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An Analytical Approach to Energy Spectrum and

Optical Properties of Gated Bilayer Graphene

Cheng-Peng Chang [*]

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Abstract

First, we present an analytical approach to access the exact energy spectrum and wave functions of the gated Bernal bilayer graphene (BBLG), with all the tight-binding parameters included. To tackle the broken mirror symmetry caused by a gated voltage V_g and interlayer interactions, we create a unitary transformation to reduce the Hamiltonian matrix of BBLG to a simple form, which can offer the analytical energy spectrum. The formula generate the gated tunable energy bands and reveal that V_g changes the subband spacing, produces the oscillating bands, and increases the band-edge states. Then, we employ the analytical model to revisit the optical dipole matrix element and optical absorption spectra. In the absence of V_g, the anisotropic dipole matrix element exhibits the maximum around the point M and zero value along the high symmetry line ΓK in the first Brillouin zone. V_g effectively induces the nonzero dipole matrix element along the high symmetry line ΓK, which makes significant contribution in the absorption spectra. Moreover, the application of V_g opens an optical gap and gives rise to a profound low-energy peak in absorption spectra. The dependence upon the gated bias V_g for the location and height of this peak clearly emerges through the analytical model. Our exact analytical model can be further used to study the many-body effect and exciton effect on the electronic and optical properties of BBLG.

[*]Center for General Education, Tainan University of Technology, 710 Tainan, Taiwan E-mail:
`t00252@mail.tut.edu.tw`

1 INTRODUCTION

Graphene, a hit topic since 2004,[1] having attracted a surge of interest for fundamental and experimental studies,[2–9] is a one atom-thick layer made up of carbon atoms arranged in a honeycomb lattice. Stemming from the specular geometrical structure, graphene is an extraordinary two dimensional material with many unique properties, e. g., linear energy dispersions crossing at Dirac point, electron-hole symmetry, Klein tunneling, high mobility at room temperature, and novel quantum Hall effect.[7–13] The unusual electric properties make graphene a possible candidate for fabricating the future electronic devices. Graphene is a zero bandgap semiconductor due to linear energy dispersions crossing at Dirac point. The touch of valence and conduction bands in its energy spectrum limits on-off current ratios achievable and prevents the use of graphene in making field transistors. It is significant for the opening of a band gap in graphene to remove the limitation in using graphene material for semiconductor applications. Many breakthrough methods are proposed to generate a band gap in monolayer graphene, e. g., using molecular doping,[14,15] the application of strain,[16,17] and patterning a graphene sheet into a nanoribbon.[18] On the other hand, a tunable band gap is induced in the Bernal bilayer graphene (BBLG) through the application of a perpendicular electric field. BBLG is made up of two monolayer graphenes, held by the weak Van der Waals force, in the AB-stacking. The experimental works demonstrate that a tunable bandgap of up to 0.25 eV is achieved for electrically gated bilayer graphene by a variable external electric field.[19–22]

The energy dispersions of the gated BBLG are usually explored within the tight-binding model.[23–31] The minimal model, considering only the intralayer and main interlayer interactions, is widely employed to study the energy dispersions of BBLG.[30,31] Around the Dirac points, the analytical low-energy dispersions of the gated BBLG are obtained through the continuum model. A 4×4 Hamiltonian matrix is solvable and gives out the analytical low-energy dispersions. A full tight-binding Hamiltonian model takes into account all hopping integrals, including the additional skew interaction (γ_3) and electron-hole asymmetry (γ_4) in the model.[23,27] γ_3 is the trigonal warping

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and γ_4 is the origin of electron-hole asymmetry. The trigonal warping can significantly modify the physical properties of BBLG.[32–34] Cserti shows that trigonal warping has a great effect on the minimal conductivity of BBLG.[32] Moreover, γ_3 gives rise to the electron-hole asymmetry and distorts the circular equi-energy contour to a trigonal symmetry.[33,34] A full tight-binding Hamiltonian matrix is a 4×4 matrix and its four energy bands are usually obtained by the numerical diagonalization. Many important physical properties do not directly emerge through the numerical calculation because of a lack of the exact energy spectrum. To fully and exactly describe the electric and optical properties in the full energy region, an analytical description of energy dispersions of the four-band model is expected.

Here, we present a model to access the analytical form of energy spectrum and eigenstates of gated BBLG, based on the tight-binding framework and all the tight-binding parameters γ_0, γ_1, γ_3 and γ_4 are all considered too (the inset of Fig. 1(a)). Unlike AA-stacking graphene,[35,36] the skew interlayer interactions γ_3 and gated bias V_g destroy the inversion symmetry of gated BBLG. The broken symmetry increases the difficulty in solving the eigenvalue problem. Through a rotation operator, we generate a new set of tight-binding basis functions to deal with the broken symmetry resulting from the γ_3 and V_g. The renormalized V_g-dependent intralayer and interlayer interactions are derived based on the new set of basis functions. Most importantly, the new basis functions exactly reduces the Hamiltonian matrix H into a band-storage matrix. As a result, the energy dispersions and wave functions are analytically solvable. Furthermore, the present work is to provide full-frequency energy bands, which is beyond the effective mass approximation. The analytical form of energy spectrum and eigenstates are further applied to studying the optical absorption spectra and exploring the origin of optical transition channels.

The rest parts of the paper are organized as follows: We develop a model to derive the analytical form of energy spectrum of gated BBLG in Sec. II. Subsequently, the electronic properties are revisited in Sec. III through the analytical energy spectrum. In Sec. IV, the energy spectrum and eigenstates are used to explore the dipole matrix element and optical absorption spectra of gated BBLG. Finally, the conclusions are

drawn in Sec. V.

2 Theory and Model

BBLG is the stack of two identical graphene layers with the AB-stacking, as shown in the inset of Fig. 1(a). On each graphene plane, two basic atoms A and B are arranged in the honeycomb lattice and the bond length between atoms A and B is $b = 1.42$ Å. The distance between two graphene layers is assumed to be 3.35Å.[37] The lower or upper graphene layer is denoted by the index $l = 1$ or 2. Atoms A_2 and A_1 have the same (x, y) projection and they are denoted as the dimer sites. And the projections of the other half, atoms B, lie in the center of the hexagons in the adjacent sheets. BBLG is a periodic system in the xy plane and has four atoms, A_1, B_1, A_2, B_2, in its primitive cell. The first Brillouin zone of BBLG, as illustrated in the inset of Fig. 1(b), is the same as that of a graphene, which is a hexagon with points Γ located at $(0,0)$, K at $(\frac{4\pi}{3\sqrt{3}b}, 0)$, and M at $(\frac{\pi}{\sqrt{3}b}, \frac{\pi}{3b})$.

