\quad + \left(A_\uparrow(\mathbf{k}) B_\downarrow(-\mathbf{k}) - B_\uparrow(\mathbf{k}) A_\downarrow(-\mathbf{k}) \frac{\beta(\mathbf{k}) - i\gamma(\mathbf{k})}{\eta(\mathbf{k})} \frac{\beta(-\mathbf{k}) + i\gamma(-\mathbf{k})}{\eta(-\mathbf{k})} \right) c_{\mathbf{k},+}^\dagger c_{-\mathbf{k},-}^\dagger] \end{aligned} \quad (1.21)$$

We will use a more convenient notation by making the following substitutions

$$\Delta_{++}(\mathbf{k}) = -\Delta f_p(\mathbf{k}) \frac{\beta(-\mathbf{k}) + i\gamma(-\mathbf{k})}{\eta(-\mathbf{k})} \quad (1.22)$$

$$\Delta_{--}(\mathbf{k}) = \Delta f_p(-\mathbf{k}) \frac{\beta(\mathbf{k}) - i\gamma(\mathbf{k})}{\eta(\mathbf{k})} \quad (1.23)$$

$$\Delta_{+-}(\mathbf{k}) = \Delta f_s(\mathbf{k}) \quad (1.24)$$

Where

$$f_s(\mathbf{k}) = \left(A_{\uparrow}(\mathbf{k})B_{\downarrow}(-\mathbf{k}) - B_{\uparrow}(\mathbf{k})A_{\downarrow}(-\mathbf{k}) \frac{\beta(\mathbf{k}) - i\gamma(\mathbf{k})}{\eta(\mathbf{k})} \frac{\beta(-\mathbf{k}) + i\gamma(-\mathbf{k})}{\eta(-\mathbf{k})} \right) \quad (1.25)$$

The pairing potential Hamiltonian then becomes

$$\mathcal{H}_{SC} = \sum_{\mathbf{k}} \Delta_{++} c_{\mathbf{k},+}^{\dagger} c_{-\mathbf{k},+}^{\dagger} + \Delta_{--} c_{\mathbf{k},-}^{\dagger} c_{-\mathbf{k},-}^{\dagger} + \Delta_{+-} c_{\mathbf{k},+}^{\dagger} c_{-\mathbf{k},-}^{\dagger} + H.c. \quad (1.26)$$

Writing the full Hamiltonian in compact form we will use the following Nambu spinor

$$\Psi = (c_{\mathbf{k},+}, c_{\mathbf{k},-}, c_{-\mathbf{k},+}^{\dagger}, c_{-\mathbf{k},-}^{\dagger})^T \quad (1.27)$$

Then we write the Hamiltonian as, where we have used the conventional BdG approach of applying the anticommutation relation and reindexing the momentum vector of the second term to give

$$\mathcal{H} = \frac{1}{2} \sum_{\mathbf{k}} \Psi^{\dagger} H_{BdG} \Psi \quad (1.28)$$

with

$$H_{BdG} = \begin{bmatrix} \epsilon_{+}(\mathbf{k}) & 0 & 2\Delta_{++}(\mathbf{k}) & \Delta_{+-}(\mathbf{k}) \\ 0 & \epsilon_{-}(\mathbf{k}) & -\Delta_{+-}(-\mathbf{k}) & 2\Delta_{--}(\mathbf{k}) \\ 2\Delta_{++}^{*}(\mathbf{k}) & -\Delta_{+-}^{*}(-\mathbf{k}) & -\epsilon_{+}(-\mathbf{k}) & 0 \\ \Delta_{+-}^{*}(\mathbf{k}) & 2\Delta_{--}^{*}(\mathbf{k}) & 0 & -\epsilon_{-}(-\mathbf{k}) \end{bmatrix} \quad (1.29)$$

where

$$\epsilon_{\pm}(\mathbf{k}) = \frac{k^2}{2m} - \mu + \epsilon'_{\pm}(\mathbf{k}) \quad (1.30)$$

