Electron transmission through the stacking domain boundary in multilayer graphenes

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We present a theoretical study on the electron transmission through the AB-BA stacking boundary in multilayer graphenes. Using the tight-binding model and the transfer matrix method, we calculate the electron transmission probability through the boundary as a function of electron Fermi energy in multilayers from bilayer to five-layer. We find that the transmission is strongly suppressed particularly near the band touching point, suggesting that the electronic conductivity in general multilayer graphenes is significantly interfered by stacking fault. The conductivity suppression by stacking fault is the strongest in the bilayer graphene, while it is gradually relaxed as increasing the number of layers. At a large carrier density, we observe an even-odd effect where the transmission is relatively lower in trilayer and five-layer than in bilayer and four-layer, and this is related to the existence of a monolayer-like linear band in odd layers. For bilayer graphene, we also study the effect of the perpendicular electric field opening an energy gap, and show that the band deformation enhances the electron transmission at a fixed carrier density.

I. INTRODUCTION

After the successful isolation of individual graphene flake, graphene and its multilayers became one of the most intensively studied topics. In multilayer graphene, the weak van der Waals interlayer interaction allows domain structure consisting of different stacking regions. Recent experiments found that bilayer graphene samples commonly contain domain boundaries, which connect two distinct Bernal-stacking structures referred as AB and BA (Fig. 1). In trilayer, similar stacking fault forms ABA-ABC stacking boundary which connects the Bernal stacked and rhombohedral stacked trilayer graphenes. This kind of domain structure is expected to rather common in graphene multilayers, and it should influence the electric conductivity through the scattering of charge carriers. The effect of the domain boundary on the electron transport was studied for graphene bilayer, and it was found that the transmission through the boundary is highly suppressed at the low carrier concentration.

In this paper, we extend the previous analyses to general graphene multilayers from bilayer to five layer and investigate the characteristic boundary effect on the electron transport in increasing the thickness. Specifically we consider a multilayer system in Fig. 2 having AB-BA boundary on the bottom layer while otherwise stacked in Bernal stacking order. We calculate the electron transmission probability through the stacking fault as a function of the Fermi energy using the tight-binding model and the transfer matrix method. The result shows that the boundaries generally suppress the electron transmission in comparison with the perfect Bernal stacked system, while the reduction becomes gradually weaker as increasing the number of layers. We also notice that the transmission shows some odd-even effect at high electron density larger than $10^{13}$ cm$^{-2}$, where the even-layer boundaries have better electron transmission than odd-layer boundaries. We present the qualitative explanation of those characteristic properties of electron transmission through domain boundary by considering the local band structure inside the boundary region.

For Bernal stacked bilayer graphene, we can open an band gap between conduction band and valence bands by applying an external electric field perpendicular to the graphene sheet. Here we also study the electron transmission in bilayer AB-BA boundary under the perpendicular electric field, and find that the band deformation induced by the electric field significantly enhances the electron transmission at a fixed carrier density.

II. FORMULATION

A. Atomic structure

Let us consider the AB-BA domain boundaries in bilayer graphene as illustrated in Fig. 1 where the uniform BA stacking in the left region ($x < 0$) is continuously deformed in the boundary region ($0 < x < W$) to connect to the uniform AB stacking in the right region ($x > W$). We assume that the system is periodic in y-direction. The side view shows the atomic positions on a $xz$-plane, where filled circles and open circles indicate A and B atoms, respectively, while dots are the centers of hexagons denoted as C sites (no atoms). The domain boundary is created by shifting two graphene layers in the right region with respect to each other, while fixing the left region. Specifically, we start with the regular BA bilayer graphene [Fig. 1(a)], and shift the top layer and the bottom layer of the right region by $\pm a/(2\sqrt{3})$ (where $a = 0.246$ nm is the graphene’s lattice constant), respectively, with the structure in the left region fixed. We assume that the atomic positions in the intermediate region linearly interpolates between left and right. The width of the intermediate region, W is written in terms of an the number of unit cells $N$ as $W = (N + \frac{1}{2}) \sqrt{3}a$. At $N = 20$, for instance, we have $W \approx 8.7$ nm, while the realistic boundary width is about 10nm. Here we focus on the boundary parallel to the zigzag direction which has the biggest effect on the transmission.
FIG. 1: Atomic structure of (a) regular BA bilayer graphene and (b) BA-AB domain boundary on bilayer graphene.