The electronic properties of BBLG subjected to a perpendicular electric field are studied within the tight-binding method framework; Hamiltonian equation of BBLG is $\mathbf{H}\Phi = E\Phi$, where the Bloch function is $\Phi = c_1|A_1\rangle + c_2|A_2\rangle + c_3|B_1\rangle + c_4|B_2\rangle$, which is the linear combination of the periodic wave functions $|A_1\rangle$, $|A_2\rangle$, $|B_1\rangle$, and $|B_2\rangle$. $\mathbf{H}\Phi = E\Phi$ is then transformed into the matrix equation $H|\mathbf{c}\rangle = E|\mathbf{c}\rangle$, here $|\mathbf{c}\rangle = |c_1, c_2, c_3, c_4\rangle^T$. The representation of Hamiltonian matrix reads

$$H = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix}, \tag{1}$$

where H is a 4×4 matrix. The elements H_{AA}, H_{AB}, H_{BA}, and H_{BB} are 2×2 matrices. The hopping integrals γ_i, usually used to describe the Bernal bilayer graphene, are illustrated in the inset of Fig. 1(a). γ_0 is the intralayer interaction. The hopping integral γ_1 is the interaction between the dimer sites A_1 and A_2. The trigonal warping integral, γ_3, is the skew interlayer hopping between atoms B_1 and B_2. γ_4 represents γ_{A_1,B_2} and

γ_{B_2,A_1}. The matrices H_{AA}, H_{AB}, H_{BA} are further to be expressed as

$$H_{AA} = \begin{pmatrix} V_g & \gamma_1 \\ \gamma_1 & -V_g \end{pmatrix}, \tag{2a}$$

$$H_{AB} = H_{BA}^* = \begin{pmatrix} \gamma_0 f_{\mathbf{k}} & \gamma_4 f_{\mathbf{k}}^* \\ \gamma_4 f_{\mathbf{k}} & \gamma_0 f_{\mathbf{k}}^* \end{pmatrix}, \tag{2b}$$

$$H_{BB} = \begin{pmatrix} V_g & \gamma_3 f_{\mathbf{k}} \\ \gamma_3 f_{\mathbf{k}}^* & -V_g \end{pmatrix}, \tag{2c}$$

where the on-site energy V_g is the electric potential caused by the external perpendicular electric field. $f_{\mathbf{k}} = \sum_{l=1}^{3} \exp(i\mathbf{k} \cdot \mathbf{b}_l)$ is the structure factor, where $\mathbf{k} = (k_x, k_y)$ is the wave vector and $\mathbf{b}_l$ represents the nearest neighbor on the same graphene plane. The three neighboring atoms are located at $\mathbf{b}_1 = (-\frac{\sqrt{3}b}{2}, -\frac{b}{2})$, $\mathbf{b}_2 = (0, b)$, and $\mathbf{b}_3 = (\frac{\sqrt{3}b}{2}, -\frac{b}{2})$ and thus, $f_{\mathbf{k}} = 2\cos(\frac{\sqrt{3}b}{2}k_x)\exp(-ik_y\frac{b}{2}) + \exp(ik_yb)$.

To find out the analytical energy dispersions of the 4×4 matrix above, we now construct the symmetrized basis functions $(|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, |\psi_4\rangle)^T$, which are linear combination of the periodic wave functions $|A_1\rangle$, $|A_2\rangle$, $|B_1\rangle$, and $|B_2\rangle$. The symmetrized basis functions are

$$\begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \\ |\psi_3\rangle \\ |\psi_4\rangle \end{pmatrix} = \begin{pmatrix} s_1^+ & s_2^+ & 0 & 0 \\ 0 & 0 & s_1^+ \frac{f_{\mathbf{k}}^*}{|f_{\mathbf{k}}|} & s_2^+ \frac{f_{\mathbf{k}}}{|f_{\mathbf{k}}|} \\ 0 & 0 & s_1^- \frac{f_{\mathbf{k}}^*}{|f_{\mathbf{k}}|} & s_2^- \frac{f_{\mathbf{k}}}{|f_{\mathbf{k}}|} \\ s_1^- & s_2^- & 0 & 0 \end{pmatrix} \begin{pmatrix} |A_1\rangle \\ |A_2\rangle \\ |B_1\rangle \\ |B_2\rangle \end{pmatrix}, \tag{3}$$

where the coefficients $s_1^\pm$ and $s_2^\pm$ are the components of eigenvector of the matrix H_{AA} (Eq.(2a)). The eigen-equation of H_{AA} is

$$\begin{pmatrix} V_g & \gamma_1 \\ \gamma_1 & -V_g \end{pmatrix} \begin{pmatrix} s_1^\pm \\ s_2^\pm \end{pmatrix} = \pm\varepsilon_{AA} \begin{pmatrix} s_1^\pm \\ s_2^\pm \end{pmatrix}, \tag{4}$$

where the eigenenergy is $\varepsilon_{AA} = \sqrt{\gamma_1^2 + V_g^2}$. The related eigen-vectors $(s_1^{\pm}, s_2^{\pm})^T$ are

$$
\begin{pmatrix} s_1^+ \\ s_2^+ \end{pmatrix} = \begin{pmatrix} \frac{\gamma_1}{\sqrt{\gamma_1^2 + (\varepsilon_{AA} - V_g)^2}} \\ \frac{\varepsilon_{AA} - V_g}{\sqrt{\gamma_1^2 + (\varepsilon_{AA} - V_g)^2}} \end{pmatrix}, \quad \begin{pmatrix} s_1^- \\ s_2^- \end{pmatrix} = \begin{pmatrix} \frac{\gamma_1}{\sqrt{\gamma_1^2 + (\varepsilon_{AA} + V_g)^2}} \\ \frac{-(\varepsilon_{AA} + V_g)}{\sqrt{\gamma_1^2 + (\varepsilon_{AA} + V_g)^2}} \end{pmatrix}. \tag{5}
$$

Similarly, the eigenenergy related to H_{BB} is $\varepsilon_{BB} = \sqrt{\gamma_3^2 |f_{\mathbf{k}}|^2 + V_g^2}$.

The Bloch function, spanned by the new basis functions $(|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, |\psi_4\rangle)^T$, is $\Phi = \mathbf{d}_1|\psi_1\rangle + \mathbf{d}_2|\psi_2\rangle + \mathbf{d}_3|\psi_3\rangle + \mathbf{d}_4|\psi_4\rangle$. According to the symmetrized basis functions $|\psi_i\rangle$, the matrix equation has the form

$$
\begin{pmatrix} \mathcal{H}_{11} & \mathcal{H}_{12} & \mathcal{H}_{13} & 0 \\ \mathcal{H}_{21} & \mathcal{H}_{22} & \mathcal{H}_{23} & \mathcal{H}_{24} \\ \mathcal{H}_{31} & \mathcal{H}_{32} & \mathcal{H}_{33} & \mathcal{H}_{34} \\ 0 & \mathcal{H}_{42} & \mathcal{H}_{43} & \mathcal{H}_{44} \end{pmatrix} \begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \\ \mathbf{d}_3 \\ \mathbf{d}_4 \end{pmatrix} = E \begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \\ \mathbf{d}_3 \\ \mathbf{d}_4 \end{pmatrix}, \tag{6}
$$

where the matrix elements are $\mathcal{H}_{ij} = \langle \psi_i | \mathbf{H} | \psi_j \rangle$. The diagonal matrix elements are

$$
\begin{cases} \mathcal{H}_{11} = \varepsilon_{AA}, \\ \mathcal{H}_{22} = \frac{V_g^2}{\varepsilon_{AA}} + \frac{\gamma_1}{\varepsilon_{AA}} \frac{\gamma_3}{2|f_{\mathbf{k}}|^2} [f_{\mathbf{k}}^3 + f_{\mathbf{k}}^{*3}], \\ \mathcal{H}_{33} = -\mathcal{H}_{22}, \\ \mathcal{H}_{44} = -\varepsilon_{AA}. \end{cases} \tag{7a}
$$

