1 Effective Hamiltonian

We begin with the low-energy bilayer Hamiltonian (in the ψ_{A_1}, ψ_{B_1}, ψ_{A_2}, ψ_{B_2} basis).

$$H = \begin{bmatrix} 0 & \frac{\sqrt{3}a}{2}\kappa\gamma_1 & 0 & \frac{\sqrt{3}a}{2}\kappa^*\beta_{nn} \\ \frac{\sqrt{3}a}{2}\kappa^*\gamma_1 & 0 & \beta_d & 0 \\ 0 & \beta_d & 0 & \frac{\sqrt{3}a}{2}\kappa\gamma_1 \\ \frac{\sqrt{3}a}{2}\kappa\beta_{nn} & 0 & \frac{\sqrt{3}a}{2}\kappa^*\gamma_1 & 0 \end{bmatrix} \tag{1}$$

We will further allow the β_{nn} coupling terms to vanish and add an additional bias voltage term to the Hamiltonian.

$$H = \begin{bmatrix} 0 & \frac{\sqrt{3}a}{2}\kappa\gamma_1 & 0 & 0 \\ \frac{\sqrt{3}a}{2}\kappa^*\gamma_1 & 0 & \beta_d & 0 \\ 0 & \beta_d & 0 & \frac{\sqrt{3}a}{2}\kappa\gamma_1 \\ 0 & 0 & \frac{\sqrt{3}a}{2}\kappa^*\gamma_1 & 0 \end{bmatrix} + h_{bias} \tag{2}$$

where the modification to the Hamiltonian due to an interlayer bias voltage is given by

$$h_{bias} = \begin{bmatrix} -\frac{V(x)}{2} & 0 & 0 & 0 \\ 0 & -\frac{V(x)}{2} & 0 & 0 \\ 0 & 0 & \frac{V(x)}{2} & 0 \\ 0 & 0 & 0 & \frac{V(x)}{2} \end{bmatrix} \tag{3}$$

If we choose to let $\pi = \kappa^\dagger = p_x + ip_y$ (for notational reasons), $\beta_d = t_\perp$, and the Fermi velocity $c = \frac{\sqrt{3}a}{2}\gamma_1$, then we have for our full Hamiltonian:

$$H = \begin{bmatrix} -\frac{V(x)}{2} & c\pi^\dagger & 0 & 0 \\ c\pi & -\frac{V(x)}{2} & t_\perp & 0 \\ 0 & t_\perp & \frac{V(x)}{2} & c\pi^\dagger \\ 0 & 0 & c\pi & \frac{V(x)}{2} \end{bmatrix} \tag{4}$$

To obtain a nicer form for the effective Hamiltonian, we begin by reorganizing the basis: $\{A_1, B_1, A_2, B_2\} \to \{A_1, B_2, A_2, B_1\}$. We obtain

$$H = \begin{bmatrix} -\frac{V(x)}{2} & 0 & 0 & c\pi^\dagger \\ 0 & \frac{V(x)}{2} & c\pi & 0 \\ 0 & c\pi^\dagger & \frac{V(x)}{2} & t_\perp \\ c\pi & 0 & t_\perp & -\frac{V(x)}{2} \end{bmatrix} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \tag{5}$$

We make use of the identity

$$det(H - E) = det(H_{11} - H_{12}(H_{22} - E)^{-1}H_{21} - E)det(H_{22} - E) \tag{6}$$

Here, we will assume that $V << t_\perp$ and since we are concerned with the low energy region where $E << t_\perp$, we can make the approximation

$$H_{22} - E \approx H_{22}^{'} = \begin{bmatrix} 0 & t_\perp \\ t_\perp & 0 \end{bmatrix}$$

This approximation allows us to write

$$det(H_{22} - E) = -t_\perp^2$$

and the effective 2×2 Hamiltonian is

$$H_{eff} = \left(H_{11} - H_{12} H_{22}^{-1} H_{21}\right) \tag{7}$$

We will make use of the fact that $V(x) << t_\perp$ to simplify H_{22}^{-1}:

$$H_{22}^{-1} = \frac{1}{-(\frac{V(x)}{2})^2 - t_\perp^2} \begin{bmatrix} \frac{-V(x)}{2} & -t_\perp \\ -t_\perp & \frac{V(x)}{2} \end{bmatrix} \approx \begin{bmatrix} \frac{V(x)}{2t_\perp^2} & \frac{1}{t_\perp} \\ \frac{1}{t_\perp} & \frac{-V(x)}{2t_\perp^2} \end{bmatrix}$$