FIG. 2: Side view of N-layer domain boundary, which consists of \( N - 1 \) Bernal stacking layers (red layers) and one distorted layer at the bottom (blue layer).

The construction of the domain boundary in general \( N \)-layer graphene is similar to the bilayer case, where we assume only the bottom layer is expanded by \( a/\sqrt{3} \) in \( x \)-axis while other \( N - 1 \) layers are fixed to the Bernal stacking without distortion as illustrated in Fig. 2. The stacking structure can be specified by the sequence of sites along a vertical line; here we see that \( \cdots \)BA\( BA \) stack at \( x = 0 \) is continuously deformed to \( \cdots \)BA\( BC \) stack at \( x = W \).

B. Tight-binding model

To model the motion of an electron in the system, we use the tight-binding method. The Hamiltonian for tight-binding model is written as

\[
H = - \sum_{i \neq j} t_i j (R_i - R_j) |R_i\rangle\langle R_j| + \text{h.c.} \tag{1}
\]

where \( R_i \) is the atomic coordinate, \( |R_i\rangle \) is the wavefunction at site \( i \), and \( t_i j (R_i - R_j) \) is the transfer integral.
between atom $i$ and $j$. We adopt an approximation \cite{17, 21}

$$-t(d) = V_{pp\sigma}(d) \left[ 1 - \left( \frac{d \cdot e_z}{d} \right)^2 \right] + V_{pp\sigma}(d) \left( \frac{d \cdot e_z}{d} \right)^2$$

(2)

$$V_{pp\sigma}(d) = V_0^{pp\sigma} \exp \left( -\frac{d - a}{a} \right),$$

(3)

$$V_{pp\sigma}(d) = V_0^{pp\sigma} \exp \left( -\frac{d - a}{a} \right),$$

(4)

where $d = R_i - R_j$ is the distance between two atoms. $e_z$ is the unit vector on $z$ axis. $V_{pp\sigma}$ is the transfer integrals between nearest-neighbor atoms of monolayer graphene which are located at distance $a_0 = a/\sqrt{3} \approx 0.142$nm. $V_0^{pp\sigma}$ is the transfer integral between two nearest-vertically aligned atoms. $d_0 \approx 0.335$nm is the interlayer spacing. The decay length $r_0$ of transfer integral is chosen at 0.184a. At $d > \sqrt{3}a$, the transfer integral is very small and can be neglected.

\section{C. Transmission probability}

Fig. 3 shows the schematic view of Fermi surface in the left region and the right region at a fixed energy $\varepsilon$. For $k_y$ falling inside the Fermi surface, we have traveling modes with real $k_y$, which can be classified as left-going and right-going modes depending on the expectation value of velocity in $x$. Since the system is translationally symmetric along $y$-direction, the wavenumber $k_y$ is conserved, so that an electronic state in the left region is only connected to one in the right region on the same horizontal line. Using the formulation in the Appendix, we calculate the transmission coefficient $t_{\mu\nu}(k_y; \varepsilon)$ from incident channel $\nu$ in the left region to outgoing channel $\mu$ in the right region. The case (a) in Fig. 3 shows a situation where we have a single channel per direction i.e., we have the right going mode 1 ($1'$) and the left going mode 2 ($2'$) in the left (right) region. The electron transmission probability is then given by $|t_{11'}|^2$. In (b), we have multiple channels per direction; two right going modes 1, 2 ($1'$, $2'$) and two left going modes 3, 4 ($3'$, $4'$) in the left (right) region. We then have multiple transmission probabilities $|t_{13'}|^2$, $|t_{14'}|^2$, $|t_{23'}|^2$, $|t_{24'}|^2$, and $|t_{22'}|^2$.