The off-diagonal terms are

$$
\begin{cases} \mathcal{H}_{12} = \mathcal{H}_{21} = (\gamma_0 + \frac{\gamma_1}{\varepsilon_{AA}} \gamma_4) |f_{\mathbf{k}}|, \\ \mathcal{H}_{13} = \mathcal{H}_{31} = -\frac{V_g}{\varepsilon_{AA}} \gamma_4 |f_{\mathbf{k}}|, \\ \mathcal{H}_{14} = \mathcal{H}_{41} = 0, \\ \mathcal{H}_{23} = \mathcal{H}_{32}^* = \frac{\gamma_1 V_g}{\varepsilon_{AA}} + \frac{\gamma_3}{2|f_{\mathbf{k}}|^2} [\frac{(\varepsilon_{AA} - V_g)}{\varepsilon_{AA}} f_{\mathbf{k}}^{*3} - \frac{(\varepsilon_{AA} + V_g)}{\varepsilon_{AA}} f_{\mathbf{k}}^3], \\ \mathcal{H}_{24} = \mathcal{H}_{42} = -\frac{V_g}{\varepsilon_{AA}} \gamma_4 |f_{\mathbf{k}}|, \\ \mathcal{H}_{34} = \mathcal{H}_{43} = (\gamma_0 - \frac{\gamma_1}{\varepsilon_{AA}} \gamma_4) |f_{\mathbf{k}}|. \end{cases} \tag{7b}
$$

Notably, in the absence of the gated bias, $V_g = 0$, $\mathcal{H}_{13}$, $\mathcal{H}_{31}$, $\mathcal{H}_{24}$ and $\mathcal{H}_{42}$ are all equal to zero.[38] Moreover, a straightforward calculation shows that $\mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32} = \varepsilon_{BB}^2 = V_g^2 + \gamma_3^2 |f|^2$ because the sub-matrix

$$\begin{pmatrix} \mathcal{H}_{22} & \mathcal{H}_{23} \\ \mathcal{H}_{32} & \mathcal{H}_{33} \end{pmatrix}$$

is the transformation of H_{BB}.

2.1 In the limit of $\gamma_4 = 0$

The exclusion of electron-hole asymmetry, $\gamma_4 = 0$, allows us to obtain a simple and exact analytical solution to energy spectrum. The interactions $\mathcal{H}_{13}$, $\mathcal{H}_{31}$, $\mathcal{H}_{24}$ and $\mathcal{H}_{42}$ in H_{red} are all equal to zero as $\gamma_4 = 0$. The reduced Hamiltonian matrix H_{red} is a band-storage matrix and is expressed as follows:

$$H_{red} = \begin{pmatrix} \mathcal{H}_{11} & \mathcal{H}_{12} & 0 & 0 \\ \mathcal{H}_{12} & \mathcal{H}_{22} & \mathcal{H}_{23} & 0 \\ 0 & \mathcal{H}_{32} & -\mathcal{H}_{22} & \mathcal{H}_{12} \\ 0 & 0 & \mathcal{H}_{12} & -\mathcal{H}_{11} \end{pmatrix}, \tag{8}$$

where $\mathcal{H}_{12} = \mathcal{H}_{34} = \gamma_0 |f_{(\mathbf{k})}|$. The analytical energy dispersions, associated with H_{red}, read

$$E(\mathbf{k})_{\pm\pm} = \pm\sqrt{\mathcal{B} \pm \sqrt{\mathcal{B}^2 - \mathcal{C}}}, \tag{9}$$

where

$$\begin{cases} \mathcal{B} &= \mathcal{H}_{11}^2/2 + \mathcal{H}_{12}^2 + (\mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32})/2 \\ &= \frac{\gamma_1^2}{2} + \gamma_0^2 |f_{\mathbf{k}}|^2 + \frac{\gamma_3^2 |f_{\mathbf{k}}|^2}{2} + V_g^2, \\ \mathcal{C} &= \mathcal{H}_{12}^4 - 2\mathcal{H}_{11}\mathcal{H}_{12}^2\mathcal{H}_{22} + \mathcal{H}_{11}^2(\mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32}). \\ &= \gamma_0^4 |f_{\mathbf{k}}|^4 - 2\gamma_1 \gamma_0^2 \gamma_3 |f_{\mathbf{k}}|^3 cos(3\phi) + \gamma_1^2 \gamma_3^2 |f_{\mathbf{k}}|^2 + V_g^2(\gamma_1^2 + V_g^2 + \gamma_3^2 |f_{\mathbf{k}}|^2 - 2\gamma_0^2 |f_{\mathbf{k}}|^2). \end{cases}$$

where $\mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32} = \gamma_3^2|f|^2 + V_g^2$ is used. $f_{\mathbf{k}} = |f_{\mathbf{k}}|e^{i\phi}$ and the angle ϕ is $\phi = tan^{-1}\frac{Im[f(\mathbf{k})]}{Re[f(\mathbf{k})]}$. There are four branches of energy bands, which are in the sequence $E(\mathbf{k})_{++} > E(\mathbf{k})_{+-} > E(\mathbf{k})_{--} > E(\mathbf{k})_{-+}$. The former tow, $E(\mathbf{k})_{++}$ and $E(\mathbf{k})_{+-}$, are the energy dispersions associated with the conduction bands. The latter two, $E(\mathbf{k})_{--}$ and $E(\mathbf{k})_{-+}$ are the energy spectrum related to the valence bands.

At the point $\mathbf{K}$, $\mathcal{B} = \gamma_1^2/2 + V_g^2$ and $\mathcal{C} = V_g^2(\gamma_1^2 + V_g^2)$. The state energies are exactly $E(\mathbf{K}) = \pm V_g$ and $\pm\sqrt{\gamma_1^2 + V_g^2}$. Around the point $\mathbf{K}$ and in the absence of the electric field, $\mathcal{B} \gg \mathcal{C}$ and $\mathcal{C} \approx (\gamma_0^2|f_{\mathbf{k}}|^2 - \gamma_1\gamma_3|f_{\mathbf{k}}|)^2$. The two branches of low energy dispersions of BBLG are $E(\mathbf{k})_{\pm-} \approx \pm\sqrt{\frac{\mathcal{C}}{2\mathcal{B}}} = \pm\frac{1}{\gamma_1}(\gamma_0^2|f_{\mathbf{k}}|^2 - \gamma_1\gamma_3|f_{\mathbf{k}}|)$. They are the eigenenergies of the effective Hamiltonian matrix

$$H_{eff} = \frac{1}{\gamma_1}\begin{pmatrix} 0 & \gamma_0^2|f_{\mathbf{k}}|^2 - \gamma_1\gamma_3|f_{\mathbf{k}}| \\ \gamma_0^2|f_{\mathbf{k}}|^2 - \gamma_1\gamma_3|f_{\mathbf{k}}| & 0 \end{pmatrix}.$$