We can rearrange our matrix into a more block diagonal form with off terms to give

$$H_{BdG} = \begin{bmatrix} \epsilon_+(\mathbf{k}) & 2\Delta_{++} & 0 & \Delta_{+-}(\mathbf{k}) \\ 2\Delta_{++}^* & -\epsilon_+(-\mathbf{k}) & -\Delta_{+-}^*(-\mathbf{k}) & 0 \\ 0 & -\Delta_{+-}(-\mathbf{k}) & \epsilon_-(\mathbf{k}) & 2\Delta_{--} \\ \Delta_{+-}^*(\mathbf{k}) & 0 & 2\Delta_{--}^* & -\epsilon_-(-\mathbf{k}) \end{bmatrix} \quad (1.31)$$

Upon studying $V_y = V_x = 0$ we see that near the fermi surface the interband pairing has little affect on the band gap. Scaling it's effect from $0 \rightarrow 1$ we see the intraband gap appears at a slightly smaller momentum as the interband pairing is turned off. We thus use the approximation $\Delta_{+-}(k_f) \approx 0$. We also set μ such that it only crosses the lower bands, thus allowing $c_+^\dagger \rightarrow 0$.

$$H_{BdG} = \begin{bmatrix} \epsilon_-(\mathbf{k}) & 2\Delta_{--}(\mathbf{k}) \\ 2\Delta_{--}^*(\mathbf{k}) & -\epsilon_-(-\mathbf{k}) \end{bmatrix} \quad (1.32)$$

Solving for the dispersion relation of the system we arrive at

$$E_{\pm}(\mathbf{k}) = \frac{\epsilon'_-(\mathbf{k}) - \epsilon'_-(-\mathbf{k})}{2} \pm \sqrt{\frac{(\epsilon_-(\mathbf{k}) + \epsilon_-(-\mathbf{k}))^2}{4} + 4|\Delta_{--}(\mathbf{k})|^2} \quad (1.33)$$

1.2 Small Applied Magnetic Field Approximation

To simplify we set $V_y \neq V_x = 0$ and look at $V_y \ll V_z$ and $\alpha k_f \ll V_z$ to get an idea of what the effective pairing term will be.

$$\epsilon'_+(\pm\mathbf{k}) = V_z \sqrt{1 + \frac{V_y^2 + \alpha^2 k^2 \mp 2\alpha k_x V_y}{V_z^2}} \quad (1.34)$$

$$\epsilon'_+(\pm\mathbf{k}) \approx V_z \left(1 + \frac{V_y^2 + \alpha^2 k^2 \mp 2\alpha k_x V_y}{2V_z^2} \right) \quad (1.35)$$

$$\epsilon'_+(\pm\mathbf{k}) - V_z \approx \frac{V_y^2 + \alpha^2 k^2 \mp 2\alpha k_x V_y}{2V_z^2} \quad (1.36)$$

$$\frac{\sqrt{\epsilon'_+(\mathbf{k}) - V_z}}{\eta(\mathbf{k})} \approx \sqrt{\frac{V_y^2 + \alpha^2 k^2 - 2\alpha k_x V_y}{2V_z^2}} \frac{\alpha}{\sqrt{V_y^2 + \alpha^2 k^2 - 2\alpha k_x V_y}} \quad (1.37)$$

$$\frac{\sqrt{\epsilon'_+(\mathbf{k}) - V_z}}{\eta(\mathbf{k})} \approx \frac{\alpha}{\sqrt{2}V_z} \quad (1.38)$$

$$\frac{\eta(-\mathbf{k})}{\sqrt{\epsilon'_+(-\mathbf{k}) - V_z}} \approx \sqrt{\frac{2V_z^2}{V_y^2 + \alpha^2 k^2 + 2\alpha k_x V_y}} \frac{\sqrt{V_y^2 + \alpha^2 k^2 + 2\alpha k_x V_y}}{\alpha} \quad (1.39)$$

$$\frac{\eta(-\mathbf{k})}{\sqrt{\epsilon'_+(-\mathbf{k}) - V_z}} \approx \frac{\sqrt{2}V_z}{\alpha} \quad (1.40)$$

$$\frac{\eta(-\mathbf{k})}{\sqrt{\epsilon'_+(-\mathbf{k}) - V_z}} \frac{\sqrt{\epsilon'_+(\mathbf{k}) - V_z}}{\eta(\mathbf{k})} \approx 1 \quad (1.41)$$

$$(\epsilon'_+(-\mathbf{k})\epsilon'_+(\mathbf{k}))^{-1/2} \approx V_z^{-1}(1 - \delta_-)^{-1/2}(1 - \delta_+)^{-1/2} \quad (1.42)$$