To characterize the total transmission for given bound-ary structure, we calculate the Landauer’s conductance

$$G(\varepsilon) = \frac{e^2}{\pi \hbar} \sum_{k_y} \sum_{\mu \nu} |t_{\mu\nu}(k_y; \varepsilon)|^2$$

$$\approx \frac{e^2}{\pi \hbar} \int \frac{dk_y}{2\pi/L_y} \sum_{\mu \nu} |t_{\mu\nu}(k_y; \varepsilon)|^2,$$

(5)

where the indexes $\mu$ and $\nu$ run over all the traveling modes, and we assumed the system is periodic in $y$-direction with a sufficiently long period $L_y$. The conductance $G$ is naturally proportional to $L_y$, and the conductance per unit width, $G/L_y$, can be used as a quantity which measures the transparency of the domain boundary for the electronic transport.

\section{III. NUMERICAL RESULT AND DISCUSSION}

\subsection{A. Bilayer graphene and the effect of asymmetric electric potential}

We first consider the AB-BA domain boundary in bilayer graphene \cite{1}. The width of the boundary region is chosen as $N = 20$, or $W = (N + 1/2)a\sqrt{3} \approx 8.7$nm. Fig. 4(a) shows the band structure of uniform AB-bilayer graphene, where the energy origin $\varepsilon = 0$ is set to the band touching point. In the top panels of Fig. 5(a), we plot the transmission probability as a function of wave vector $k_y$ around the K-point at several Fermi energies. Here we choose the energy range $0 < \varepsilon_F < 0.15$eV, where we have at most a single traveling channel in one-direction at each $k_y$, where we have the only transmission probability $|t_{11'}|^2$.

We observe that the electron transmission is very small near the bottom of conduction band ($\varepsilon_F = 0.03$eV) where the electron waves mostly get reflected at the boundary, while the transmission probability sharply rises up in-
FIG. 5: Electron transmission probability $|t_{\mu \nu}(k_y)|^2$ through AB-BA domain boundary ($W = 8.7$ nm) on the bilayer graphene with the interlayer asymmetric potential (a) $\Delta = 0$ and (b) $\Delta = 0.1$ eV. The lower panels show the local Fermi surfaces and their corresponding local atomic structures.

Increasing the Fermi level [25] This behavior can also be seen in Fig. [5] which plots the total transmission $G/L_y$ as a function of electron density. In Fig. [6] we also compare the total transmission for the AB-BA domain boundary (blue) with that for the uniform AB bilayer graphene without domain boundary (black). We see that, that ratio of the former to the latter is almost zero near the zero energy, while rapidly increases at higher energy levels. This result suggests that the existence of the domain boundary dramatically reduces the conductivity of the bilayer graphene near the charge neutral point.

These characteristic features can be roughly explained from two different aspects. First, we generally expect a bigger transmission in a smoothly changing boundary than in the sharply changing boundary. The smoothness / sharpness is characterized by the ratio of the wave length of the incident wave $\lambda$ to the width of the boundary region $W$. In the low Fermi energy ($\varepsilon_F = 0.03$ eV), the effective wavenumber measured from $K$ point is about $k \approx 0.04a^{-1}$, and then the wavelength $\lambda = 2\pi/k \sim 40$ nm is actually larger than the width of boundary region at $W \approx 8.7$ nm ($N = 20$). So this case is regarded as a sharp boundary, suggesting that we have a considerable reflection. In increasing the Fermi level, the ratio $\lambda/W$ simply decreases, i.e., the boundary becomes relatively smoother and gives a larger transmission.

Another important aspect is the wavenumber matching in local Fermi surface [2]. In Fig. [5] we see that the stacking structure gradually changes from AB to BA in increasing $x$, and the local structure at any particular $x$ approximates the uniform bilayer graphene with a certain interlayer translation. Then we can consider the local Fermi surface corresponding to the local atomic structure as a function of $x$, which is shown in the lower panels of Fig. [5]. At $\varepsilon_F = 0.03$ eV, for instance, the Fermi surface in the intermediate region shifts along the $k_y$ direction, leaving only a small overlap with initial Fermi surface when projected to $k_y$ axis. As a result, for a traveling wave of $k_y$ off the overlapping region does not have corresponding traveling waves in the intermediate region, then it does not reach the other side. Meanwhile, at higher Fermi levels, the intermediate Fermi surface better overlaps with the initial one on the $k_y$ axis, so that the boundary becomes more transparent.
FIG. 6: Total transmission $G/L_y$ as a function of the electron density calculated for bilayer graphene of $\Delta = 0$ with (blue, solid) and without (black dotted) AB-BA domain boundary ($W = 8.7 \text{ nm}$). The red dashed curve is for the domain boundary in presence of the interlayer asymmetric potential $\Delta = 0.1 \text{ eV}$.