2.2 The effect of γ_4 on the energy dispersions

A plainly analytical energy dispersions of the Hamiltonian matrix (Eq.(6)), involving all hopping integrals, is in fact inaccessible. The energy dispersions are generally obtained by the numerical diagonalization method. To obtain a simply analytical solution to energy spectrum, we treat γ_4 as a perturbation and neglect the matrix elements $\mathcal{H}_{13}$, $\mathcal{H}_{31}$, $\mathcal{H}_{24}$ and $\mathcal{H}_{42}$ because they make nonsignificant contributions to the energy spectrum. $\mathcal{H}_{13}$, $\mathcal{H}_{31}$, $\mathcal{H}_{24}$ and $\mathcal{H}_{42}$ are right dependent on the magnitude of gated voltage V_g and interlayer interaction γ_4. The magnitude of γ_4 is smaller than that of γ_0 and γ_3, so that $\mathcal{H}_{13}$, $\mathcal{H}_{31}$, $\mathcal{H}_{24}$ and $\mathcal{H}_{42}$ are negligible. γ_4 affects the matrix elements $\mathcal{H}_{12}$ and $\mathcal{H}_{34}$ in such a manner as $\mathcal{H}_{12} = (\gamma_0 + \frac{\gamma_1}{\varepsilon}\gamma_4)|f_{\mathbf{k}}|$ and $\mathcal{H}_{34} = (\gamma_0 - \frac{\gamma_1}{\varepsilon}\gamma_4)|f_{\mathbf{k}}|$. The Hamiltonian equation with the band-storage Hamiltonian matrix is expressed as follows:

$$\begin{pmatrix} \mathcal{H}_{11} & \mathcal{H}_{12} & 0 & 0 \\ \mathcal{H}_{21} & \mathcal{H}_{22} & \mathcal{H}_{23} & 0 \\ 0 & \mathcal{H}_{32} & -\mathcal{H}_{22} & \mathcal{H}_{34} \\ 0 & 0 & \mathcal{H}_{43} & -\mathcal{H}_{11} \end{pmatrix}\begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \\ \mathbf{d}_3 \\ \mathbf{d}_4 \end{pmatrix} = E_{\pm,\pm}\begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \\ \mathbf{d}_3 \\ \mathbf{d}_4 \end{pmatrix}. \quad (10)$$

The eigen-energies, determined by the criterion $Det|\mathcal{H}| = 0$, are the roots of the secular equation $E^4 - \mathtt{B}E^2 - \mathtt{B}'E + \mathtt{C} = 0$, where $\mathtt{B} = \mathcal{H}_{11}^2 + \mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32} + \mathcal{H}_{12}^2 + \mathcal{H}_{34}^2$, $\mathtt{B}' = (\mathcal{H}_{11} + \mathcal{H}_{22})(\mathcal{H}_{12}^2 - \mathcal{H}_{34}^2)$, and $\mathtt{C} = \mathcal{H}_{12}^2\mathcal{H}_{34}^2 - \mathcal{H}_{11}\mathcal{H}_{22}(\mathcal{H}_{12}^2 + \mathcal{H}_{34}^2) + \mathcal{H}_{11}^2(\mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32})$. The analytical form of the eigen-energies looks so complicated and tedious just because the coefficient $\mathtt{B}' \neq 0$. To acquire the simple analytical result, we further approximate $\mathtt{B}' \approx 0$ because $\mathcal{H}_{12} \approx \mathcal{H}_{34}$. As a result, the eigen-energies $\mathcal{E}(\mathbf{k})$ are

$$\mathcal{E}(\mathbf{k})_{\pm\pm} = \pm\sqrt{\mathtt{B}/2 \pm \sqrt{(\mathtt{B}/2)^2 - \mathtt{C}}}. \tag{11}$$

To check out the accuracy of the afore-presented model, we first calculate energy dispersions $\mathcal{E}(\mathbf{k})_{\pm\pm}$ at $V_g = 0$ in the high symmetry line K-Γ-M-K, shown by the dashed red curves in Fig. 1(a). There are four energy subbands $\mathcal{E}(\mathbf{k})_{\pm\pm}$. For comparison, energy dispersions, $E_{\pm\pm}$, obtained through the numerical diagonalization of Hamiltonian matrix (Eq. 1), are also drawn by the black curves in Fig. 1(a). The tight binding parameters $\gamma_i's$ used to calculate the energy bands are: $\gamma_0 = -3.12$ eV, $\gamma_1 = 0.38$ eV, $\gamma_3 = 0.280$ eV, and $\gamma_4 = 0.12$ eV.[39] Obviously, the red curves are not identical to those in black in higher energy region $\mathcal{E} > 3.0$ eV. The higher the energy $\mathcal{E}$ is, the more discrepancy between two curves is. Plus, the energy spectrum $\mathcal{E}$ in the presence of the gated voltage $V_g = 200$ meV are presented in Fig. 1(b). The applied gated voltage does not significantly affect the profile of energy bands in the high symmetry line K-Γ-M-K. The disagreement between the red and black curves reveals that the derived analytical formula can not exactly describe the energy spectra in the energy region $E(eV) > 3.0$ eV. Energy dispersions around the the point K at different $V_g's$ are shown in the Fig.2 for comparison. The calculation result illustrates that the presented analytical model can not replicate the exact energy dispersions around the point K. Notably, in the absence of the gate voltage, the presented analytical model $\mathcal{E}_{\pm\pm}$ can not reproduce the analytical formula of BBLG at $V_g = 0$.[38]

We here modify and improve the aforementioned analytical model to approach the exact energy dispersions at any V_g. In the absence of the gated voltage $V_g = 0$, the matrix elements $\mathcal{H}_{23}$ and $\mathcal{H}_{32}$ in Eq. (10) play a minor role and can be then neglected.[38]

E_{++} and E_{--} (E_{+-} and E_{-+}) belong to the symmetrical states (the anti-symmetrical states). E_{++} and E_{--} depend only upon $\mathcal{H}_{12} = \mathcal{H}_{21} = (\gamma_0 + \frac{\gamma_1}{\varepsilon}\gamma_4)|f_{\mathbf{k}}|$ while E_{+-} and E_{-+} on $\mathcal{H}_{34} = \mathcal{H}_{43} = (\gamma_0 - \frac{\gamma_1}{\varepsilon}\gamma_4)|f_{\mathbf{k}}|$.[38] We thus replace both $\mathcal{H}_{34}$ and $\mathcal{H}_{43}$ with $\mathcal{H}_{12}$ and $\mathcal{H}_{21}$ in Eq. (10) during the calculation of E_{++} and E_{--} at any V_g. Then, we obtain the energy dispersions

$$E(\mathbf{k})_{++} = \sqrt{\mathcal{B} + \sqrt{\mathcal{B}^2 - \mathcal{C}}}, \tag{12a}$$

$$E(\mathbf{k})_{--} = -\sqrt{\mathcal{B} - \sqrt{\mathcal{B}^2 - \mathcal{C}}}, \tag{12b}$$

where $\mathcal{B} = \mathcal{H}_{12}^2 + (\mathcal{H}_{11}^2 + \mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32})/2$ and $\mathcal{C} = \mathcal{H}_{12}^4 - 2\mathcal{H}_{12}^2\mathcal{H}_{11}\mathcal{H}_{22} + \mathcal{H}_{11}^2(\mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32})$. The other two energy bands E_{+-} and E_{-+} are acquired by utilizing $\mathcal{H}_{34} = (\gamma_0 - \frac{\gamma_1}{\varepsilon}\gamma_4)|f_{\mathbf{k}}|$ to calculate $\mathcal{B}' = \mathcal{H}_{34}^2 + (\mathcal{H}_{11}^2 + \mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32})/2$ and $\mathcal{C}' = \mathcal{H}_{34}^4 - 2\mathcal{H}_{34}^2\mathcal{H}_{11}\mathcal{H}_{22} + \mathcal{H}_{11}(\mathcal{H}_{22}^2 + \mathcal{H}_{23}\mathcal{H}_{32})$. E_{+-} and E_{-+} are, respectively, expressed as

$$E(\mathbf{k})_{+-} = \sqrt{\mathcal{B}' - \sqrt{\mathcal{B}'^2 - \mathcal{C}'}}, \tag{12c}$$

$$E(\mathbf{k})_{-+} = -\sqrt{\mathcal{B}' + \sqrt{\mathcal{B}'^2 - \mathcal{C}'}}. \tag{12d}$$

