Electronic and Optical Properties of a Graphene Monolayer in a Spatially Modulated Magnetic Field

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Tight-binding Model
in a Graphene Monolayer

Bloch Function: $\psi_{\mathbf{k}}(\mathbf{r})$

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$$

$$u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}+\mathbf{T})$$

$u_{\mathbf{k}}(\mathbf{r})$ **is a periodic function with the period T**

Tight-binding Model

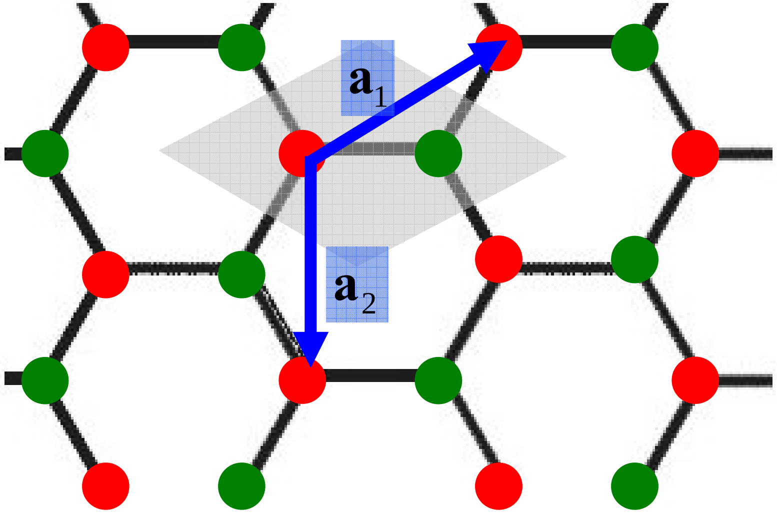
$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} \phi(\mathbf{r} - \mathbf{r}_j)$$

$$= e^{i\mathbf{k}\cdot\mathbf{r}} \frac{1}{\sqrt{N}} \sum_j e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_j)} \phi(\mathbf{r} - \mathbf{r}_j)$$

$\psi_{\mathbf{k}}(\mathbf{r})$: **Tight-binding function (Bloch function)**

$\phi(\mathbf{r} - \mathbf{r}_j)$: **atomic orbital at r=r$_j$**

Graphene Monolayer



$$\Psi = a_A \psi_A + a_B \psi_B \qquad \textbf{(1)}$$

$$\psi_A = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}_A} e^{i\mathbf{k}\cdot\mathbf{r}_A} \phi(\mathbf{r} - \mathbf{r}_A)$$

$$\psi_B = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}_B} e^{i\mathbf{k}\cdot\mathbf{r}_B} \phi(\mathbf{r} - \mathbf{r}_B)$$

Ref: P. R. Wallace, Phys. Rev. 71, 622 (1947)

$$H\Psi = E\Psi$$

$$\Rightarrow \langle \psi_A | H | \Psi \rangle = E \langle \psi_A | \Psi \rangle$$

$$\Rightarrow \langle \psi_A | H | \psi_A \rangle a_A + \langle \psi_A | H | \psi_B \rangle a_B = E \langle \psi_A | \psi_A \rangle a_A$$

$$\Rightarrow \langle \psi_A | H | \psi_A \rangle a_A + \langle \psi_A | H | \psi_B \rangle a_B = E a_A$$

同理 $\langle \psi_B | H | \psi_A \rangle a_A + \langle \psi_B | H | \psi_B \rangle a_B = E a_B$

Define: $H_{11} = \langle \psi_A | H | \psi_A \rangle$ $H_{22} = \langle \psi_B | H | \psi_B \rangle$

$H_{12} = \langle \psi_A | H | \psi_B \rangle$ $H_{21} = \langle \psi_B | H | \psi_A \rangle$

H_{12} **(**H_{21}**): Hopping integral**

$$\begin{cases} H_{11}a_A + H_{12}a_B = Ea_A \\ H_{21}a_A + H_{22}a_B = Ea_B \end{cases}$$

$$\Rightarrow \det \begin{vmatrix} H_{11} - E & H_{12} \\ H_{21} & H_{22} - E \end{vmatrix} = 0$$

where $H_{11} = H_{22} \quad H_{21} = H_{12}^*$

$$\Rightarrow (H_{11} - E)^2 = H_{12} \cdot H_{12}^* = | H_{12} |^2$$

$$\Rightarrow E - H_{11} = \pm | H_{12} |$$

$$H_{12} = \langle \psi_A | H | \psi_B \rangle$$

$$= \frac{1}{N} \left\langle \sum_{\mathbf{r}_A} e^{i\mathbf{k}\cdot\mathbf{r}_A} \phi(\mathbf{r}-\mathbf{r}_A) \,|\, H \,|\, \sum_{\mathbf{r}_B} e^{i\mathbf{k}\cdot\mathbf{r}_B} \phi(\mathbf{r}-\mathbf{r}_B) \right\rangle$$

$$= \frac{1}{N} \sum_{\mathbf{r}_A,\mathbf{r}_B} e^{i\mathbf{k}\cdot(\mathbf{r}_B-\mathbf{r}_A)} \langle \phi(\mathbf{r}-\mathbf{r}_A) \,|\, H \,|\, \phi(\mathbf{r}-\mathbf{r}_B) \rangle$$

$$\overset{\mathbf{r}\to\mathbf{r}+\mathbf{r}_A}{\Longrightarrow} H_{12} = \frac{1}{N} \sum_{\mathbf{r}_A,\mathbf{r}_B} e^{i\mathbf{k}\cdot(\mathbf{r}_B-\mathbf{r}_A)} \langle \phi(\mathbf{r}) \,|\, H \,|\, \phi(\mathbf{r}-(\mathbf{r}_B-\mathbf{r}_A)) \rangle$$

$$\overset{\mathbf{r}_B-\mathbf{r}_A=\boldsymbol{\rho}_A}{\Longrightarrow} H_{12} = \sum_{\boldsymbol{\rho}_A} e^{i\mathbf{k}\cdot\boldsymbol{\rho}_A} \langle \phi(\mathbf{r}) \,|\, H \,|\, \phi(\mathbf{r}-\boldsymbol{\rho}_A) \rangle$$

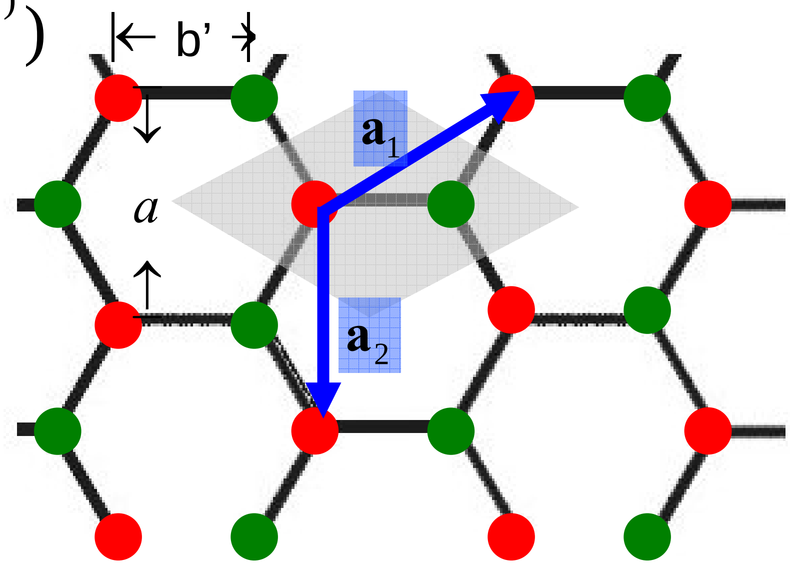
$$\equiv \sum_{nn} e^{i\mathbf{k}\cdot\boldsymbol{\rho}_{nn}} \langle \phi(\mathbf{r}) \,|\, H \,|\, \phi(\mathbf{r}-\boldsymbol{\rho}_{nn}) \rangle = -\gamma_0 \sum_{nn} e^{i\mathbf{k}\cdot\boldsymbol{\rho}_{nn}} \quad \mathbf{(2)}$$

$$H_{12} = -\gamma_0 \sum_{nn} e^{i\mathbf{k}\cdot\boldsymbol{\rho}_{nn}}$$

$$= -\gamma_0 (e^{ik_x b'} + e^{i(-k_x b'/2 + k_y a/2)} + e^{i(-k_x b'/2 - k_y a/2)})$$

$$= -\gamma_0 [e^{ik_x b'} + e^{-ik_x b'/2} (e^{ik_y a/2} + e^{-ik_y a/2})]$$

$$= -\gamma_0 [e^{ik_x b'} + 2\cos(k_y \, a/2) e^{-ik_x b'/2}]$$



$$H_{21} = -\gamma_0 [e^{-ik_x b'} + 2\cos(k_y \, a/2) e^{ik_x b'/2}]$$

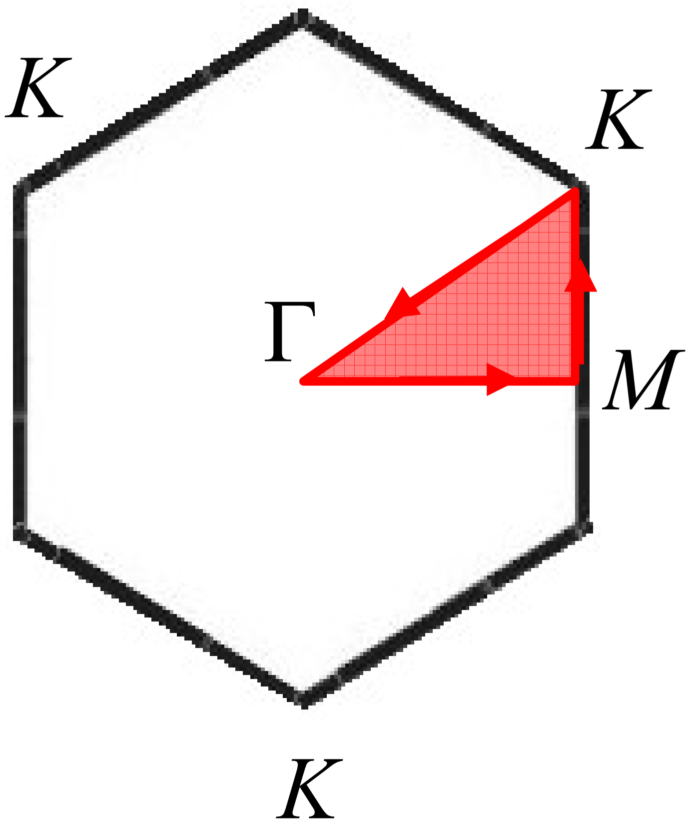
$$\varepsilon = E - H_{11} = \pm | H_{12} |$$

$$= \pm \gamma_0 [1 + 4\cos^2(k_y \, a/2) + 4\cos(k_y \, a/2)\cos(k_x \, 3b'/2)]^{1/2}$$

$$= \pm \gamma_0 [1 + 4\cos^2(\frac{\sqrt{3}b'k_y}{2}) + 4\cos(\frac{\sqrt{3}b'k_y}{2})\cos(\frac{3b'k_x}{2})]^{1/2} \quad \textbf{(3)}$$

H_{11} **and** H_{22} **are assumed to be zero**

$\gamma_0 = 2.56$ **eV**



$$K\left(\frac{2\pi}{3b'}, \frac{2\pi}{3b'} \times \frac{1}{\sqrt{3}}\right)$$

$$\varepsilon_K = \pm\gamma_0\left(1 + 4\cos^2\frac{\pi}{3} + 4\cos\frac{\pi}{3}\cos\pi\right)^{1/2}$$

$$= \pm\gamma_0(1 + 1 - 2)^{1/2} = 0$$

$$\Gamma(0,0)$$

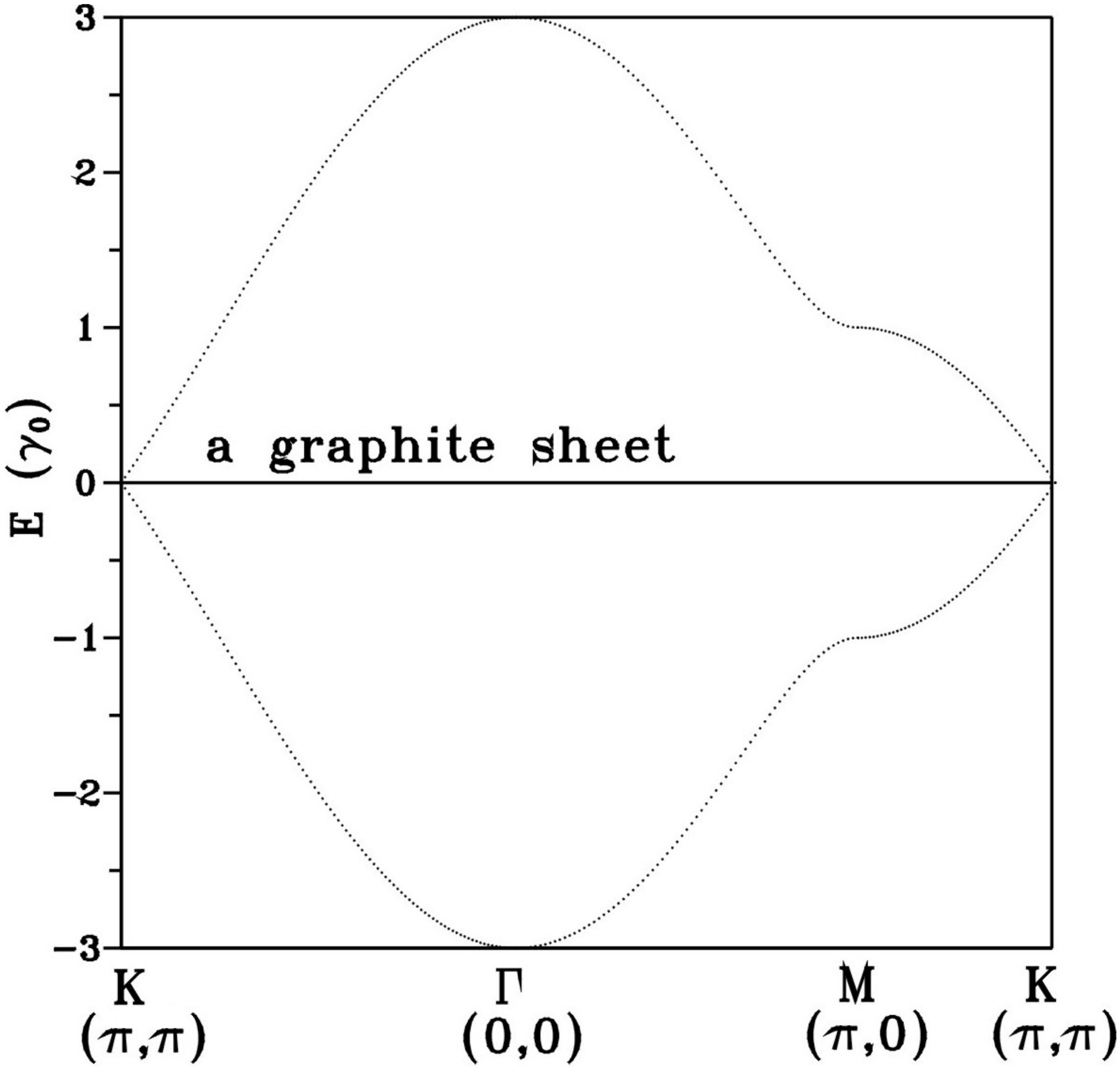
$$\varepsilon_\Gamma = \pm\gamma_0\left(1 + 4\cos^2 0 + 4\cos 0\cos 0\right)^{1/2}$$