That is,

$$H_{eff} = \begin{bmatrix} \frac{-V(x)}{2} & 0 \\ 0 & \frac{V(x)}{2} \end{bmatrix} - \begin{bmatrix} 0 & c\pi^\dagger \\ c\pi & 0 \end{bmatrix} \begin{bmatrix} \frac{V(x)}{2t_\perp^2} & \frac{1}{t_\perp} \\ \frac{1}{t_\perp} & \frac{-V(x)}{2t_\perp^2} \end{bmatrix} \begin{bmatrix} 0 & c\pi^\dagger \\ c\pi & 0 \end{bmatrix} \tag{8}$$

$$= \begin{bmatrix} \frac{-V(x)}{2} & 0 \\ 0 & \frac{V(x)}{2} \end{bmatrix} - \begin{bmatrix} \frac{-V(x)c^2|\pi|^2}{2t_\perp^2} & \frac{(c\pi^\dagger)^2}{t_\perp} \\ \frac{(c\pi)^2}{t_\perp} & \frac{V(x)c^2|\pi|^2}{2t_\perp^2} \end{bmatrix}$$

We finally obtain

$$H_{eff} = \begin{bmatrix} \frac{-V(x)}{2}(1 - \frac{c^2|\pi|^2}{t_\perp^2}) & -\frac{(c\pi^\dagger)^2}{t_\perp} \\ -\frac{(c\pi)^2}{t_\perp} & \frac{V(x)}{2}(1 - \frac{c^2|\pi|^2}{t_\perp^2}) \end{bmatrix} \tag{9}$$

The basis of which is the non-dimer sites A_1, B_2. Diagonalizing the effective Hamiltonian, we can now see that the energies are given by

$$E^2 = \frac{(c|\pi|)^4}{t_\perp^2} + \frac{V(x)^2}{4}\left(1 - \frac{c^2|\pi|^2}{t_\perp^2}\right)^2 \tag{10}$$

But if V(x) is significantly less than the hopping parameter $t_\perp$, then we can simplify the effective Hamiltonian and corresponding spectrum as

$$H_{eff} = \begin{bmatrix} \frac{-V(x)}{2} & -\frac{(c\pi^\dagger)^2}{t_\perp} \\ -\frac{(c\pi)^2}{t_\perp} & \frac{V(x)}{2} \end{bmatrix} \tag{11}$$

$$E^2 = \frac{(c|\pi|)^4}{t_\perp^2} + \frac{V(x)^2}{4} \tag{12}$$

In order to rewrite the effective Hamiltonian in a quasiclassical form, we begin by factoring out $\frac{c^2}{t_\perp}$

$$H_{eff} = \begin{bmatrix} \frac{-V(x)t_\perp}{2c^2} & -(\pi^\dagger)^2 \\ -\pi^2 & \frac{V(x)t_\perp}{2c^2} \end{bmatrix} \tag{13}$$

$$= \begin{bmatrix} \frac{-V(x)t_\perp}{2c^2} & -(p_x^2 - p_y^2 - 2ip_xp_y) \\ -(p_x^2 - p_y^2 + 2ip_xp_y) & \frac{V(x)t_\perp}{2c^2} \end{bmatrix} \tag{14}$$

Finally, if we define the momenta to be measured in units of $1/a$, then we finally obtain

$$H_{qc} = -\phi(x)\sigma_z - (p_x^2 - p_y^2)\sigma_x - 2p_xp_y\sigma_y \tag{15}$$

where we define

$$\phi(x) = \frac{V(x)t_\perp a^2}{2c^2}$$

We can also further define a function $\vec{g}(\vec{p}, x)$ such that

$$H_{qc} = \vec{g}(\vec{p}, x) \cdot \vec{\sigma} \tag{16}$$

The corresponding wave equation is given by

$$H(\vec{p}, x)\psi = \epsilon\psi \tag{17}$$

For $\psi = [u(x), v(x)]$, we obtain

$$\begin{aligned} -\phi(x)u(x) + (ip_x + p_y)^2 v(x) &= \epsilon u(x) \\ \phi(x)v(x) + (ip_x - p_y)^2 u(x) &= \epsilon v(x) \end{aligned} \tag{18}$$

And using $\partial_x = -ip_x$ in natural units where $\hbar = 1$,

$$\begin{aligned} -\phi(x)u(x) + (\partial_x + p_y)^2 v(x) &= \epsilon u(x) \\ \phi(x)v(x) + (\partial_x - p_y)^2 u(x) &= \epsilon v(x) \end{aligned} \tag{19}$$