$$(\epsilon'_+(-\mathbf{k})\epsilon'_+(\mathbf{k}))^{-1/2} \approx V_z^{-1}(1 - \frac{1}{2}(\delta_- + \delta_+)) \quad (1.43)$$

$$(\epsilon'_+(-\mathbf{k})\epsilon'_+(\mathbf{k}))^{-1/2} \approx V_z^{-1} \left(1 - \frac{V_y^2 + \alpha^2 k^2}{2V_z^2} \right) \quad (1.44)$$

$$(1.45)$$

With all of the appropriate approximations we can now write out the intraband pairing term as

$$\Delta_{--}(\mathbf{k}) \approx -\frac{\Delta}{2V_z} \left(1 - \frac{V_y^2 + \alpha^2 k^2}{2V_z^2} \right) (\alpha k_y - i(\alpha k_x - V_y)) \quad (1.46)$$

$$\Delta_{--}(\mathbf{k}) \approx -\frac{\Delta}{2V_z} (\alpha k_y - i(\alpha k_x - V_y)) \quad (1.47)$$

If we instead turn the applied field from y to x we arrive at a similar answer as above. Combining both solutions for any arbitrary magnetic field pointing in the x - y plane we arrive at

$$\Delta_{--}(\mathbf{k}) \approx -\frac{\Delta}{2V_z} ((\alpha k_y + V \cos \phi) - i(\alpha k_x - V \sin \phi)) \quad (1.48)$$

Where $V = \sqrt{V_x^2 + V_y^2}$ and $\phi = \arg(V_x + iV_y)$

1.3 Perturbation of Band Gap due to Magnetic Field

Let us now consider what has more of an affect on the energy band gap, the diagonal or off-diagonal terms in the Hamiltonian. To start we seperate the Hamiltonian in to two terms using only an applied field in the y -direction,

$$H_{BdG} = H_0 + H_y \quad (1.49)$$

Where

$$H_0 = \begin{bmatrix} \epsilon_0(k) & 2\Delta_0(\mathbf{k}) \\ 2\Delta_0^*(\mathbf{k}) & -\epsilon_0(k) \end{bmatrix} \quad (1.50)$$

$$H_y = \begin{bmatrix} \epsilon_y(k_x) & 2\Delta_y \\ 2\Delta_y^* & -\epsilon_y(-k_x) \end{bmatrix} \quad (1.51)$$

Here we define

$$\epsilon_0(k) = \frac{k^2}{2m} - \mu - V_z - \frac{\alpha^2 k^2}{2V_z} \quad (1.52)$$

$$\Delta_0(\mathbf{k}) = -\frac{\alpha\Delta}{2V_z}(k_y - ik_x) \quad (1.53)$$

$$\epsilon_y(\pm k_x) = \frac{V_y}{V_z}(\pm \alpha k_x - \frac{1}{2}V_y) \quad (1.54)$$

$$\Delta_y = -\frac{i\Delta V_y}{2V_z} \quad (1.55)$$

To start we look at when $\epsilon_0(k_0) = 0$, which is the momentum value we would see an energy band gap appear. Determining the orthonormal eigensystem of the base Hamiltonian gives us

$$|\pm = \pm 2|\Delta_0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} \mp \frac{\Delta_0}{|\Delta_0|} \\ 1 \end{bmatrix} \quad (1.56)$$

We then perform the basis transformation

$$\langle +|H_y|+ \rangle = \frac{\alpha k_x V_y}{V_z} \quad (1.57)$$

$$\langle +|H_y|- \rangle = \frac{V_y}{V_z} \left(\frac{1}{2} V_y + i\Delta \right) \quad (1.58)$$

$$\langle -|H_y|+ \rangle = \frac{V_y}{V_z} \left(\frac{1}{2} V_y - i\Delta \right) \quad (1.59)$$

$$\langle -|H_y|- \rangle = \frac{\alpha k_x V_y}{V_z} \quad (1.60)$$

Which can be written in a more compact form as

$$H_y = \frac{V_y}{V_z} \begin{bmatrix} \alpha k_x & \frac{1}{2} V_y + i\Delta \\ \frac{1}{2} V_y - i\Delta & \alpha k_x \end{bmatrix} \quad (1.61)$$

Here we claim that all elements of the matrix are of equal importance due to them all being within the same order of magnitude.