The correspondence between the transmission and the band structure is only approximate, but the agreement should become almost perfect when $W$ becomes much larger than the typical wavelength. To see this, we calculate the transmission probability at various widths of boundary region, $W$. In Fig. 7 we show the transmission probability in the top panel, and the local band structure in the bottom. The blue shading indicates the region of $k_y$ which has traveling modes throughout the intermediate region. For small boundary region $W = 8.7 \text{ nm}$ ($N = 20$), we still have a finite transmission probability in the region outside of the blue shading region, because there the wavelength $\lambda$ is actually larger than $W$ as already argued, and thus the local Fermi surface is not well defined. Increasing $W$, the transmission outside the shaded region vanishes, and at the same time the transmission probability in the shaded region rapidly rises and reaches almost 1 at $W = 85.4 \text{ nm}$. This is because the wave is hardly reflected in a smoothly-changing boundary which is much longer than the electron wave length, as long as a traveling mode exists throughout the intermediate region.

Next, we apply a perpendicular external electric field to the system by adding the asymmetric electrostatic potential $+\Delta$ and $-\Delta$ to the top and bottom layers. As shown in Fig. 8 (b), $\Delta$ actually opens up a band gap between the touching conductance and valence band, and near the band edge, the energy dispersion exhibits a complex feature where the Fermi surface split into several different parts due to the trigonal warping. In Fig. 8 (b), we compare the transmission probabilities in gapped case ($\Delta = 0$) and that in gapless case ($\Delta = 0.1 \text{ eV}$) at the two different electron densities. At the lower density $n_s = 1.0 \times 10^{12} \text{ cm}^{-2}$, we have two right-going channels in the gapped case so that we plot multiple transmission probabilities $|t_{11}|^2$, $|t_{21}|^2 = |t_{12}|^2$, and $|t_{22}|^2$. We see that the transmission probability is much greater in the gapped case than in the gapless case. The total transmission calculation in Fig. 9 also shows that the suppression at low electron density observed in the gapless case is considerably relaxed in the gapped case, suggesting that applying the external electric field definitely increases the electron transmission near the charge neutral point. Here it should be noted that the total electron transmission can be changed purely by deforming the band structure, with the electron density fixed. This feature can also be explained in terms of the local Fermi surface structure shown in the lower panels Fig. 5. At $n_s = 1.0 \times 10^{12} \text{ cm}^{-2}$, the Fermi surface spreads in a wider $k$-space region than in gapless case due to the complex structure of band bottom. This results in a shorter Fermi wavelength and also a better overlap with the intermediate Fermi surface, and both of them contribute to a larger transmission.

B. Trilayer, four-layer and five-layer graphene

In more than three-layer stack, the left and right regions have generally different energy bands as shown in Fig. 8. When we consider a realistic experimental situation with a single gate electrode underneath the sample, we have a homogeneous carrier density over the whole system, where the left and right regions and share the same Fermi energy, while the origins of band energies are relatively shifted to achieve the same charge density in the both regions. The situation is schematically illustrated in Fig. 9 for the trilayer case. The shift of the band energy is given by the different electrostatic potentials between the two regions, which automatically arises to satisfy the electrostatic equation in the field-effect transistor geometry. In the intermediate region, we simply assume the electrostatic potential $V(x)$ linearly changing in the intermediate region to connect left and right as shown in the lower panel of Fig. 9, i.e.,

$$V(x) = \begin{cases} 
0 & (x < 0) \\
\frac{x}{W} & (0 \leq x \leq W) \\
0 & (x > W).
\end{cases}$$

We calculate the transmission probability for the tight-binding Hamiltonian with $V(x)$ is included.