$$= \pm\gamma_0(1 + 4 + 4)^{1/2} = \pm 3\gamma_0$$

$$M\left(\frac{2\pi}{3b'}, 0\right)$$

$$\varepsilon_M = \pm\gamma_0\left(1 + 4\cos^2 0 + 4\cos 0\cos\pi\right)^{1/2}$$

$$= \pm\gamma_0(1 + 4 - 4)^{1/2} = \pm\gamma_0$$

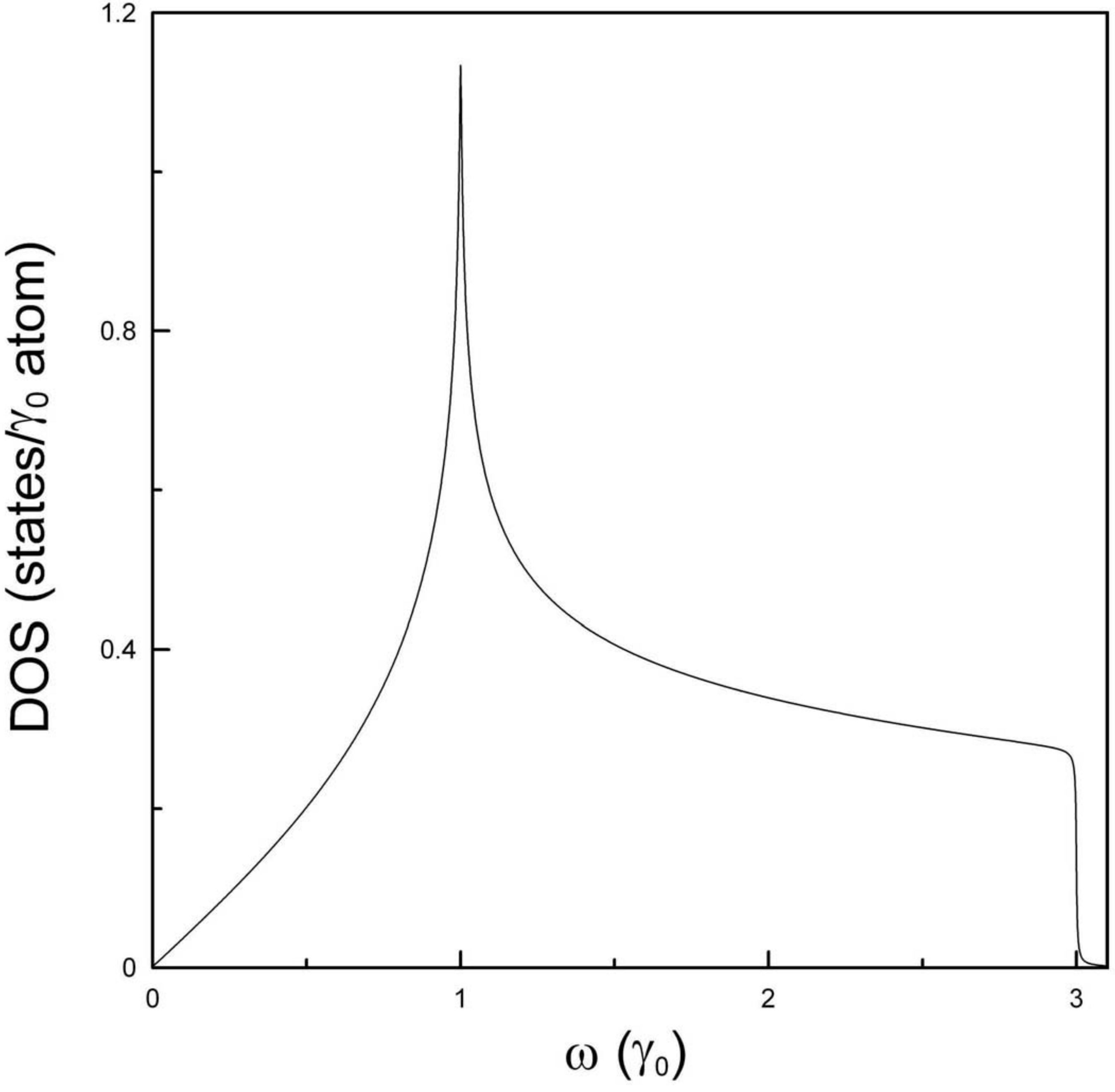


3
2
1
0
−1
−2
−3
E (γ0)
a graphite sheet
K
(π,π)
Γ
(0,0)
M
(π,0)
K
(π,π)

Density of states (DOS)

$$D(\omega) = \sum_{h=c,v} \int_{1st\ BZ} \frac{d\mathbf{k}}{(2\pi)^2} \frac{\Gamma}{\pi} \frac{1}{\left[E^h(\mathbf{k}) - \omega\right]^2 + \Gamma^2} \quad \textbf{(4)}$$

Γ **: phenomenological brodening parameter**



1.2
0.8
0.4
0
DOS (states/γ_0 atom)
0
1
2
3
ω (γ_0)

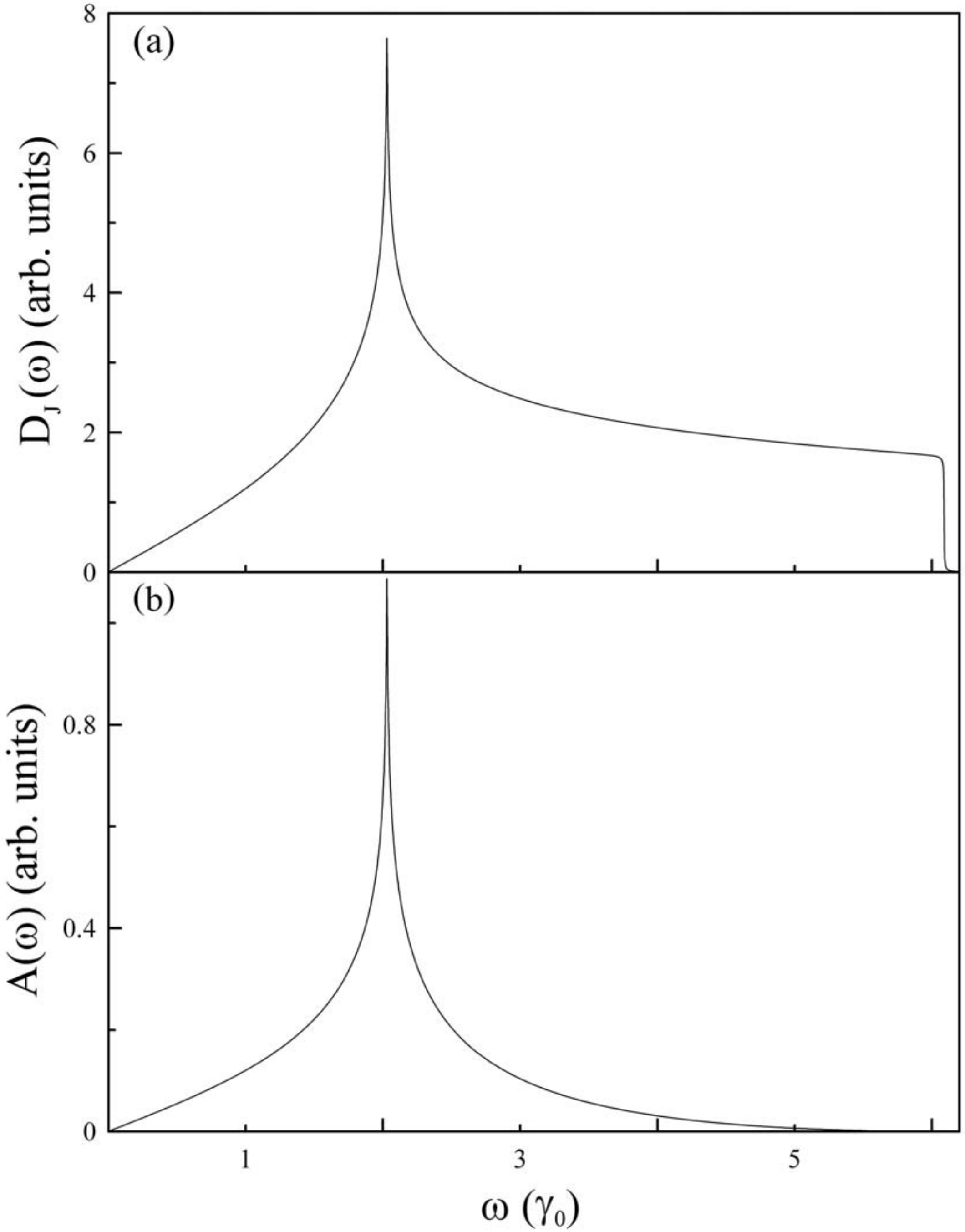
Optical absorption spectra:

$$A(\omega) \propto \sum_{c,v,\tilde{n},\tilde{n}'} \int_{1st\ BZ} \frac{d\mathbf{k}}{(2\pi)^2} \left| \left\langle \Psi^c(\mathbf{k},\tilde{n}) \middle| \frac{\hat{\mathbf{E}}\bullet\mathbf{P}}{m_e} \middle| \Psi^v(\mathbf{k},\tilde{n}') \right\rangle \right|^2$$

$$\times \mathrm{Im}\left[\frac{f\left(E^c(\mathbf{k},\tilde{n})\right) - f\left(E^v(\mathbf{k},\tilde{n}')\right)}{E^c(\mathbf{k},\tilde{n}) - E^v(\mathbf{k},\tilde{n}') - \omega - i\Gamma} \right] \qquad \textbf{(5a)}$$

Joint density of states:

$$D_J\text{: }\textbf{Set } \left\langle \Psi^c(\mathbf{k},\tilde{n}) \middle| \frac{\hat{\mathbf{E}}\bullet\mathbf{P}}{m_e} \middle| \Psi^v(\mathbf{k},\tilde{n}') \right\rangle = 1 \qquad \textbf{(5b)}$$



(a)
(b)
D$_J$(ω) (arb. units)
A(ω) (arb. units)
ω (γ_0)
0
2
4
6
8
0
0.4
0.8
1
3
5

The Bloch functions in a static magnetic field:

$$\Phi\left(\vec{k},\vec{r}\right)=\frac{1}{\sqrt{N}}\sum_{\vec{R}}\exp\left(i\vec{k}\cdot\vec{r}+i\frac{e}{\hbar}G_{\vec{R}}\right)\phi\left(\vec{r}-\vec{R}\right) \quad \textbf{(6)}$$

$$G_{\vec{R}}=\int_{R}^{r}A\left(\xi\right)d\xi=\int_{0}^{1}\left(\vec{r}-\vec{R}\right)\cdot\vec{A}\left(\vec{R}+\lambda\left[\vec{r}-\vec{R}\right]\right)d\lambda \quad \textbf{(7)}$$

$G_{\vec{R}}$: **Peierls phase**

Ref: J. M. Luttinger, Phys. Rev. 84, 814~817 (1951)

$$H\Phi\left(\vec{k},\vec{r}\right)$$

$$=\frac{1}{\sqrt{N}}\sum_{\vec{R}}\exp\left(i\vec{k}\cdot\vec{R}+i\frac{e}{\hbar}G_{\vec{R}}\right)\left(\frac{\vec{P}^{2}}{2m}+V\right)\phi\left(\vec{r}-\vec{R}\right)$$

$$H_{\vec{k}\vec{k}'}=\left\langle\Phi_{\vec{k}'}\middle|H\middle|\Phi_{\vec{k}}\right\rangle$$

$$=\frac{1}{N}\sum_{\vec{R}\vec{R}'}e^{i\left(\vec{k}\cdot\vec{R}-\vec{k}'\cdot\vec{R}'\right)+\left(ie/\hbar\right)\left(G_{\vec{R}}-G_{\vec{R}'}\right)}H_{\vec{R}\vec{R}'}$$

$$H_{\vec{R}\vec{R}'}=\left\langle\Phi\left(\vec{r}-\vec{R}\right)\middle|\frac{\vec{P}^{2}}{2m}+V\middle|\Phi\left(\vec{r}-\vec{R}'\right)\right\rangle\quad(8)$$

$$G_{\vec{R}} - G_{\vec{R'}} = \int_0^1 \left(\overrightarrow{R'} - \vec{R}\right) \cdot \vec{A}\left(\vec{R} - \lambda\left[\overrightarrow{R'} - \vec{R}\right]\right) d\lambda \quad (9)$$

The flux quantum ϕ_0

$$\phi_0 = \frac{h}{e} = 4.1356 \times 10^{-15}\left[T/m^2\right] \qquad (10)$$

For a graphene monolayer, $\Phi_0 \approx 79000$ T through a hexagon area.