The analytical formula (Eqs. (12a)-(12d)) are now employed to calculate the energy dispersions of gated BBLG. We first present the analytical energy dispersions $E(\mathbf{k})_{\pm\pm}$ at $V_g = 0$ in Fig. 3(a). $E(\mathbf{k})_{\pm\pm}$ in the high-symmetry line K-Γ-M-K are drawn in red to be distinguished from those obtained through the numerical diagonalization of Hamiltonian matrix in black. The red curves are exactly identical to the black ones except for the conduction bands in the high-symmetry line KM, where 3.0 eV $< E <$ 3.5 eV [Fig. 3(b)]. The energy spectrum in the presence of the gated voltage $V_g = 200$ meV is also exhibited in Fig. 3(c). The identity between the red and black curves reveals that the derived analytical formula can well describe the energy spectrum of the gated BBLG except for the conduction bands in the energy region 2.6 eV $< E < 3.4$ eV [Fig. 3(d)]. The results of the calculation show that the analytical model is able to provide us with the exact energy dispersions of the gated BBLG as $E < 2.6$ eV or $E > 3.5$ eV. The analytical energy dispersions and conjugated eigenstates are useful for

exploring the electronic properties, such as energy dispersions, density of states (DOS), and absorption spectra.

3   Discussion: Electronic Properties

Characteristics of the low energy spectrum are explored. BBLG owns two pairs of parabolic conduction and valence bands, as shown in Fig. 4 in the dashed and solid curves, which are obtained, respectively, by the analytical formula and numerical di-agonalization method. The dashed curves are in good agreement with the solid curves. With the comparison shown above, the exact solution to the low energy spectrum of BBLG emerges through our analytical model. While the high energy bands arouse some focus of our discussion, we are more interested in the lowest-energy electronic properties. At $V_g = 0$, $E(\mathbf{k})_{+-}$ and $E(\mathbf{k})_{-+}$, the first pair located near the chemical potential $\mu = 0$ exhibits a tiny overlap. $E(\mathbf{k})_{+-}$ and $E(\mathbf{k})_{--}$ are asymmetrical about $\mu = 0$, i.e., the electron-hole asymmetry, which is caused by the interlayer interaction γ_4. The minimum of $E(\mathbf{k})_{+-}$ and the maximum of $E(\mathbf{k})_{-+}$ are located at almost the same wavevector($\sim$ the K point). $E(\mathbf{k})_{+-}$ and $E(\mathbf{k})_{--}$ along high symmetry lines Γ-K and M-K are strongly anisotropic, which originates in the vanishing of $\mathcal{H}_{23}$ and $\mathcal{H}_{32}$ in Eqs. (12a)-(12d) along the line Γ-K.

The gated voltage V_g has a great influence on the low energy spectrum. First, the low energy subbands are significantly modified by V_g and change from monotonically parabolic dispersions into oscillating ones, referred to as a Mexican hat. Then, the asymmetry between the conduction $E(\mathbf{k})_{+-}$ and the valence $E(\mathbf{k})_{-+}$ bands along the Γ-K direction about the chemical potential is also enhanced. In addition to the K point, two extra band-edge states emerge in all directions. There exists a band-edge state with the minimum (maximum) energy along the Γ-K direction. The energy difference between the lowest band-edge state of $E_{+-}(\mathbf{k})$ and the highest one of $E_{--}(\mathbf{k})$ decides the band gap E_g. The locations of band-edge state are determined by $\frac{\partial E_{+-}}{\partial k_x}|_{k_c} = 0$ and $\frac{\partial E_{--}}{\partial k_x}|_{k_v} = 0$. By taking the main interactions γ_0 and γ_1 into consideration, E_{+-} (E_{--})

has a minimum (maximum) at

$$k_c = \frac{V_g}{\hbar v}\sqrt{\frac{2\gamma_1^2 + 4V_g^2}{\gamma_1^2 + 4V_g^2}},$$

where the Fermi velocity v is $\hbar v = 3b\gamma_0/2$. Therefore, the energy gap is

$$E_g = \frac{2\gamma_1 V_g}{\sqrt{\gamma_1^2 + 4V_g^2}},$$

The size of the band gap $E_g = E_{-+}(k_c) - E_{--}(k_v)$, which at first grows rapidly but then gradually declines with the increase in V_g. Another band-edge state along the KM direction belongs to the saddle point. Such states are the critical points in the energy-wavevector space and thus have a high DOS.

The DOS is useful for understanding the essential physical properties of BBLG. DOS is defined as

$$D(\omega) = \sum_{\eta_1,\eta_2} D(\omega)_{\eta_1,\eta_2}, \tag{13a}$$

$$D_{\eta_1,\eta_2}(\omega) = \frac{2}{\pi}\int\limits_{1stBZ}\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{\Gamma}{(E_{\eta_1,\eta_2}(\mathbf{k}) - \omega)^2 - \Gamma^2}, \tag{13b}$$

where $\eta_1, \eta_2 = \pm, \pm$ represents the subband index. The broadening energy width Γ is set as 3.0 meV. The full density of state $D(\omega)$ is the summation of $D_{\eta_1,\eta_2}(\omega)$, resulting from each subband E_{η_1,η_2}. $D(\omega)$ and $D_{\eta_1,\eta_2}(\omega)$ of BBLG at $V_g = 0$ are illustrated in Fig. 5(a). DOS exhibits logarithmic peaks, originating in the saddle point M around $\omega = \pm 3$ eV, which directly reflects the main features of the energy dispersions. The detailed structure of DOS at low energy is presented in Fig. 5(b). $D_{+-}(\omega)$ $(D_{-+}(\omega))$ makes contributions to $D(\omega)$ as $0 < \omega < \gamma_1$ $(-\gamma_1 < \omega < 0)$. BBLG at $V_g = 0$ is a semimetal due to nonvanished DOS at $\omega = 0$. The gated voltage V_g can open a band

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gap and induce two van hove singularities in the energy region $-\gamma_1 < \omega < \gamma_1$, as shown in Figs. 5(c)-5(e), where band gap is labeled by vertical red bars and van hove singularities are indicated by the blue arrows. One can modulate the band gap in BBLG using an external electric field. The increase in V_g not only enlarges the size of the band gap but enhances the height of van hove singularities. The predicted size of band gap and locations of van hove singularities can be verified by experimental measurements.