Figures 10 (a) (b) and (c) plot the total transmission $G/L_y$ as a function of the electron density for trilayer, four-layer and five-layer cases, respectively, where the black and blue curves are for with and without domain boundary, respectively. Figure 10 (d) shows the ratio of the transmission with the boundary to without the boundary. The overall behavior in the trilayer boundary is pretty much similar to the bilayer case, i.e., the transmission is suppressed near the charge neutral point and gradually rises at the high Fermi energy. In adding more layer, however, we see that the reduction near $n_s = 0$ becomes gradually weaker. It is a natural consequence
because the wave amplitude per single layer becomes relatively smaller in a larger stack so that the transmission is less sensitive to the existence of the domain boundary on the surface layer. When it comes to high density region, we observe some odd-even effect in Fig. 10 (d), where the boundaries with even number of layers show relatively better transmission than in the odd layers. It is particularly conspicuous when comparing bilayer and trilayer, where the transmission at \( n = 20 \times 10^{12}\text{cm}^{-2} \) is almost 90% in bilayer while it is only 60% in trilayer.

The even-odd characteristics is closely related to the left and right band structures presented in Fig. 8. There the horizontal dashed lines indicate the Fermi energies corresponding to several carrier densities \( n_s \). In trilayer at \( n_s \leq 20 \times 10^{12}\text{cm}^{-2} \), for example, we have two right-going channels \( \nu = 1, 2 \) in the left region, and a single right-going channel \( \mu = 1' \) in the right region. We notice that the odd layer always has one more channel in left region than in right region, and this is due to the existence of the monolayer-like band in Bernal stacked odd layer graphene.\(^\text{23,28}\) Fig. 11 shows the transmission probability \( |t_{1'1}(k_y)|^2 \) in trilayer, four-layer and five-layer at \( n_s = 20 \times 10^{12}\text{cm}^{-2} \). In the odd-layers, the incident carriers from the linear band (green curve) are not very well transmitted, and at the same time, the carriers from the other non-linear bands are considerably reflected only in the region of \( k_y \) where a linear band state exists. This suggests that the reflection matrix elements between the linear band and the other bands are particularly strong, and it significantly interferes the total transmission. The strong reflection in presence of the linear band is presumably related to the fact that a linear band state has a relatively large wave amplitude on the surface layer compared to other bands.\(^\text{26}\) This fact explains why the transmission at the high carrier density is generally higher in even layer cases where the linear band state is absent.

IV. CONCLUSION

We studied the electron transmission properties in stacking domain boundary in multilayer graphenes from bilayer to five-layer. We find the boundary significantly reduces the electron transmission at low Fermi energies, while the reduction becomes gradually weaker as increas-
FIG. 8: Energy band structures in the vicinity of K-point of the left region (left panel) and right region (right panel) in trilayer (top), four-layer(middle) and five layer (bottom) domain boundary. The dashed lines indicate the Fermi levels corresponding to several specific carrier densities $n_s$.

FIG. 9: Schematics of the electrostatic potential $V(x)$ to achieve the same electron density in ABA stack and ABC stack regions in trilayer graphene.

Our result indicates the electron transmission in a general graphitic system is significantly suppressed in presence of domain boundaries. The present result also suggests that a boundary between two different stacking structures may provide a mechanism to control the electron current on multilayer graphene. In particular, the fact that the system being almost insulator near bottom of conduction band and quickly becoming transparent when increasing Fermi levels gives a possibility to be applied to switching devices.

Appendix: Transfer matrix method

In this section, we present the formula to calculate the transmission probability in the domain boundary. We first consider the semi-infinite left and right regions separately, and specify the traveling modes in each region. Then we consider the intermediate region and calculate the transfer matrix connecting the traveling modes in the left and right.

In uniform AB-stacked bilayer graphene, for example, we define a unit cell as in Fig. 12 which consists of eight atoms. The Schrödinger equation reads

$$\bigl(\varepsilon - H_0\bigr) C_j = -T^\dagger C_{j-1} - T C_{j+1}, \quad \text{(A.1)}$$

where $C_j, C_{j-1}, C_{j+1}$ are 8-component vectors consisting of 8 wavefunctions of 8 atoms in each unit cell, and $H_0, T^\dagger, T$ are $8 \times 8$ matrices. $H_0$ consists of transfer integrals between atoms inside each unit cell, while $T^\dagger, T$ consists of transfer integrals between atoms in $j$-th cell and atoms in $j - 1$-th, $j + 1$-th cell respectively. The
equation is transformed as

\[
\lambda \left( \begin{array}{c} C_j \\ C_{j-1} \end{array} \right) = \left( \begin{array}{cc} -T^{-1}(\varepsilon - H_0) & -T^{-1}T^\dagger \\ 1 & 0 \end{array} \right) \left( \begin{array}{c} C_j \\ C_{j-1} \end{array} \right),
\]