For a single-layer graphene:

(1). Modulated magnetic field :

$$\vec{B} = \left(0, 0, B\sin\left(k_B x\right)\right) \text{ and } \vec{A} = \left(0, \frac{-B}{k_B}\cos\left(k_B x\right), 0\right)$$

(i). Armchair

(ii). Zigzag

Modulated magnetic field:

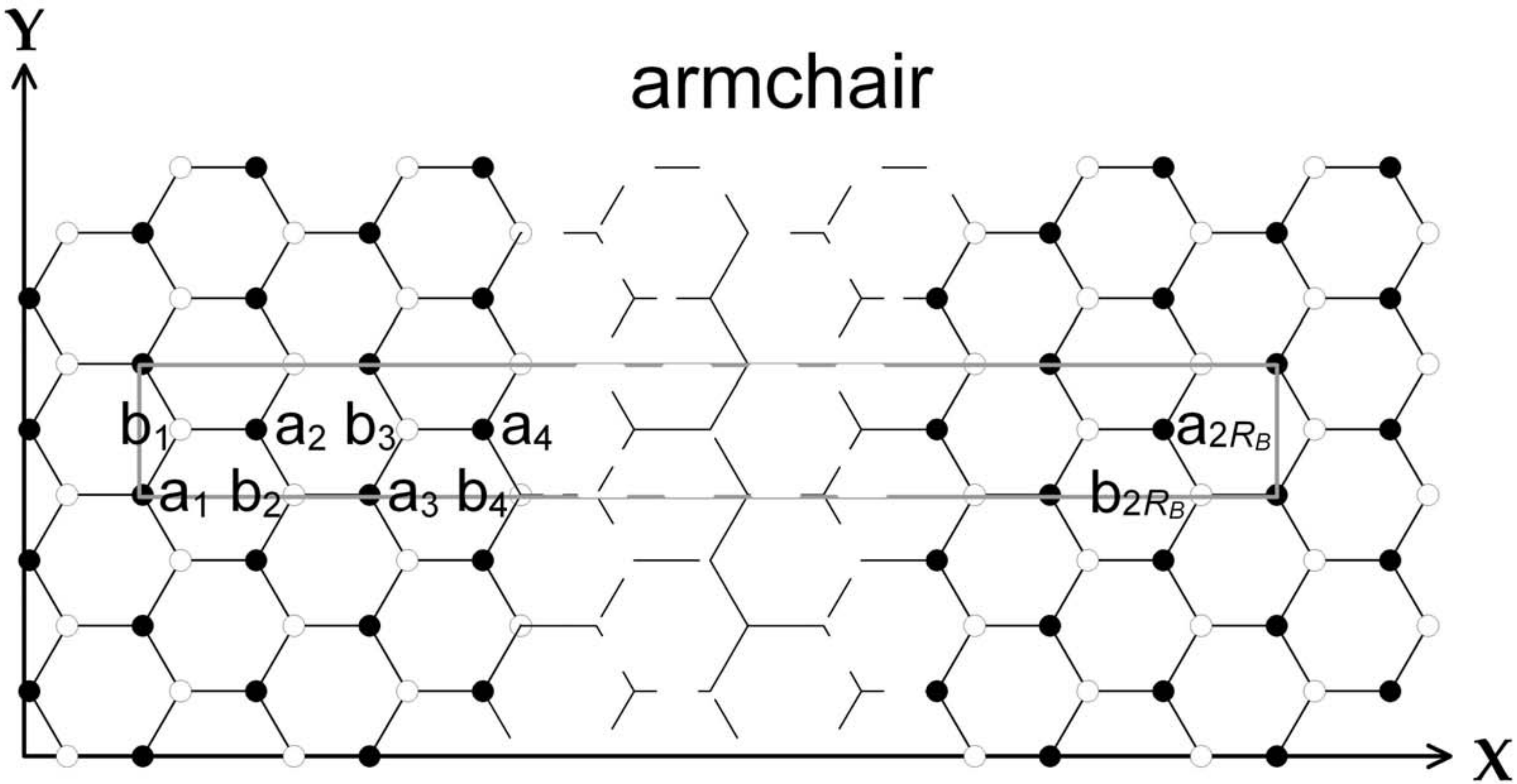
$$\vec{B} = \left(0, 0, B\sin\left(k_B x\right)\right) \quad \vec{A} = \left(0, \frac{-B}{k_B}\cos\left(k_B x\right), 0\right)$$

Along the armchair direction:

$$k_B = 2\pi / l_B = 2\pi / 3b' R_B$$

Along the zigzag direction:

$$k_B = 2\pi / l_B = 2\pi / \sqrt{3} b' R_B$$



Y
armchair
b1
a2 b3
a4
a1 b2
a3 b4
a2RB
b2RB
X

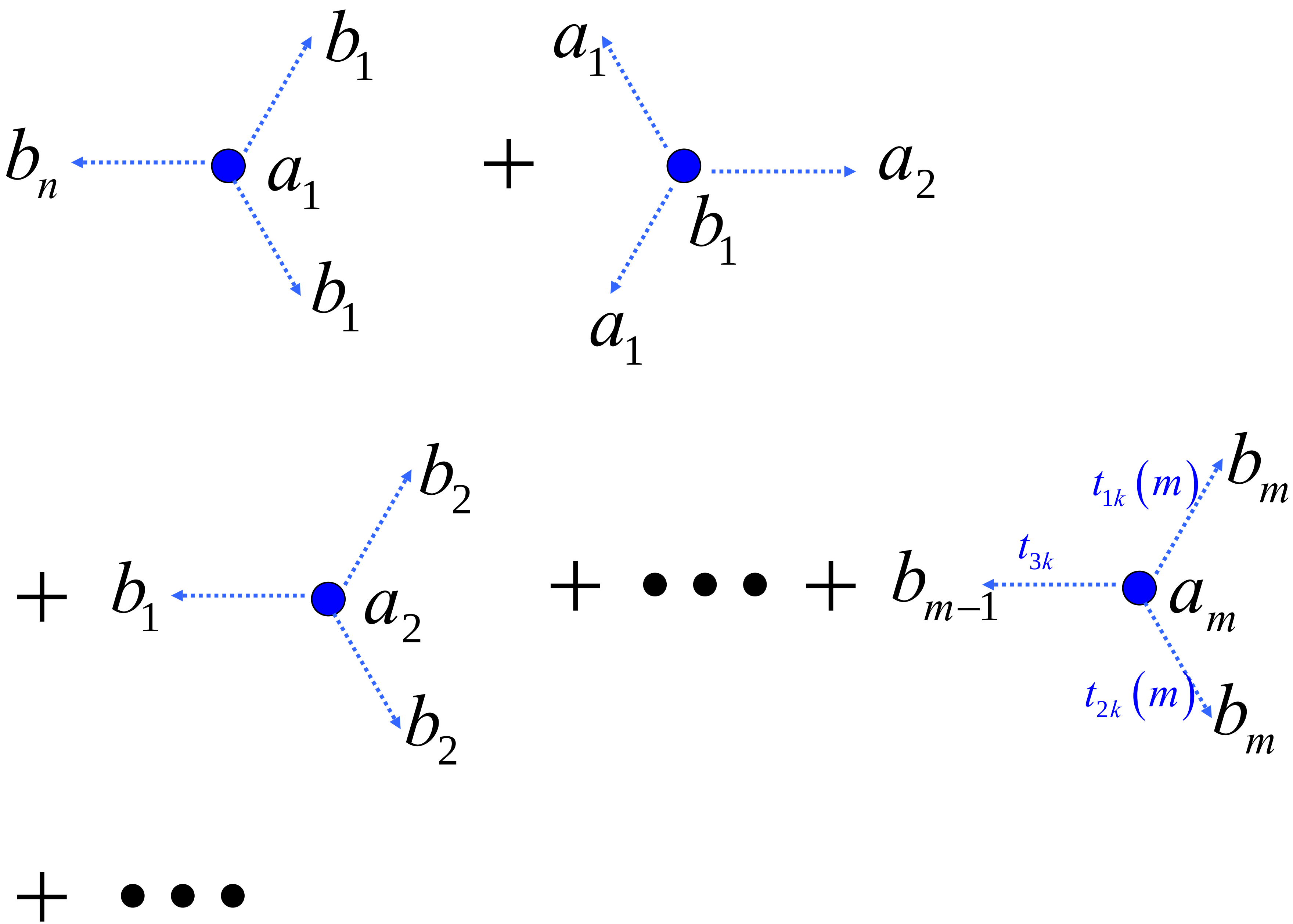
The positions of atoms a and b:

The original point $a_1=(0,0)$, then

$$\begin{cases} a_m^x = \dfrac{3b'}{2}(m-1) \\ b_m^x = \dfrac{3b'}{2}(m-1)+\dfrac{b'}{2} \end{cases} \qquad (11)$$

The π-electronic wave functions

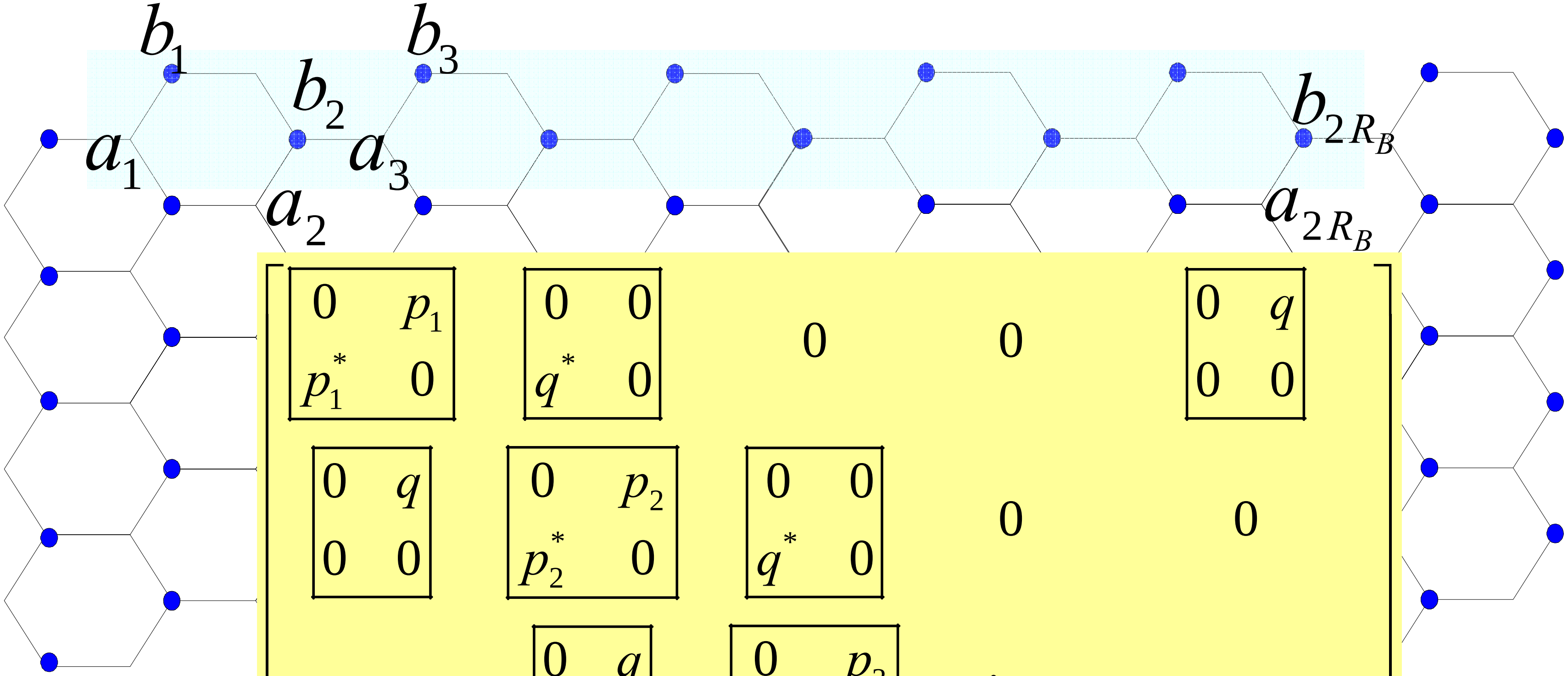
$$\left|\Psi_{\mathbf{k}}\right\rangle = \sum_{m=1}^{2R_B} C_{a\mathbf{k}}^{m}\left|a_{m\mathbf{k}}\right\rangle + C_{b\mathbf{k}}^{m}\left|b_{m\mathbf{k}}\right\rangle \quad \textbf{(12)}$$


b1
bn
a1
b1
+
a1
a2
b1
a1
b2
+ b1
a2
b2
+ • • • + bm−1
t3k
t1k (m)
bm
am
t2k (m)
bm
+ • • •

$$\langle a_{n\mathbf{k}} | H_B | a_{m\mathbf{k}} \rangle = \langle b_{n\mathbf{k}} | H_B | b_{m\mathbf{k}} \rangle = 0 \quad \textbf{(13)}$$