4 Absorption Spectra

Utilizing the analytical model, we revisit the low-energy absorption spectra of the gated BBLG, which has been studied through the numerical method.[40–42] The absorption function of the bilayer graphene at zero temperature (T = 0) is given by[38]

$$A(\omega) \propto \sum_{i,f} \int_{1stBZ} \frac{d\mathbf{k}}{(2\pi)^2} \, \text{Im}\left[\frac{F_f - F_i}{E_{ex} - \omega - i\Gamma} \right] \times |\mathbf{M}_{fi}(\mathbf{k})|^2, \tag{14}$$

where Γ is the broadening parameter owing to various nonradiative processes. f (i) denotes the final (initial) state and F_f (F_i) is the Fermi-Dirac distribution function. $E_{ex} = E_f(\mathbf{k}) - E_i(\mathbf{k})$ is the excitation energy. $\mathbf{M}_{fi}(\mathbf{k}) = \langle \Phi_f(\mathbf{k}) | \frac{\hat{E} \cdot \vec{P}}{m_e} | \Phi_i(\mathbf{k}) \rangle$, the dipole matrix element, is the velocity operator between the initial and final wave functions $\Phi_i(\mathbf{k})$ and $\Phi_f(\mathbf{k})$. The absorption spectra $A_x(\omega)$ originates in electronic transitions that correspond to excitations from the occupied valence bands to the unoccupied conduction bands, excited by the electromagnetic field. In this work, the direction of electromagnetic field is assumed to be parallel to the x-axis. Within the gradient approximation,[43,44] the dipole matrix element $M_{fi}(\mathbf{k}) = \langle \Phi_f(\mathbf{k}) | \frac{\partial H}{\partial k_x} | \Phi_i(\mathbf{k}) \rangle$, where $\frac{\hat{E} \cdot \vec{P}}{m_e}$ is derived from the gradient of Hamiltonian operator, $\frac{\partial H}{\partial k_x}$. Because of the zero momentum of photon, the optical selection rule is $\Delta k = 0$. The optical transition channels are determined by the thermal factor $F_F - F_i$ and the dipole matrix element.

The dipole matrix element, by inserting the tight-binding wave functions $\Phi =$

$c_1|A_1\rangle + c_2|A_2\rangle + c_3|B_1\rangle + c_4|B_2\rangle$, is expressed as

$$\mathbf{M}_{fi} = \sum_{l,m} \mathbf{c}_l^f (\frac{\partial H}{\partial k_x})_{lm} \mathbf{c}_m^i, \tag{15a}$$

where $(\frac{\partial H}{\partial k_x})_{lm} = \frac{\partial H_{lm}}{\partial k_x}$ and H_{lm} is the element of the Hamiltonian matrix (Eq. (1)). After the action of rotation operator (Eq. (3)), the dipole matrix element is then changed into

$$\mathbf{M}_{fi} = \sum_{l,m} \mathbf{d}_l^f \mathscr{V}_{lm} \mathbf{d}_m^i, \tag{15b}$$

where the analytical form of matrix elements $\mathscr{V}_{lm}$ is given explicitly in the appendix. $|\mathbf{d}_1^{i,f}, \mathbf{d}_2^{i,f}, \mathbf{d}_3^{i,f}, \mathbf{d}_4^{i,f}\rangle$ are the initial (final) eigenstates associated with the Bloch function, Eq. (6). The eigenstate corresponding to each energy dispersion $E_{\pm\pm}$ can be exactly specified, which is

$$\begin{cases} \mathbf{d}_1 = \frac{1}{\sqrt{N_c}}, \\ \mathbf{d}_2 = \frac{1}{\sqrt{N_c}} \left[\frac{E_{\pm\pm} - \mathscr{H}_{21}}{\mathscr{H}_{12}} \right], \\ \mathbf{d}_3 = \frac{1}{\sqrt{N_c}} \left[\frac{(E_{\pm\pm} - \mathscr{H}_{22})\mathbf{d}_2 - \mathscr{H}_{11}}{\mathscr{H}_{23}} \right], \\ \mathbf{d}_4 = \frac{1}{\sqrt{N_c}} \left[\frac{(E_{\pm\pm} - \mathscr{H}_{33})\mathbf{d}_3 - \mathscr{H}_{32}\mathbf{d}_2}{\mathscr{H}_{34}} \right]. \end{cases} \tag{16}$$

The analytical expression for dipole matrix element can be used to efficiently evaluate the magnitude of M_{fi} and the optical absorption spectra $A(\omega)$. M_{fi} depends on energy spectrum, velocity operator, and eigenstates.

The square of the absolute value of dipole matrix element $|M_{fi}(\mathbf{k})|^2$ in the high-symmetry line Γ-K-M for the transition $E_{--} \to E_{+-}$ at different V_g's is drawn in Fig. 6, where the solid (dashed) curves are calculated with the energy spectrum and eigenstates obtained through the numerical method (analytical model). The dashed curves are exactly in agreement to solid ones along the high-symmetry line ΓK while they exhibit some discrepancy around the point M. In the absence of the gated voltage ($V_g = 0$), $|M_{fi}(\mathbf{k})|^2$ exhibits a highly anisotropic characteristic with a maximal value around the point M in the high-symmetry line Γ-K-M. $|M_{fi}|$ is equal to zero in the line Γ-K, along

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which the structure factor $f(\mathbf{k})$ is a real number and the matrix elements $\mathcal{H}_{23}$ and $\mathcal{H}_{32}$ in Eq. (6) is equal to zero. The 4×4 Hamiltonian matrix is decomposed into the two 2×2 blocks. The eigen-vector corresponding to the final (initial) state is $|\mathbf{d}^f\rangle = |d_1, d_2, 0, 0\rangle$ ($|\mathbf{d}^i\rangle = |0, 0, d_3, d_4\rangle$). The six matrix elements $\mathcal{V}_{13}$, $\mathcal{V}_{23}$, $\mathcal{V}_{24}$, $\mathcal{V}_{31}$, $\mathcal{V}_{32}$, and $\mathcal{V}_{42}$ are all equal to zero as $Im[f(\mathbf{k})] = 0$ and $V_g = 0$. The straightforward calculation exhibits that the magnitude of the dipole matrix element vanishes, i.e., $|M_{fi}| = 0$.

In the presence of the gated voltage, $|\mathrm{M}_{fi}|^2$ shows different aspects, as illustrated in Figs. 6(b)-6(d). V_g alters the Hamiltonian matrix elements, energy spectrum and eigenstates $|\mathbf{d}^i\rangle$ and $|\mathbf{d}^f\rangle$. Moreover, the V_g-dependent $\mathcal{V}_{lm}$'s are also modified by the gated voltage. As a result, at $V_g = 100$ meV, $|\mathrm{M}_{fi}|^2$ (blue solid curve in Fig. 6(b)) around the point M exhibits a different aspect and magnitude. The maximum is located in the vicinity of the point M. The increase in V_g does not alter the profile of $|\mathrm{M}_{fi}|^2$ around the point M. Most importantly, the application of V_g enhances $|\mathrm{M}_{fi}|^2$ in the high-symmetry line KΓ. V_g introduces the nonzero matrix elements $\mathcal{H}_{23}$ and $\mathcal{H}_{32}$ in Eq. (6), which mixes the symmetrical and anti-symmetrical wave functions, i.e., the alternation of the eigenstates. Moreover, V_g also produces the six matrix elements $\mathcal{V}_{13}$, $\mathcal{V}_{23}$, $\mathcal{V}_{24}$, $\mathcal{V}_{31}$, $\mathcal{V}_{32}$, and $\mathcal{V}_{42}$, being unequal to zero. As a result, V_g intensifies $|\mathrm{M}_{fi}|^2$ in the symmetry line KΓ. Such a characteristic strongly modifies the low energy absorption spectra in the presence of V_g.