(A.2)

which gives 16 eigenvalues of \( \lambda \). These modes are classified as traveling modes if \( |\lambda| = 1 \), and as evanescent modes if \( |\lambda| \neq 1 \). For traveling modes, we can define the real wave number \( k_x \) by

\[
\lambda = \exp(ik_x \sqrt{3a}),
\]

and it is even classified to left-going or right-going modes depending on the expectation value of the velocity along \( x \)-direction. For evanescent modes, we categorize \(|\lambda| > 1\) and \(|\lambda| < 1\) as left-going and right-going modes, respectively, for the sake of convenience. The 16 eigenmodes are always composed of 8 right-going and 8 left-going modes. Let \( \lambda_1^\pm \), \( \lambda_2^\pm \), ..., \( \lambda_8^\pm \) be the eigenvalues of the right and left going modes, respectively.

The wavefunction is written as \( C_j = \lambda^j \hat{u} \) with 8-component eigenvector \( \hat{u} \). We define \( u_i^\pm \) as the eigenvectors corresponding to \( \lambda_i^\pm \). We then define the \( 8 \times 8 \) matrices

\[
U^\pm = (u_1^\pm, u_2^\pm \cdots u_8^\pm),
\]

(A.3)

\[
\Lambda^\pm = \left( \begin{array}{cccc} \lambda_1^\pm & & & \\ & \ddots & & \\ & & \lambda_8^\pm & \\ & & & \lambda_1^\pm \end{array} \right).
\]

(A.4)

Now any left and right-going waves can be written as the superposition of the waves functions \( u_j^- \) or \( u_j^+ \). For example, wave function at site 0 is written as

\[
C_0^\pm = \sum_i u_i^\pm \alpha_i = U^\pm \alpha^\pm,
\]

(A.5)

where

\[
\alpha^\pm = \left( \begin{array}{c} \alpha_1^\pm \\ \vdots \\ \alpha_8^\pm \end{array} \right).
\]

(A.6)

Then the wave amplitude at \( j \)-th site becomes

\[
C_j^\pm = \sum_i (\lambda_i^\pm)^j u_i^\pm \alpha_i^\pm = U^\pm (\Lambda^\pm)^j \alpha^\pm,
\]

(A.7)

leading to the relation

\[
C_{j+1}^\pm = [U^\pm (\Lambda^\pm)^j (U^\pm)^{-1}] C_j^\pm = F^\pm C_j^\pm,
\]

(A.8)
Transmission Probability

\[
0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1.0
\]

Wave vector \(k_y\) (unit of \(a^{-1}\))

\(0.2\) \(0.4\) \(0.6\) \(0.8\) \(1.0\)

FIG. 11: Transmission probability \(\sum_n |t_{\nu n}(k_y)|^2\) through the domain boundary \((W = 8.7\, \text{nm})\) from the incident channel \(\nu\) in (a) trilayer, (b) four-layer and (c) five-layer at \(n_s = 20 \times 10^{12}\, \text{cm}^{-2}\). The channel index \(\nu = 1, 2, \ldots\) corresponds to the numbers in Fig. 5.

FIG. 12: Unit cell of AB-bilayer graphene.

FIG. 13: Schematic view of the AB-BA domain boundary.

which is similar to the Bloch theorem. The wavefunction at site \(j\) can be generally written as summation of left-going wave and right-going wave.

\[ C_j = C_j^+ + C_j^- \quad (A.9) \]

By doing the similar process for BA bilayer graphene (the right region), we are also able to get the eigenvectors and eigenvalues. We define \(U_L^\pm, \Lambda_L^\pm, F_L^\pm\) for the left region (AB-stack), and \(U_R^\pm, \Lambda_R^\pm, F_R^\pm\) for the right region (BA-stack).