If we enforce an antisymmetric potential profile (i.e. $\phi(-x) = -\phi(x)$), then,

$$\begin{aligned} -\phi(x)u(x) + (\partial_x + p_y)^2 v(x) &= \epsilon u(x) \\ -\phi(x)v(-x) + (\partial_x + p_y)^2 u(-x) &= \epsilon v(-x) \end{aligned} \tag{20}$$

and we can see that if $v(x) = \pm u(-x)$, then we have two systems of equations given by:

$$\begin{aligned} -\phi(x)u(x) + (\partial_x + p_y)^2 u(-x) &= \epsilon u(x) \\ -\phi(x)u(x) + (\partial_x + p_y)^2 u(-x) &= \epsilon u(x) \end{aligned}$$

and

$$\begin{aligned} -\phi(x)w(x) + (\partial_x + p_y)^2(-w(-x)) &= \epsilon w(x) \\ -\phi(x)(-w(x)) + (\partial_x + p_y)^2(w(-x)) &= -\epsilon w(x) \end{aligned}$$

But all of these equations can be solved in the same way, as they are just the same equation. So, for a particular value of p_y, we can obtain an eigenvector $\Psi_{p_y} = [u_{p_y}(x), u_{p_y}(-x)]$ with eigenvalue ϵ_{p_y} that solves the first set of equations. We can also obtain a second eigenvector $\Phi_{p_y} = [w_{p_y}(x), -w_{p_y}(-x)]$ that solves the second set of equations. From the first eigenvector solution, we have:

$$-\phi(x)u(x) + (\partial_x + p_y)^2 u(-x) = \epsilon u(x)$$

$$-\phi(x)u(x) + (\partial_x + p_y)^2 u(-x) = \epsilon u(x)$$

Inverting the sign on x gives us

$$-\phi(-x)u(-x) + (-\partial_x + p_y)^2 u(x) = \epsilon u(-x)$$

$$-\phi(-x)u(-x) + (-\partial_x + p_y)^2 u(x) = -\epsilon(-u(-x))$$

And using the antisymmetry of the potential profile:

$$-\phi(x)(-u(-x)) + (-\partial_x + p_y)^2 u(x) = \epsilon u(-x)$$

$$-\phi(x)(-u(-x)) + (-\partial_x + p_y)^2 u(x) = -\epsilon(-u(-x))$$

We know the solutions to these equations are [] If we swap the sign of x, we obtain the equivalent result

$$-\phi(-x)u(-x) + (\partial_x - p_y)^2 u(x) = \epsilon u(-x)$$

And making use of the antisymmetry of the potential profile, we can write this as

$$-\phi(x)(-u(-x)) + (\partial_x - p_y)^2 u(x) = -\epsilon(-u(-x))$$

So, we therefore obtain another solution $\Phi_{p_y} = [-u_{-p_y}(-x), u_{-p_y}(x)]$ with eigenvalue $-\epsilon_{-p_y}$. Our goal now is to analyze the dispersion $\epsilon(p_y)$ to observe the effect of the form of $\phi(x)$.

2 Step Kink

We will consider a step-like kink $\phi(x) = \phi_0 sgn(x)$, where

$$sgn(x) = \begin{cases} 1 & x > 0 \\ 0 & x = 0 \\ -1 & x < 0 \end{cases} \tag{21}$$

Our wave equation becomes

$$\begin{aligned} -u(x) + (\partial_x + p_y)^2 v(x) = \epsilon u(x) \quad & x > 0 \\ u(x) + (\partial_x + p_y)^2 v(x) = \epsilon u(x) \quad & x < 0 \end{aligned} \tag{22}$$

For $\Psi = [u(x), v(x) = u(-x)]$, we have

$$\begin{aligned} -\phi_0 u(x) + (\partial_x + p_y)^2 u(-x) = \epsilon u(x) \quad & x > 0 \\ \phi_0 u(x) + (\partial_x + p_y)^2 u(-x) = \epsilon u(x) \quad & x < 0 \end{aligned} \tag{23}$$

In the $x > 0$ region, we can rewrite this as

$$-\phi_0 u(x) + (\partial_x^2 + \partial_x p_y + p_y^2)u(-x) = \epsilon u(x) \tag{24}$$

where we use the operator algebra $\partial_x p_y = p$

In both the $+x$ and $-x$ regions, the wave equation takes the form of a second order differential equation, which has general solution $\Psi \propto e^{-\lambda x}$, where λ can be a complex root.