The low-energy absorption spectra $A(\omega)$ of AB BLG reflect the characteristics of energy dispersions. There are six possible interband excitations resulting from four branches of energy dispersion. The optical excitation from the subband E_{-+} to E_{--} and transition between E_{+-} and E_{++} are forbidden by the thermal factor $F_f - F_i$. Four allowed excitations, $A_1(\omega)$, $A_2(\omega)$, $A_3(\omega)$ and $A_4(\omega)$, are shown by the vertical lines in the inset on the left panel of Fig. 7(a). $A_1(\omega)$ stems from the transition between the highest valence subband E_{--} and the top conduction subband E_{++}, and $A_2(\omega)$ origi- nates in the excitation $E{-+} \rightarrow E_{+-}$. Moreover, the transition from the subband E_{--} to E_{+-} generates the spectra $A_3(\omega)$ and the excitation between the subbands E_{-+} and E_{++} leads to $A_4(\omega)$. $A_1(\omega)$ [$A_2(\omega)$] shows a discontinuous structure at $\omega \approx 380$ meV, as illustrated in Fig. 7(a). Such an optical gap originates in the interband transition

between E_{--} and E_{++} subbands [E_{-+} and E_{-+} subbands]. $A_4(\omega)$, resulting from the transition from E_{-+} to E_{++} subbands, exhibits an absorption edge at $\omega \approx 800$ meV. There is no optical gap found in the spectra $A_3(\omega)$ (red curve) because of the overlap between the subbands E_{--} and E_{+-}. As a result of the superposition of sub-spectra, the total spectra exhibit two discontinuities at $\omega \approx 380$ and $\omega \approx 800$ meV, and no optical gap is found in $A(\omega)$.

The application of V_g has a great effect on the low-energy absorption spectra $A_3(\omega)$, as depicted in Fig. 7(b). V_g not only opens a band gap but gives rise to a sharp peak in $A_3(\omega)$. In the presence of V_g, the steep rise of the spectra, due to the transition between the band-edge states of E_{--} and that of E_{+-} subband in the ΓK direction, can be used to determine the size of energy gap E_g. The energy gaps are equal to $\omega = 0.17, 0.25$, and 0.28 eV as $V_g = 100, 200$, and 300 meV. The first absorption peak is a compound one, consisting of a shoulder on the low energy side and a main peak. The former (shoulders) result from the transition between the E_{-+} and E_{+-} subbands, denoted by the vertical red arrow in Fig. 4. The excitation indicated by the vertical blue arrow in Fig. 4 brings about the main peak. As $V_g = 100, 200$, and 300 meV, the main peaks are located at $\omega = 0.18, 0.30$, and 0.35 eV. The main peak is in the logarithmic form, stemming from the saddle point in energy dispersions in the high-symmetry line MK. The frequency of the main peak depends on the magnitude of V_g. These peaks make a blue-shift with the increase in V_g. The height of the first peak also enhances with the increase in V_g because DOS around the band-edge state of E_{-+} (E_{+-}) and $|M_{fi}|^2$ in the high-symmetry line ΓK are enhanced by V_g, as shown in Figs. 5 and 6.

How the tight-binding parameters $\gamma_i's$ influence the low energy absorption spectra $A(\omega)$ is deliberated. The dashed brown curve in Fig. 7(c) presents $A(\omega)$ at $V_g = 200$ meV, through the analytical model, including all the tight-binding parameters γ_0, γ_1, γ_3, and γ_4. The close of the interlayer interaction γ_4 has no effect on $A(\omega)$, shown by cyan curve in Fig. 7(c). According to Eq. (7b), the magnitude of $\frac{\gamma_1}{\varepsilon_{AA}}\gamma_4|f_{\mathbf{k}}|$ gradually declines with the increase in V_g. As a result, absorption spectra at $V_g = 200$ meV are not affected by the interlayer interaction γ_4. $A(\omega)$, illustrated by the red curve, exhibits a larger band gap $E_g = 270$ meV and a sharp peak located at $\omega = E_g$ as the main

intralayer interaction (γ_0) and interlayer interaction (γ_1) are taken into consideration. Moreover, $A(\omega)$ presents a simple feature and weaker intensity of absorption relative to those in the brown curve. The chief cause is that the close of the interlayer interaction γ_3 not only changes energy dispersions and wave functions but turns off some optical transition channels.

Comparison of the study results with those obtained through ab initio calculation is made. The analytical formula can exactly describe four energy dispersions and generate the energy bands with "Mexican hat" structure. Our research demonstrates that the gated voltage V_g alters the subband spacing, changes the energy band gap, produces the oscillating bands, and induces more band-edge states. The aforementioned electronic properties, e. g., band feature, tunable band gap, and electric-field-modified oscillating bands, are also produced through the ab initio calculation.[41] That is, the electronic properties derived from the analytical model are in qualitative agreement with those given by the ab initio calculation. To be more specific, we quantitatively compare the sizes of gated tunable band gaps acquired by the two methods. The calculated tunable band gaps, shown in Fig. 8 in the cross symbols, are taken from the ab initio calculation.[45] The band gap first increases monotonically as the strength of electric field increases. Then, the energy gaps saturate to a value $E_g \approx 270$ meV as the field strength $|\mathbf{F}|$ is greater than $0.2 V/\text{Å}$. We now evaluate E_g by employing the analytical model for $\gamma_3 = \gamma_4 = 0$ (black curve) and $\gamma_3 \neq 0$ and $\gamma_4 \neq 0$ (red curve). The red curve exhibits that E_g first increases sublinearly as the strength of electric field ($|\mathbf{F}| = 2V_g/c$ and c is the layer distance) is less than $0.05 V/\text{Å}$. While the energy gaps approach to a value $E_g \approx 300$ meV as $|\mathbf{F}| > 0.2 V/\text{Å}$. The behavior of E_g predicted by the analytical method (red curve) is similar to that of the ab initio method. The comparison between the black and red curves illustrates that as the field strength is weaker than $0.05 V/\text{Å}$, the tunable band gaps are independent of the hopping integral γ_3. After that, the hopping integral γ_3 reduces the size of E_g.

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5 Conclusions

We develop a method to access the analytical form of the energy spectrum and eigenstates of the gated BBLG within the tight-binding model with all the tight-binding parameters included. The trigonal warping γ_3 and applied gated bias V_g destroy the mirror symmetry of BBLG. To deal with the broken symmetry caused by γ_3 and V_g, a new set of tight-binding basis functions is constructed through a rotation operator. The renormalized intralayer and interlayer interactions exhibit a gated bias dependence. Most importantly, the Hamiltonian matrix H is transformed into a band-storage matrix in the subspace spanned by the new basis functions. The formula of energy dispersions and wave functions are then obtained, analytically. γ_4, the electron-hole asymmetry, is treated as a perturbation and included in the analytical formula. The electronic properties, density of states, optical dipole matrix element and optical absorption spectra are explored by employing this analytical formula. The study shows that V_g can open an optical gap and produce a profound low-energy peak in absorption spectra. The dipole matrix element **M** and absorption spectra are strongly modified by V_g. Finally, the characteristics of absorption spectra, e.g., the location and height of this low-energy peak, are significantly presented and explored through the analytical model.