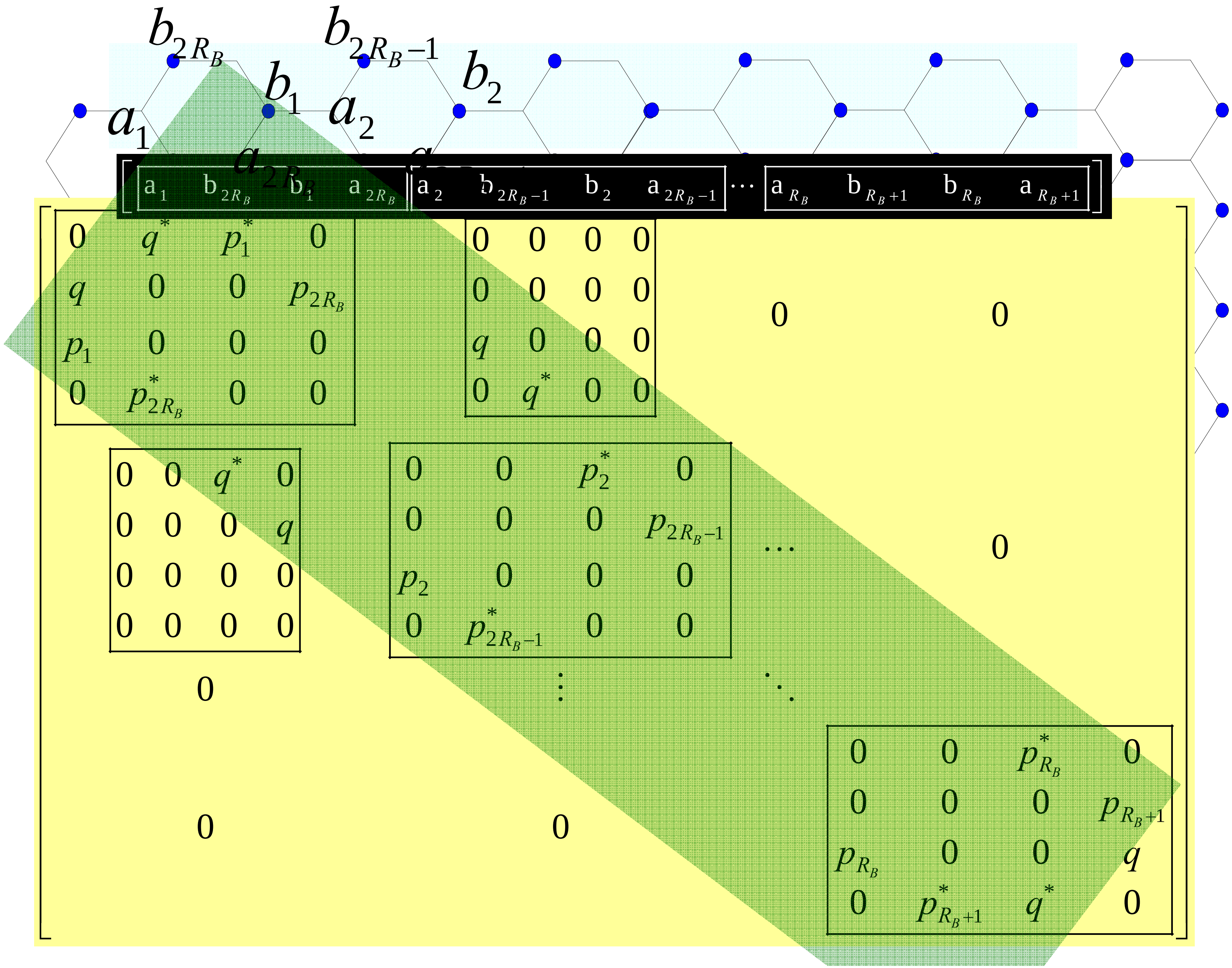
$$\langle a_{n\mathbf{k}} | H_B | b_{m\mathbf{k}} \rangle$$
$$= \left[t_{1k}(m) + t_{2k}(m) \right] \delta_{m,n} + t_{3k} \delta_{m,n-1} \quad \textbf{(14)}$$

$$
\begin{cases}
t_{1k}(m) = \gamma_0 \exp i\left[\left(\dfrac{k_x b'}{2} + \dfrac{k_y \sqrt{3} b'}{2}\right) + G_m\right] \\
t_{2k}(m) = \gamma_0 \exp i\left[\left(\dfrac{k_x b'}{2} - \dfrac{k_y \sqrt{3} b'}{2}\right) - G_m\right] \\
t_{3k} = \gamma_0 \exp\left(-ik_x b'\right) \\
\text{where } G_m = -\left[6\dfrac{\left(R_B\right)^2 \Phi}{\pi}\right]\cos\left[\pi\left(m - \dfrac{5}{6}\right)/R_B\right]\sin\left(\dfrac{\pi}{6R_B}\right), \\
\Phi = B/\Phi_0,\ b' = 1.42\ \text{Å}
\end{cases}
\qquad (15)
$$



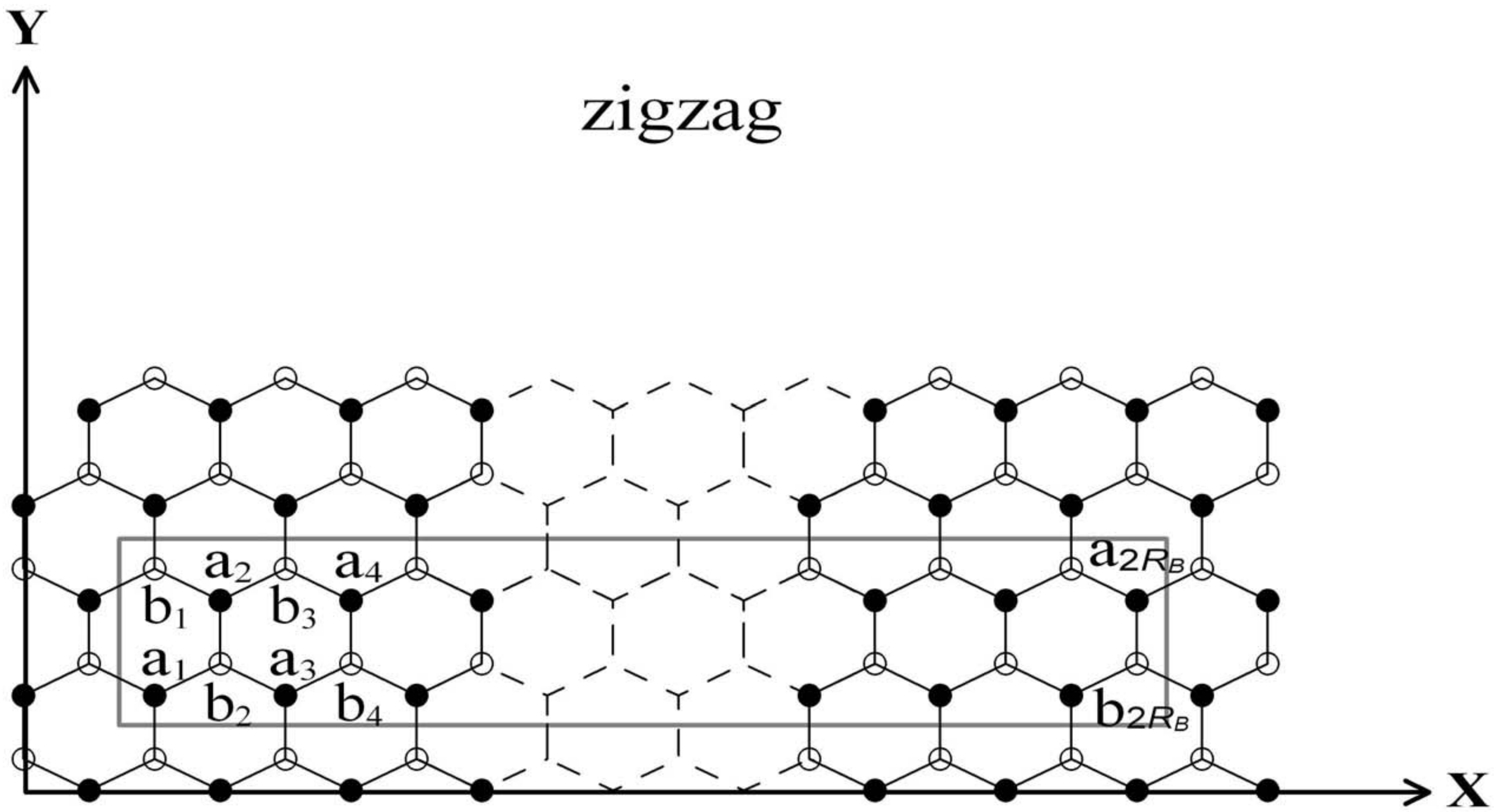
$$
\begin{bmatrix}
\boxed{\begin{matrix}0 & p_1\\ p_1^* & 0\end{matrix}} & \boxed{\begin{matrix}0 & 0\\ q^* & 0\end{matrix}} & 0 & 0 & \boxed{\begin{matrix}0 & q\\ 0 & 0\end{matrix}} \\
\boxed{\begin{matrix}0 & q\\ 0 & 0\end{matrix}} & \boxed{\begin{matrix}0 & p_2\\ p_2^* & 0\end{matrix}} & \boxed{\begin{matrix}0 & 0\\ q^* & 0\end{matrix}} & 0 & 0 \\
0 & \boxed{\begin{matrix}0 & q\\ 0 & 0\end{matrix}} & \boxed{\begin{matrix}0 & p_3\\ p_3^* & 0\end{matrix}} & \ddots & 0 \\
0 & 0 & \ddots & \ddots & \boxed{\begin{matrix}0 & 0\\ q^* & 0\end{matrix}} \\
\boxed{\begin{matrix}0 & 0\\ q^* & 0\end{matrix}} & 0 & 0 & \boxed{\begin{matrix}0 & q\\ 0 & 0\end{matrix}} & \boxed{\begin{matrix}0 & p_{2R_B}\\ p_{2R_B}^* & 0\end{matrix}}
\end{bmatrix}
$$

$\mathrm{p}_m = t_{1\mathrm{k}}\,(m$



$$
\begin{bmatrix}
\begin{pmatrix} 0 & q^* & p_1^* & 0 \\ q & 0 & 0 & p_{2R_B} \\ p_1 & 0 & 0 & 0 \\ 0 & p_{2R_B}^* & 0 & 0 \end{pmatrix} &
\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ q & 0 & 0 & 0 \\ 0 & q^* & 0 & 0 \end{pmatrix} & 0 & 0 \\
\begin{pmatrix} 0 & 0 & q^* & 0 \\ 0 & 0 & 0 & q \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} &
\begin{pmatrix} 0 & 0 & p_2^* & 0 \\ 0 & 0 & 0 & p_{2R_B-1} \\ p_2 & 0 & 0 & 0 \\ 0 & p_{2R_B-1}^* & 0 & 0 \end{pmatrix} & \cdots & 0 \\
0 & \vdots & \ddots & \\
0 & 0 & & \begin{pmatrix} 0 & 0 & p_{R_B}^* & 0 \\ 0 & 0 & 0 & p_{R_B+1} \\ p_{R_B} & 0 & 0 & q \\ 0 & p_{R_B+1}^* & q^* & 0 \end{pmatrix}
\end{bmatrix}
$$

$$
\begin{pmatrix}
0 & q^* & p_1^* & 0 & \dots & \dots & 0 & 0 \\
q & 0 & 0 & p_{2R_B} & 0 & \dots & \dots & 0 \\
p_1 & 0 & 0 & 0 & q & 0 & \dots & 0 \\
0 & p_{2R_B}^* & 0 & 0 & 0 & q^* & 0 & 0 \\
\vdots & \ddots & q^* & 0 & 0 & \ddots & \ddots & 0 \\
\vdots & \dots & \ddots & q & \ddots & \ddots & 0 & p_{R_B+1} \\
0 & \vdots & \vdots & \ddots & \ddots & 0 & \ddots & q \\
0 & 0 & 0 & 0 & 0 & p_{R_B+1}^* & q^* & 0
\end{pmatrix}, \quad (16)
$$

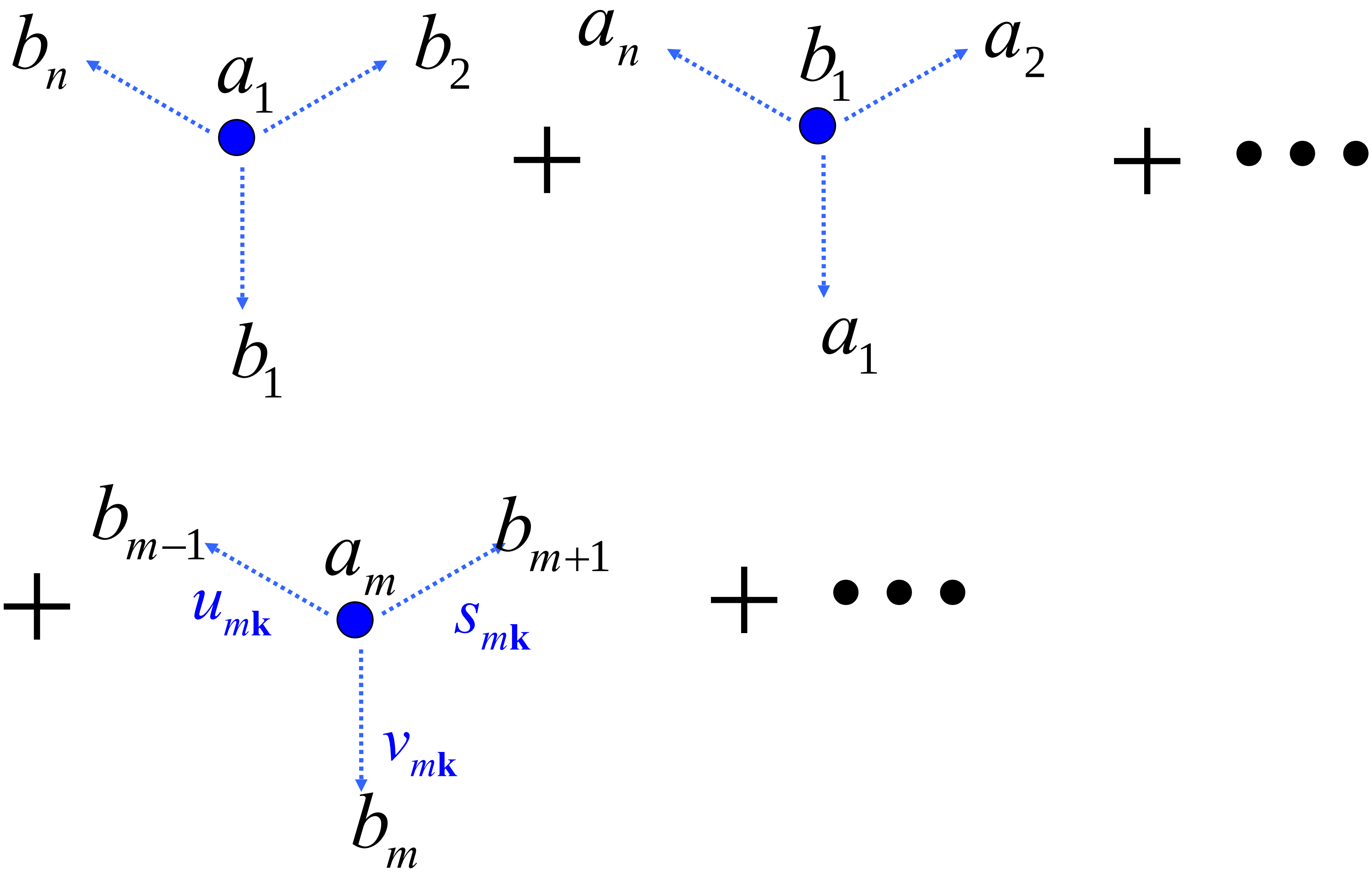


Y
zigzag
a2
a4
a2RB
b1
b3
a1
a3
b2
b4
b2RB
X

The positions of atoms a and b:

The original point $a_1=(0,0)$, then

$$\begin{cases} a_m^x = \dfrac{\sqrt{3}b'}{2}(m-1) \\ b_m^x = \dfrac{\sqrt{3}b'}{2}(m-1) \end{cases} \qquad (17)$$

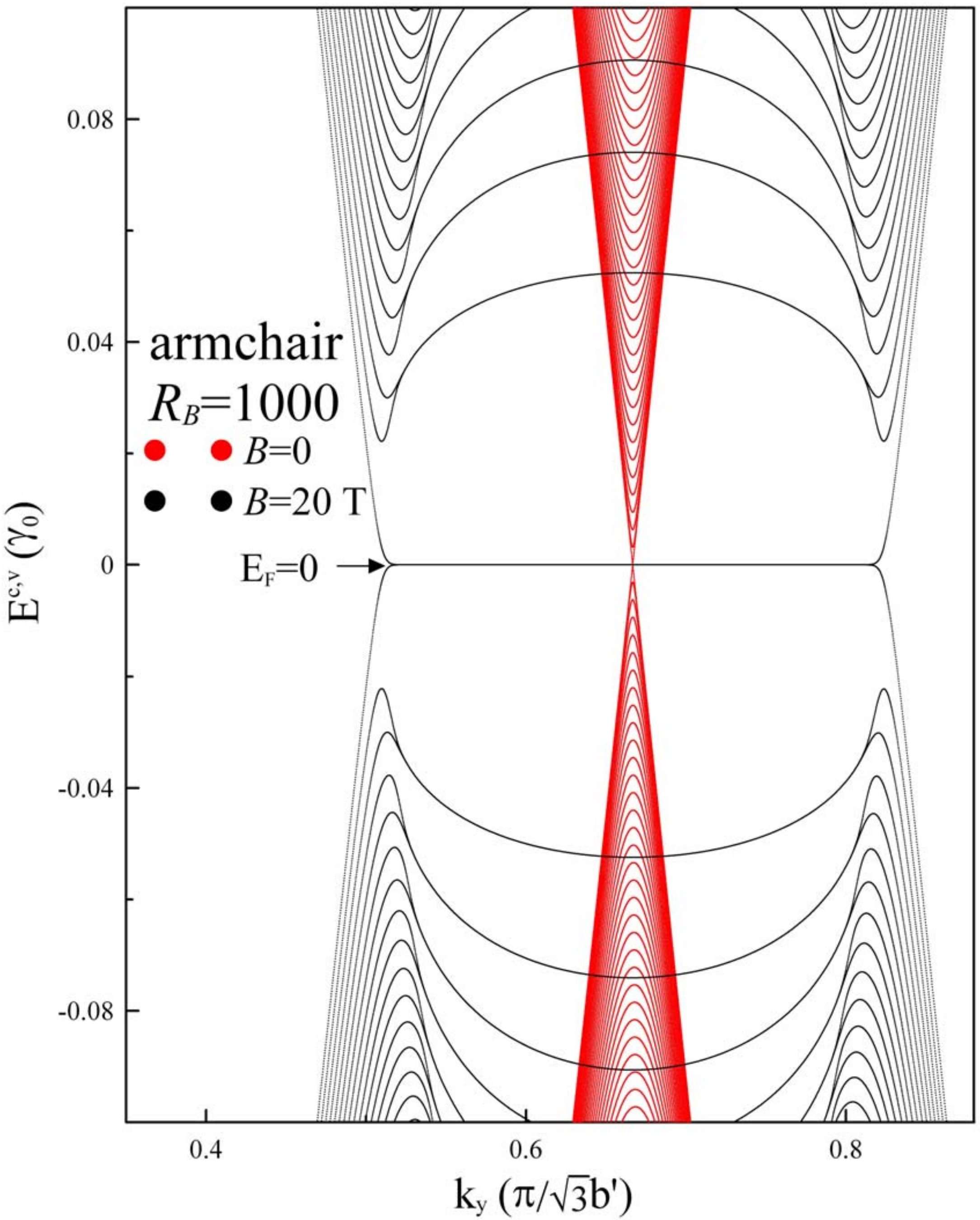


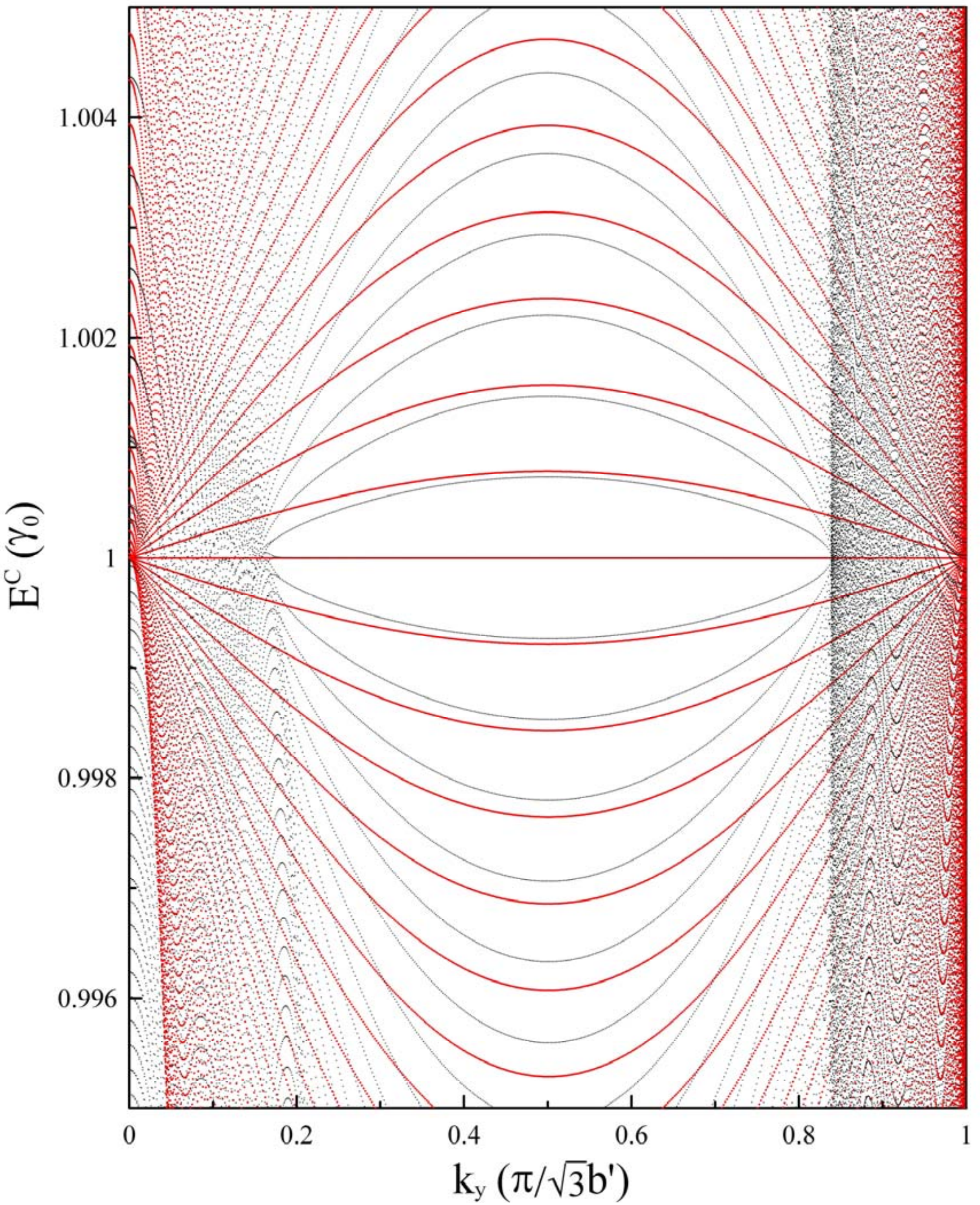
b_n
a_1
b_2
b_1
$+$
a_n
b_1
a_2
a_1
$+ \cdots$
$+$
b_{m-1}
a_m
b_{m+1}
$u_{m\mathbf{k}}$
$s_{m\mathbf{k}}$
$v_{m\mathbf{k}}$
b_m
$+ \cdots$

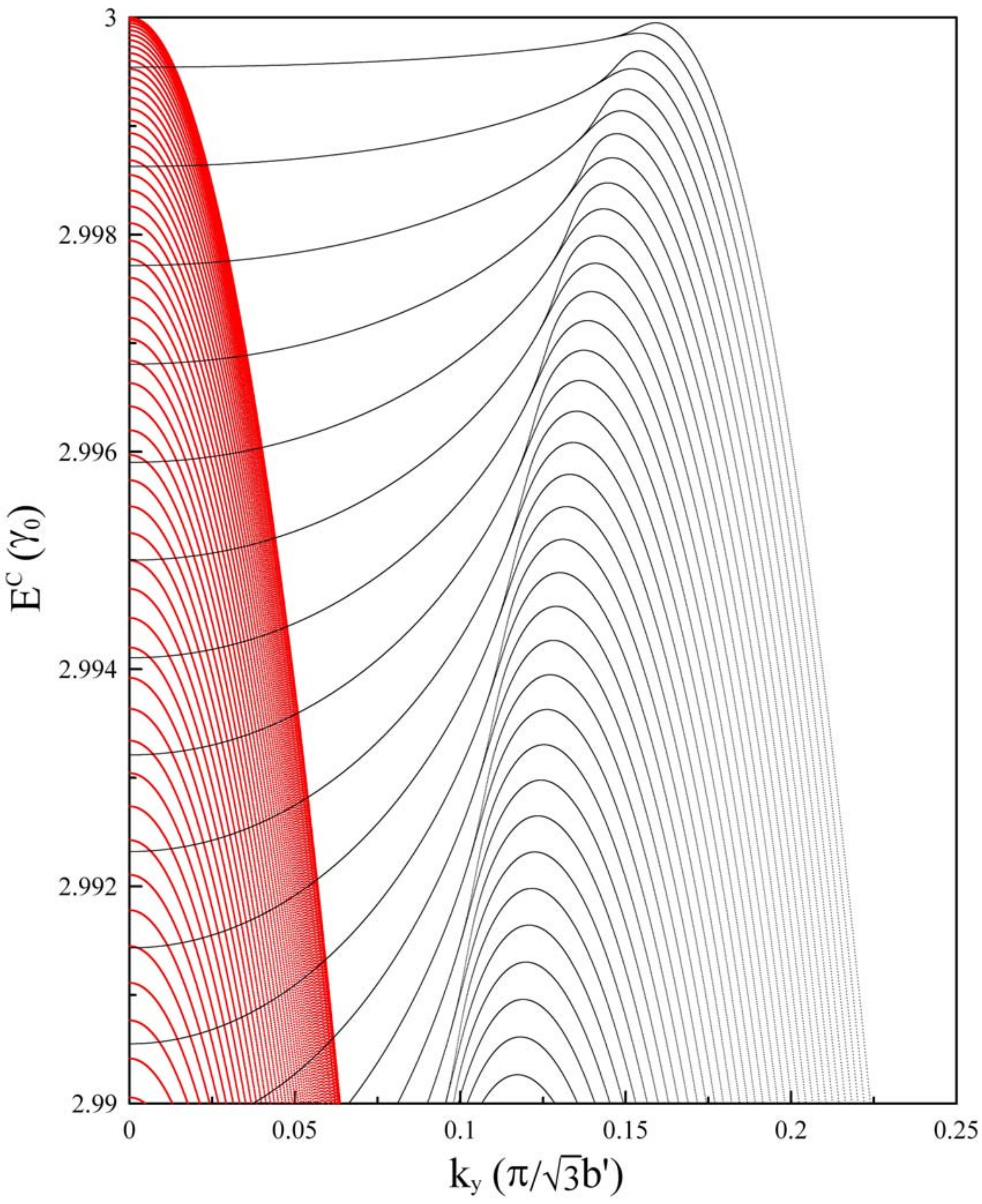
$$\left\langle a_{m\mathbf{k}} \middle| H_B \middle| a_{n\mathbf{k}} \right\rangle = \left\langle b_{m\mathbf{k}} \middle| H_B \middle| b_{n\mathbf{k}} \right\rangle = 0 \quad \textbf{(18)}$$

$$\left\langle a_{n\mathbf{k}} \middle| H_B \middle| b_{m\mathbf{k}} \right\rangle$$
$$= s_{m\mathbf{k}}\delta_{m,n+1} + u_{m\mathbf{k}}\delta_{m,n-1} + v_{m\mathbf{k}}\delta_{m,n} \quad \textbf{(19)}$$