Figure 13 schematically illustrates the Hamiltonian of the AB-BA domain boundary. The tight-binding equations read

\[
\begin{align*}
\mathcal{H}_0 & = -T_0 C_{\text{inter}} - T_1 C_{-1}, \\
\mathcal{H}_\text{inter} & = -T_0^\dagger C_0 - T_{N+1} C_{N+1}, \\
\mathcal{H}_{N+1} & = -T_{N+1}^\dagger C_{\text{inter}} - T_R C_{N+2}.
\end{align*}
\]

(A.10)

Here \(C_0, C_{-1}, C_{N+1}, C_{N+2}\) are 8-component vectors, \(C_{\text{inter}}\) is \(n\)-component vector, with \(n\) being the number of atoms in the intermediate region. \(\mathcal{H}_0, \mathcal{H}_{N+1}\) are \(8 \times 8\) matrices, \(\mathcal{H}_\text{inter}\) is a \(n \times n\) matrix, and \(T_0, T_{N+1}\) are \(8 \times n\) and \(8 \times n\) matrices, respectively.

In the following, we consider a situation where the incident wave comes from the left region, and transmits to the right or reflects back to the left. From (A.8), we have

\[
\begin{align*}
C_{-1} = (F_L^{\dagger})^{-1} C_0^+ + (F_L^{-})^{-1} C_0^- \\
C_{N+2} = F_R^+ C_{N+1}^+ = F_R^- C_{N+1}.
\end{align*}
\]

(A.11)

Note that there are only right-going waves in the right region. Then (A.10) becomes

\[
\begin{align*}
\mathcal{H}_0 & = -T_0 C_{\text{inter}} - T_1 [(F_L^{-})^{-1}] C_0^+, \\
\mathcal{H}_\text{inter} & = -T_0^\dagger C_0 - T_{N+1} C_{N+1}, \\
\mathcal{H}_{N+1} & = -T_{N+1}^\dagger C_{\text{inter}}.
\end{align*}
\]

(A.12)

which leads to

\[
\begin{pmatrix}
C_0 \\
C_{\text{inter}} \\
C_{N+1}
\end{pmatrix} = \frac{1}{E - \mathcal{H}}
\begin{pmatrix}
-T_1 [(F_L^{-})^{-1}] - (F_L^{-})^{-1} C_0^+ \\
0 \\
0
\end{pmatrix}.
\]

(A.13)
Similarly, the right-going waves at site \( N + 1 \) is written as

\[
C_{N+1}^+ = C_{N+1}^- = -G_1 T_0^L[(F_L^+)^{-1} - (F_L^-)^{-1}] C_0^+.
\]  
(A.18)

To calculate the transmission and reflection probability, we first write the left and right-going waves at site 0, \( N + 1 \) in terms of left-going waves and right-going waves

\[
C_0^+ = U_R^+ \alpha_i, \quad (A.19)
\]

\[
C_0^- = U_L^- \alpha_r, \quad (A.20)
\]

\[
C_{N+1}^+ = U_R^+ \alpha_i. \quad (A.21)
\]

The transmission and reflection matrices are defined by \( \alpha_i = T \alpha_i \) and \( \alpha_r = R \alpha_r \), and they are given by

\[
T = (U_R^+)^{-1} \left(-G_2 T_0^L[(F_L^+)^{-1} - (F_L^-)^{-1}]\right) U_L^+, \quad (A.22)
\]

\[
R = (U_L^-)^{-1} \left(-G_1 T_0^L[(F_L^+)^{-1} - (F_L^-)^{-1}]\right) U_L^+. \quad (A.23)
\]

The transmission coefficient for incident wave \( \nu \) with velocity \( v_\nu \) and out-going channel \( \mu \) with velocity \( v_\mu \) is written as

\[
t_{\mu \nu} = \left(\frac{v_\mu}{v_\nu}\right)^{1/2} T_{\mu \nu}, \quad (A.24)
\]

and the reflection coefficient for incoming channel \( \nu \) with velocity \( v_\nu \), and out-going channel \( \mu \) with velocity \( v_\mu \) as

\[
r_{\mu \nu} = \left(\frac{v_\mu}{v_\nu}\right)^{1/2} R_{\mu \nu}. \quad (A.25)
\]

These formula can also be used to derive the transmission probability for trilayer case.

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