Acknowledgement

Appendix

The element $\mathscr{V}_{lm}$ is the operator $\left(\frac{\partial H}{\partial k_x} \right)$ sandwiched by the symmetrized basis functions $\langle \phi_l |$ and $| \phi_m \rangle$, i. e. $\mathscr{V}_{lm} = \langle \phi_l | \frac{\partial H}{\partial k_x} | \phi_m \rangle$, where H is the Hamiltonian representation Eq. (1). The analytical form of each a $\mathscr{V}_{lm}$ is listed as follows.
$\mathscr{V}_{11} = 0,$

$$\mathscr{V}_{12} = \frac{\gamma_0}{2|f|}\left(\frac{\gamma_1^2\, f^*\frac{\partial f}{\partial k_x} + (\varepsilon - V_g)^2 f\frac{\partial f^*}{\partial k_x}}{\varepsilon(\varepsilon - V_g)}\right) + \frac{\gamma_1}{\varepsilon}\gamma_4\left(\frac{f^*}{2|f|}\frac{\partial f}{\partial k_x} + \frac{f}{2|f|}\frac{\partial f^*}{\partial k_x}\right),$$

$$\mathscr{V}_{13} = (\gamma_0\frac{\gamma_1}{\varepsilon} - \gamma_4)\left(\frac{f^*}{2|f|}\frac{\partial f}{\partial k_x} - \frac{f}{2|f|}\frac{\partial f^*}{\partial k_x}\right) - (\gamma_4\frac{V_g}{\varepsilon})\left(\frac{f}{2|f|}\frac{\partial f^*}{\partial k_x} + \frac{f^*}{2|f|}\frac{\partial f}{\partial k_x}\right),$$

$$\mathscr{V}_{14} = 0,$$

$$\mathscr{V}_{21} = \mathscr{V}_{12}^*,$$

$$\mathscr{V}_{22} = \frac{\gamma_1}{\varepsilon}\frac{\gamma_3}{2}\left(\frac{f^*}{|f|}\frac{\partial f^*}{\partial k_x}\frac{f^*}{|f|} + \frac{f}{|f|}\frac{\partial f}{\partial k_x}\frac{f}{|f|}\right),$$

$$\mathscr{V}_{23} = \frac{\gamma_3}{2}\left(\frac{f^*}{|f|}\frac{\partial f^*}{\partial k_x}\frac{f^*}{|f|} - \frac{f}{|f|}\frac{\partial f}{\partial k_x}\frac{f}{|f|}\right) - \frac{V_g}{\varepsilon}\frac{\gamma_3}{2}\left(\frac{f^*}{|f|}\frac{\partial f^*}{\partial k_x}\frac{f^*}{|f|} + \frac{f}{|f|}\frac{\partial f}{\partial k_x}\frac{f}{|f|}\right),$$

$$\mathscr{V}_{24} = (-\gamma_0\frac{\gamma_1}{\varepsilon} + \gamma_4)\left(\frac{f^*}{2|f|}\frac{\partial f}{\partial k_x} - \frac{f}{2|f|}\frac{\partial f^*}{\partial k_x}\right) - (\gamma_4\frac{V_g}{\varepsilon})\left(\frac{f}{2|f|}\frac{\partial f^*}{\partial k_x} + \frac{f^*}{2|f|}\frac{\partial f}{\partial k_x}\right),$$

$$\mathscr{V}_{31} = \mathscr{V}_{13}^*,$$

$$\mathscr{V}_{32} = \mathscr{V}_{23}^*,$$

$$\mathscr{V}_{33} = -\mathscr{V}_{22},$$

$$\mathscr{V}_{34} = \frac{\gamma_0}{2|f|}\left(\frac{\gamma_1^2\, f\frac{\partial f^*}{\partial k_x} + (\varepsilon + V_g)^2 f^*\frac{\partial f}{\partial k_x}}{\varepsilon(\varepsilon + V_g)}\right) + \frac{-\gamma_1}{\varepsilon}\gamma_4\left(\frac{f}{2|f|}\frac{\partial f^*}{\partial k_x} + \frac{f^*}{2|f|}\frac{\partial f}{\partial k_x}\right),$$

$$\mathscr{V}_{42} = \mathscr{V}_{24}^*,$$

$$\mathscr{V}_{34} = \mathscr{V}_{43}^*,$$

$$\mathscr{V}_{44} = 0.$$

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Figure Captions

FIG. 1. (a) The energy spectra, obtained by Eq. (11), are illustrated in the red dashed curves. The black curves are the energy spectrum by the numerical diagonalization. The geometric structure of the AB-stacking bilayer graphene and the intralayer and interlayer interactions are shown in the inset. (b) Same plots as (a) but the gated voltage $V_g = 200$ meV. The inset exhibits the first Brillouin zone. M is the saddle point and K and K' are the Dirac points.

FIG. 2. The dashed curves are the low energy spectrum at different V_g's acquired by Eq. (11). For comparison, the energy spectrum by the numerical diagonalization are drawn in the black curves.

FIG. 3. (a) The energy dispersions at $V_g = 0$ illustrated in the red dashed curves are obtained by the exact analytical model. The black curves are the energy spectrum by the numerical diagonalization. (b) The conduction bands around the point M. (c) The same plot as (a) but for $V_g = 200$meV. (d) The conduction bands around the point M.

FIG. 4. Dashed and solid curves are energy dispersions obtained by exact analytical formula and numerical diagonalization. For comparison, the exact energy dispersions are illustrated by the colorful curves.

FIG. 5. (a) DOS $D_{\eta_1\eta_2}$, associate with each subband $E_{\eta_1\eta_2}$, of BBLG at $V_g = 0$. (b)-(e) are the low-energy DOS at $V_g = 0, 100, 200$, and 300 meV. The vertical red bars indicate the energy band gap. The blue arrows label the van Hove singularities in DOS.

FIG. 6. (a)-(d) The solid curves are the square of the absolute values of optical matrix $|M_{fi}|$, obtained by the numerical diagonalization method. The same plots obtained by analytical formula are given in the dashed curves.

FIG. 7. (a) $A_1(\omega), A_2(\omega), A_3(\omega)$, and $A_4(\omega)$, the sub-optical spectra, are shown by blue, green, red and brown curves. Four allowed optical transitions are indicated by

the vertical lines in the inset in left panel. (b) The low-energy absorption spectra $A_i(\omega)$ at $V_g = 0$, 100, 200, and 300 meV are drawn in the red, green, brown and blue. (c) the low energy absorption spectra with the different tight-binding parameters.

FIG. 8. The cross symbols are band gaps acquired through the ab initio calculation (data are taken from APL **98**, 2011, 263107). E_g is obtained by the analytical model for $\gamma_3 = \gamma_4 = 0$ (black curve) and $\gamma_3 \neq 0$ and $\gamma_4 \neq 0$ (red curve).