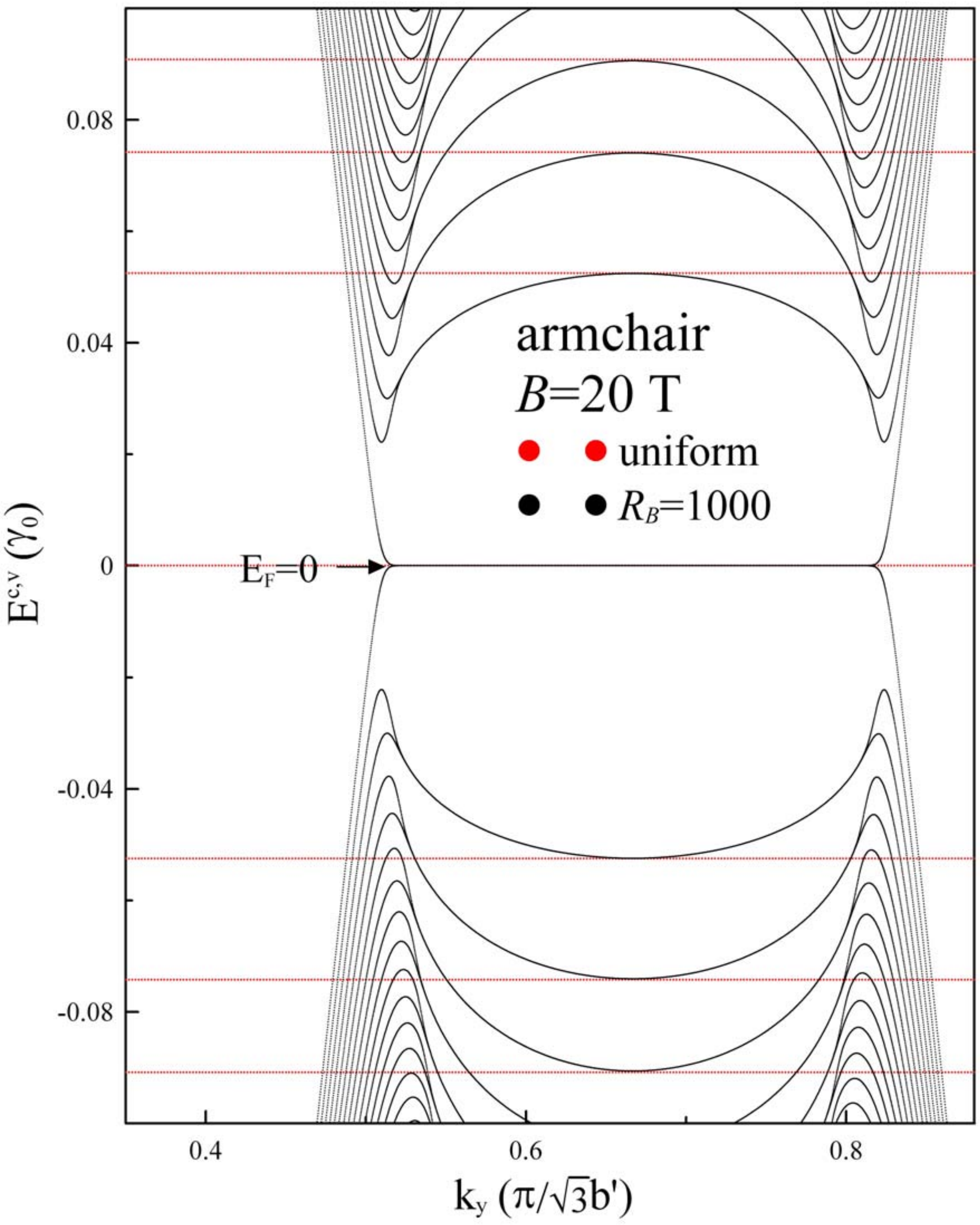
$$\begin{pmatrix}
0 & u_{2R_B}^* & v_1^* & 0 & s_1^* & 0 & \dots & 0 & 0 & 0 \\
u_{2R_B} & 0 & 0 & v_{2R_B} & 0 & s_{2R_B-1} & 0 & 0 & 0 & 0 \\
v_1 & 0 & 0 & s_{2R_B} & \ddots & \ddots & \ddots & \ddots & 0 & 0 \\
0 & v_{2R_B}^* & s_{2R_B}^* & 0 & \ddots & & & \ddots & 0 & \vdots \\
s_1 & 0 & \ddots & \ddots & \ddots & & & \ddots & s_{R_B-1}^* & 0 \\
0 & s_{2R_B-1}^* & \ddots & & & \ddots & \ddots & \ddots & 0 & s_{R_B+1} \\
\vdots & 0 & \ddots & & & \ddots & 0 & s_{R_B}^* & v_{R_B}^* & 0 \\
0 & 0 & \ddots & \ddots & \ddots & \ddots & s_{R_B} & 0 & 0 & v_{R_B+1} \\
0 & 0 & 0 & 0 & s_{R_B-1} & 0 & v_{R_B} & 0 & 0 & u_{R_B} \\
0 & 0 & 0 & \dots & 0 & s_{R_B+1}^* & 0 & v_{R_B+1}^* & u_{R_B}^* & 0
\end{pmatrix} \tag{20}$$


armchair
R_B=1000
B=0
B=20 T
E_F=0
$E^{c,v}$ (γ_0)
0.08
0.04
0
-0.04
-0.08
0.4
0.6
0.8
k_y ($\pi/\sqrt{3}b'$)

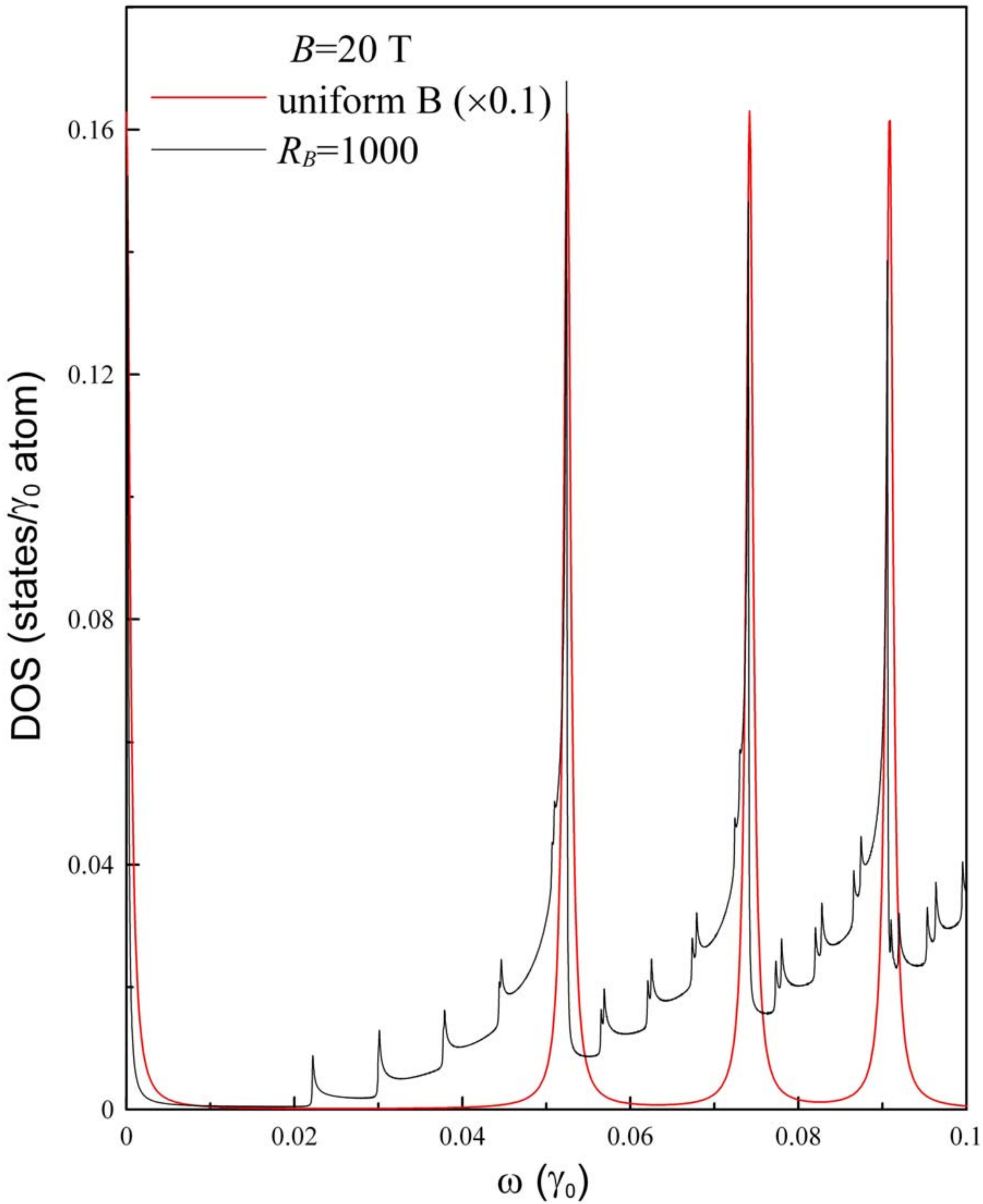

1.004
1.002
1
0.998
0.996
E^C (γ0)
0
0.2
0.4
0.6
0.8
1
ky (π/√3b')



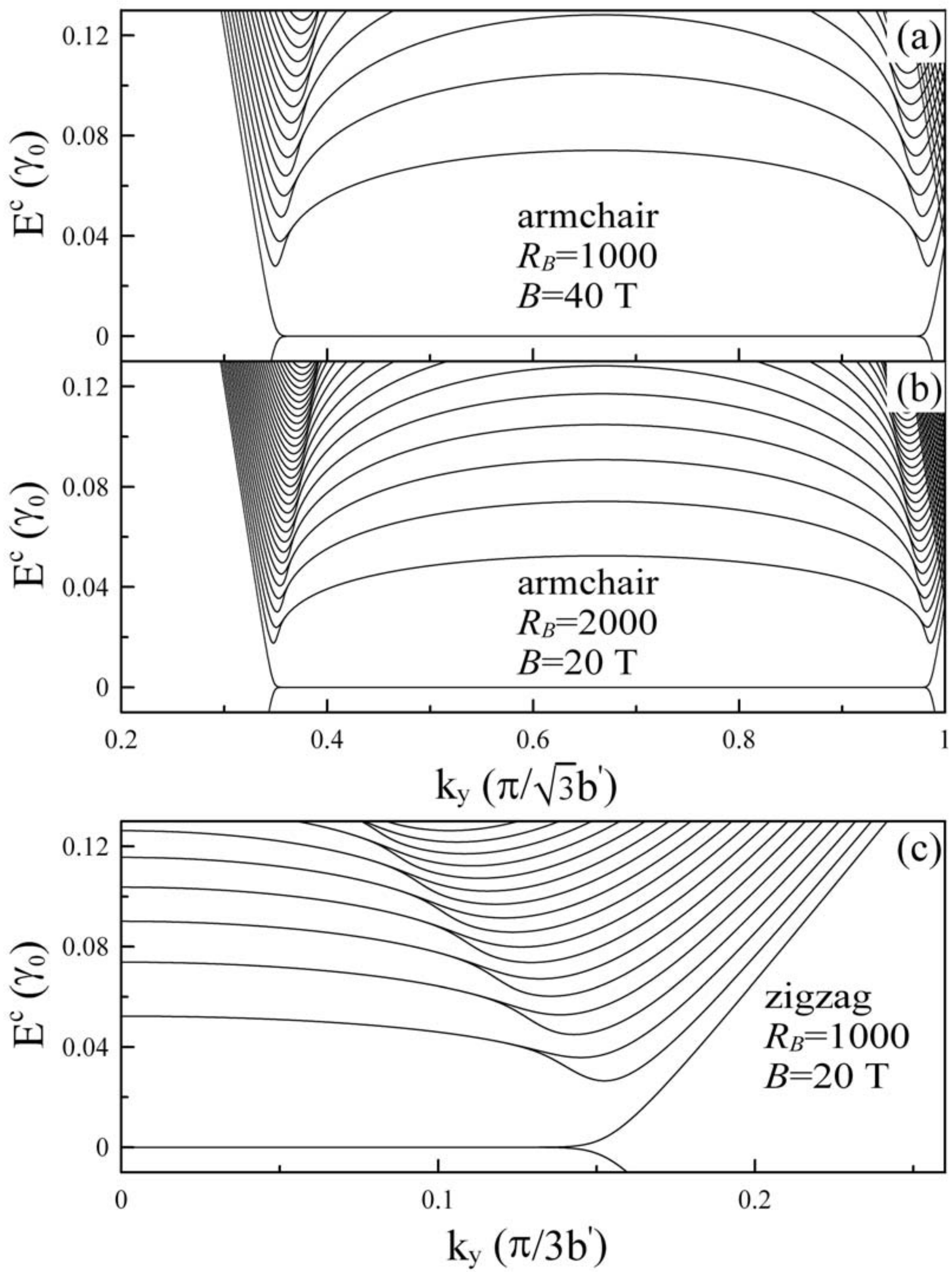
3
2.998
2.996
2.994
2.992
2.99
E^C (γ_0)
0
0.05
0.1
0.15
0.2
0.25
k_y ($\pi/\sqrt{3}b'$)

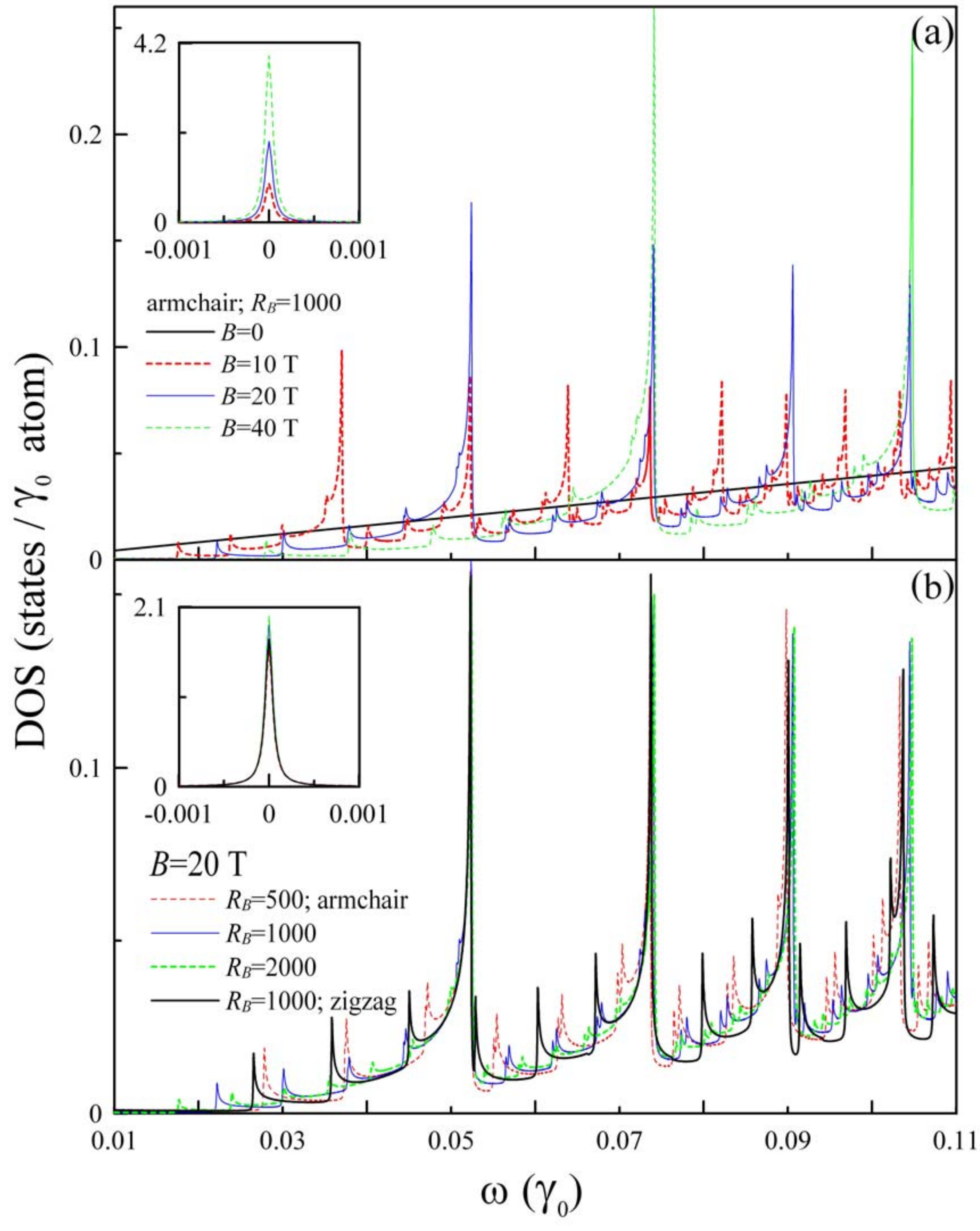


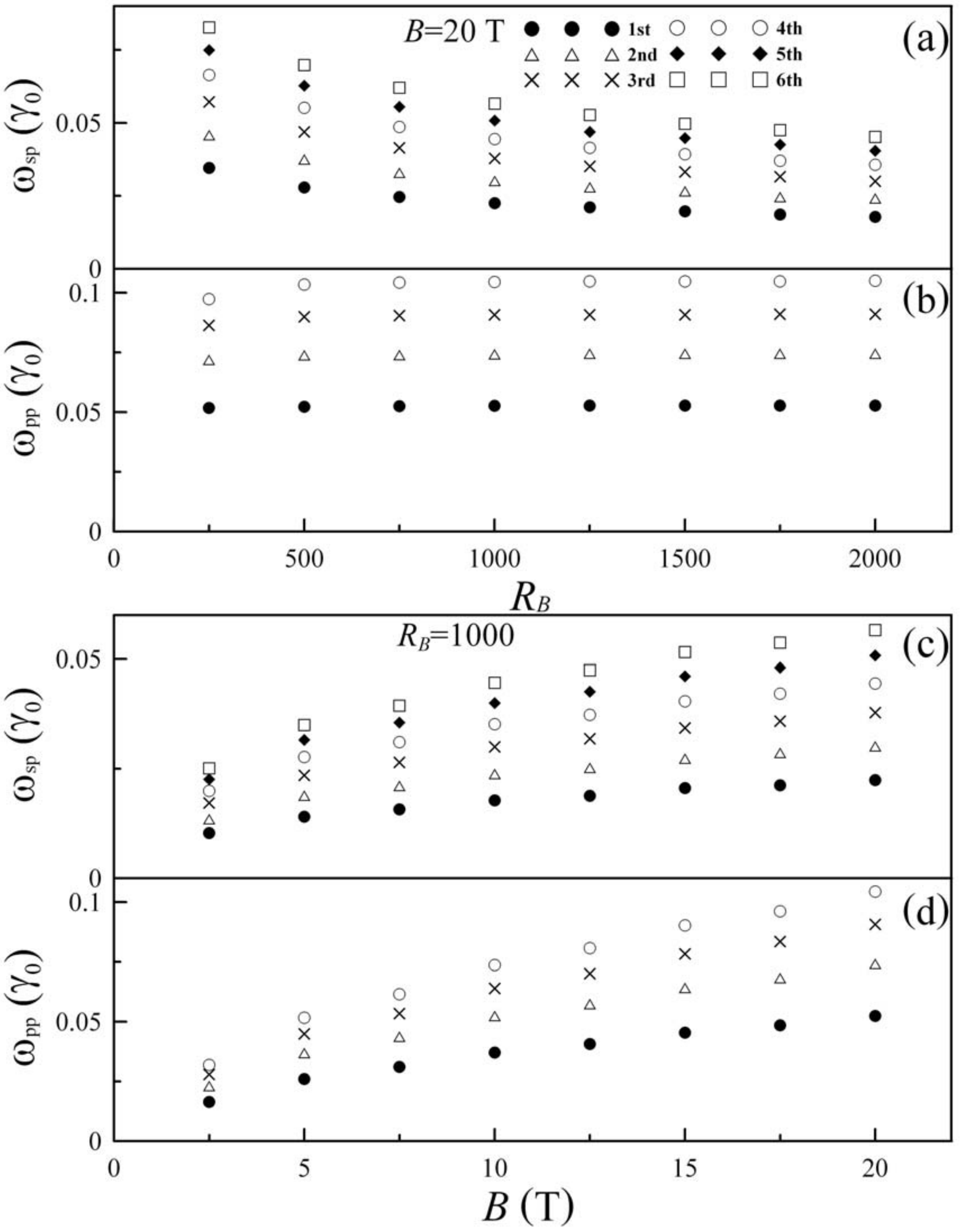
armchair
B=20 T
uniform
R_B=1000
E_F=0
0.08
0.04
0
-0.04
-0.08
0.4
0.6
0.8
E^{c,v} (γ_0)
k_y (π/√3b')



B=20 T
uniform B (×0.1)
R_B=1000
DOS (states/γ0 atom)
0
0.04
0.08
0.12
0.16
0
0.02
0.04
0.06
0.08
0.1
ω (γ0)


(a)
armchair
R_B=1000
B=40 T
(b)
armchair
R_B=2000
B=20 T
(c)
zigzag
R_B=1000
B=20 T
E^c (γ_0)
k_y ($\pi/\sqrt{3}b'$)
k_y ($\pi/3b'$)
0.12
0.08
0.04
0
0.2
0.4
0.6
0.8
1
0.1


(a)
4.2
0.2
0
-0.001
0
0.001
armchair; R_B=1000
B=0
B=10 T
B=20 T
B=40 T
0.1
0
(b)
2.1
0.1
0
-0.001
0
0.001
B=20 T
R_B=500; armchair
R_B=1000
R_B=2000
R_B=1000; zigzag
0
0.01
0.03
0.05
0.07
0.09
0.11
DOS (states / γ_0 atom)
ω (γ_0)

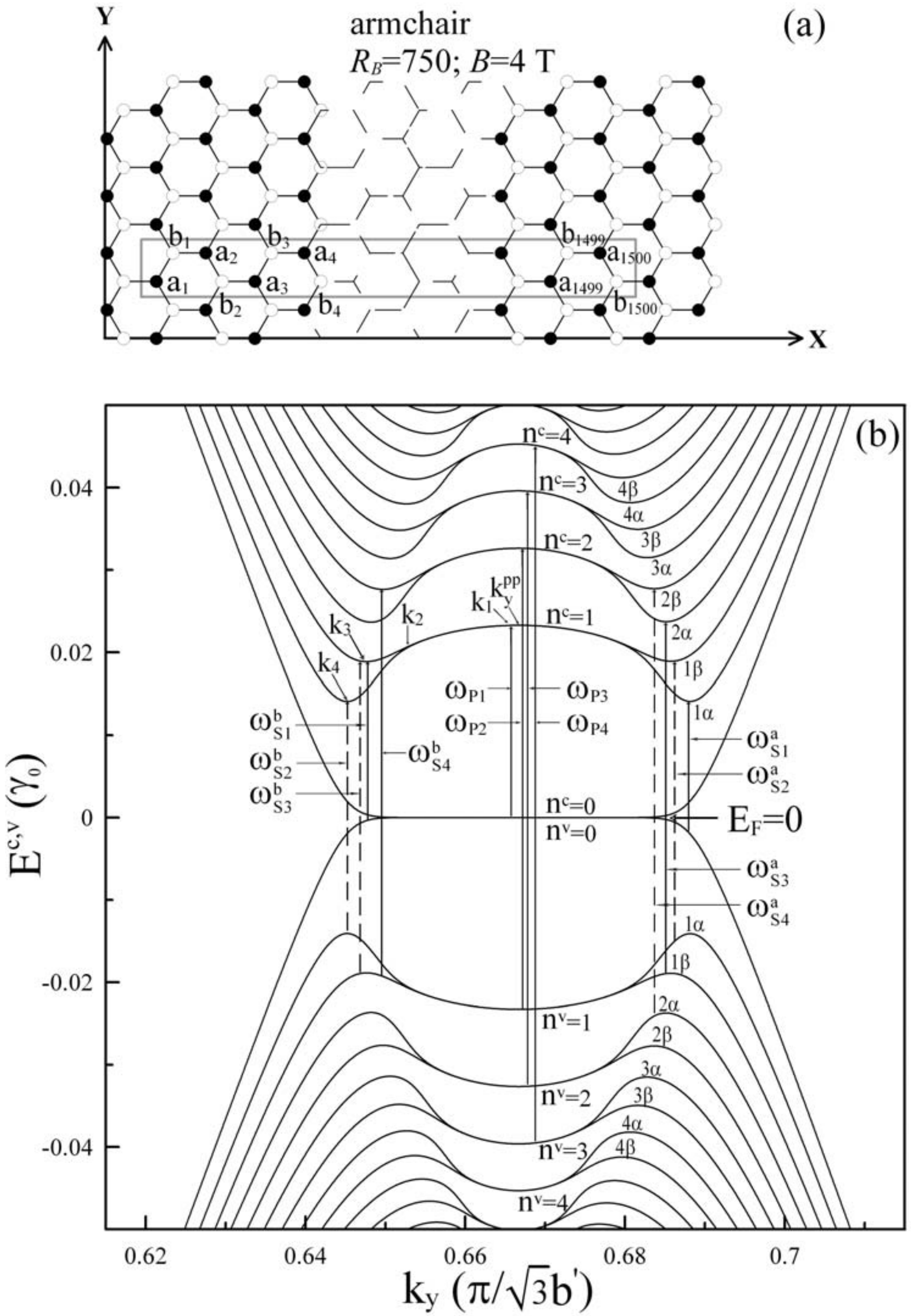


B=20 T
1st
2nd
3rd
4th
5th
6th
(a)
(b)
(c)
(d)
ωsp (γ0)
ωpp (γ0)
0
0.05
0.1
0
500
1000
1500
2000
R_B
R_B=1000
0
5
10
15
20
B (T)

Rewrite Eq. (12)

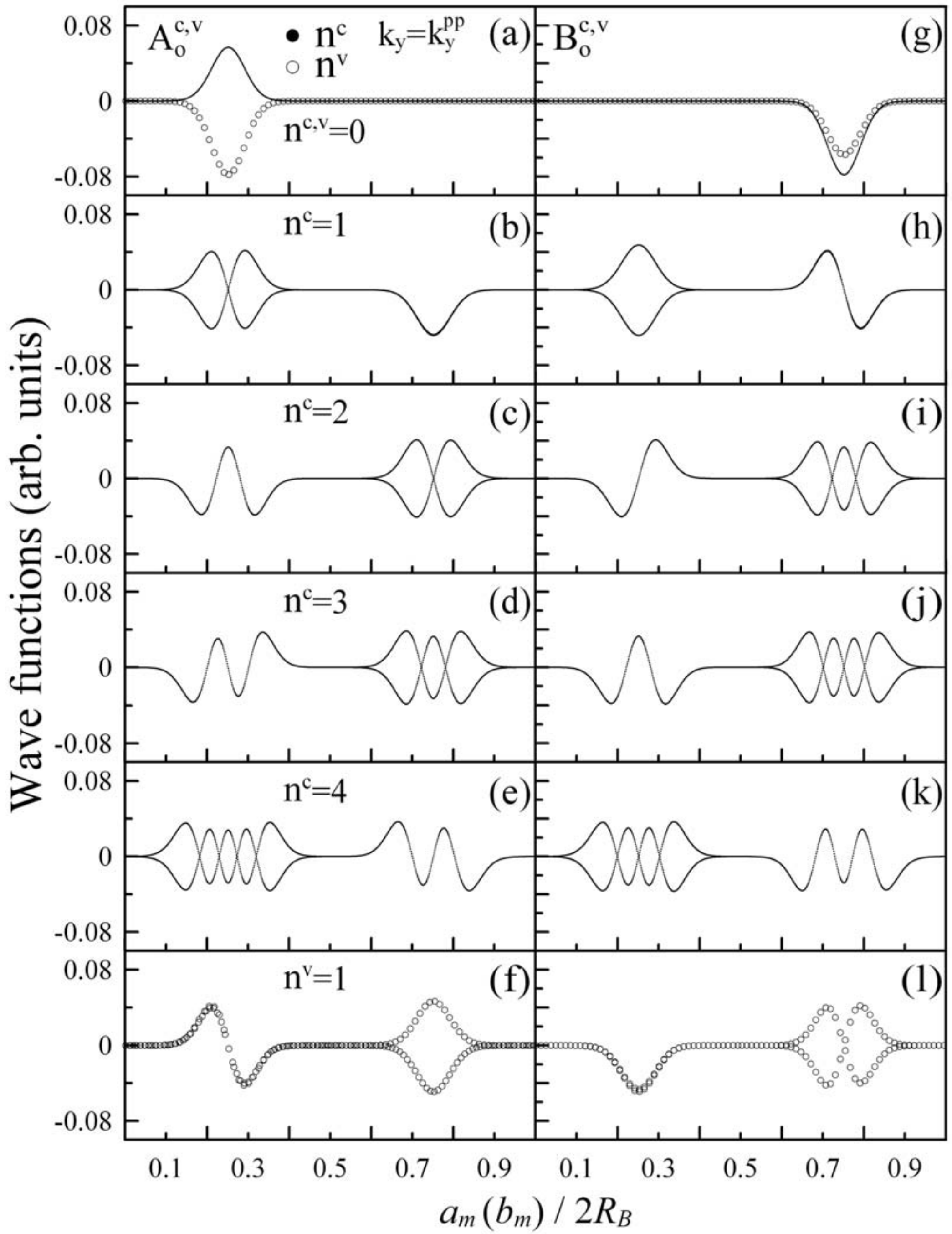
The wave function becomes:

$$\left|\Psi_{\mathbf{k}}^{c,v}\right\rangle = \sum_{m=1}^{2R_B-1}\left(A_o^{c,v}\left|a_{m\mathbf{k}}\right\rangle + B_o^{c,v}\left|b_{m\mathbf{k}}\right\rangle\right) + \sum_{m=2}^{2R_B}\left(A_e^{c,v}\left|a_{m\mathbf{k}}\right\rangle + B_e^{c,v}\left|b_{m\mathbf{k}}\right\rangle\right) \quad \textbf{(21)}$$

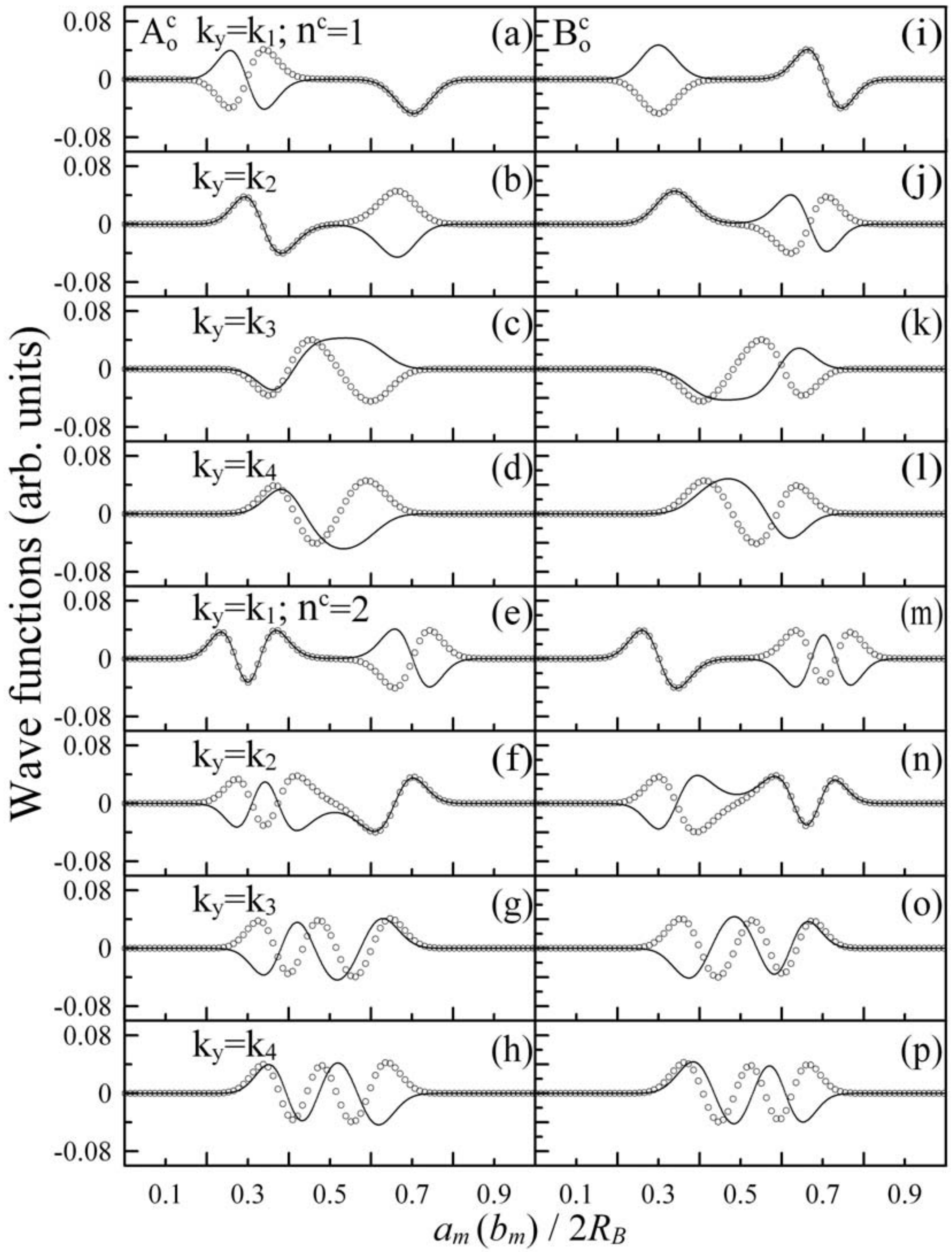


Effective quantum number :

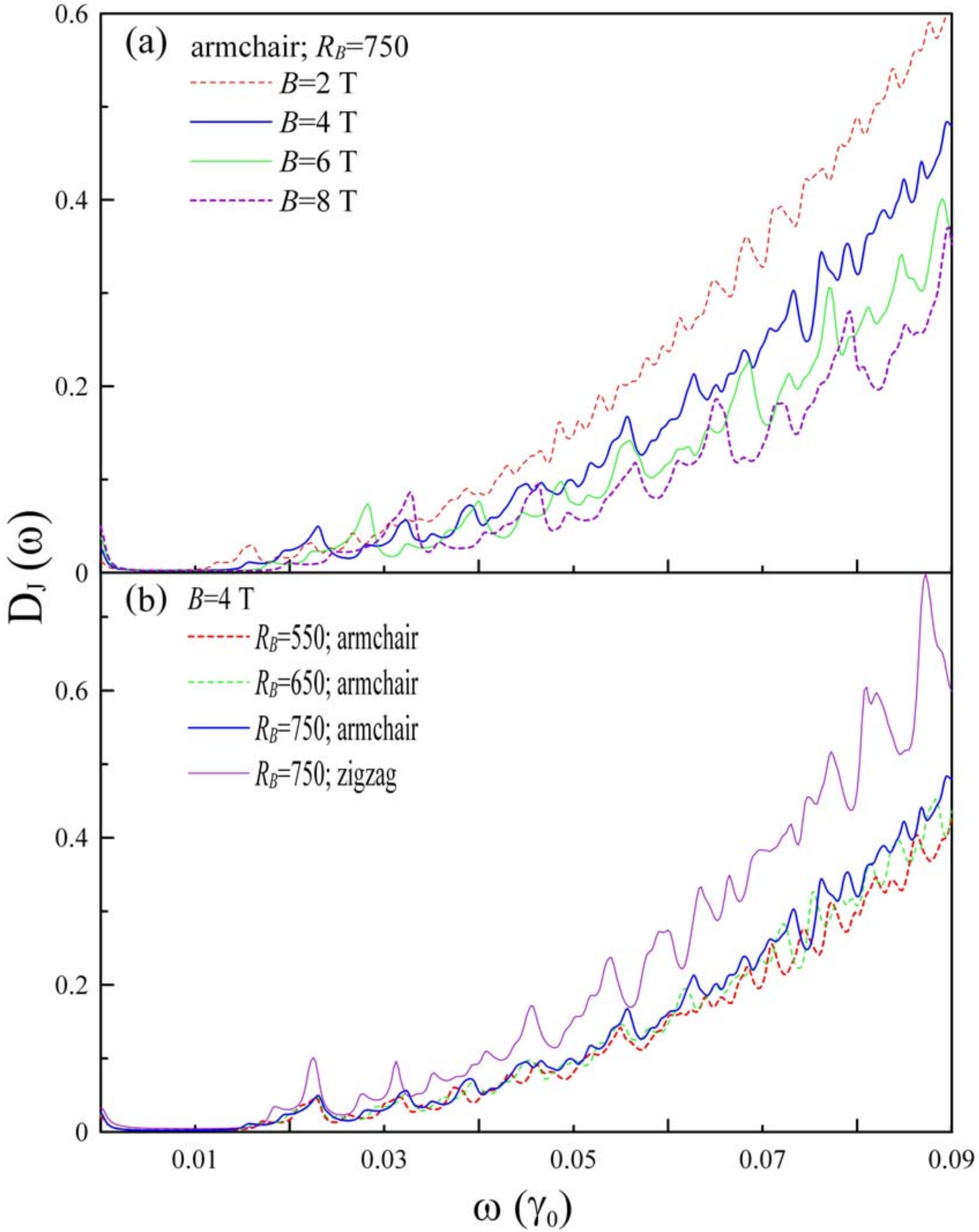
$$n^{c,v} = \tilde{n} - 1 \text{ for the } \tilde{n}\text{th QLL}$$



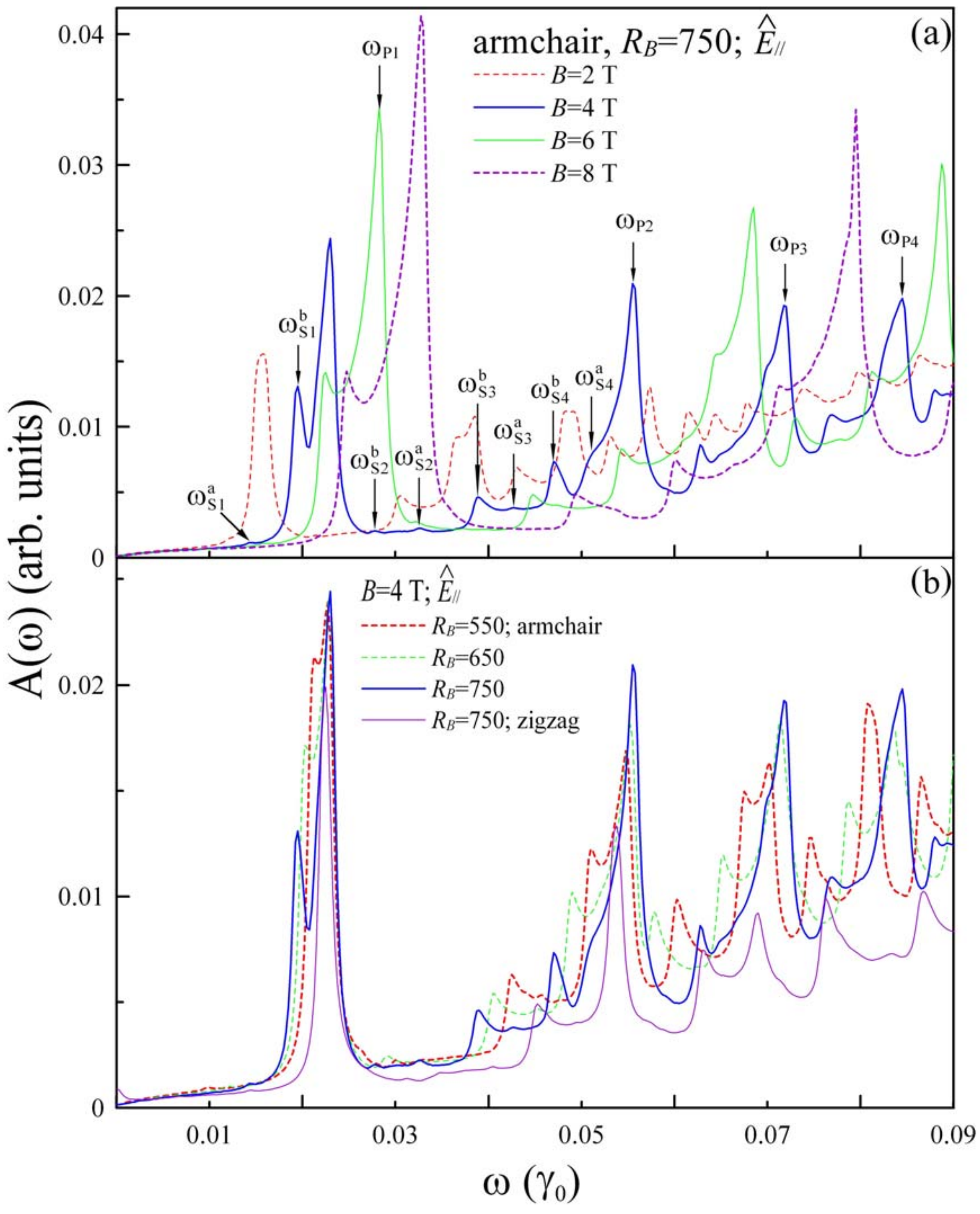
$A_o^{c,v}$
n^c
n^v
$k_y=k_y^{pp}$
(a)
$n^{c,v}=0$
$B_o^{c,v}$
(g)
$n^c=1$
(b)
(h)
$n^c=2$
(c)
(i)
$n^c=3$
(d)
(j)
$n^c=4$
(e)
(k)
$n^v=1$
(f)
(l)
0.08
0
-0.08
Wave functions (arb. units)
0.1
0.3
0.5
0.7
0.9
$a_m\,(b_m)\,/\,2R_B$



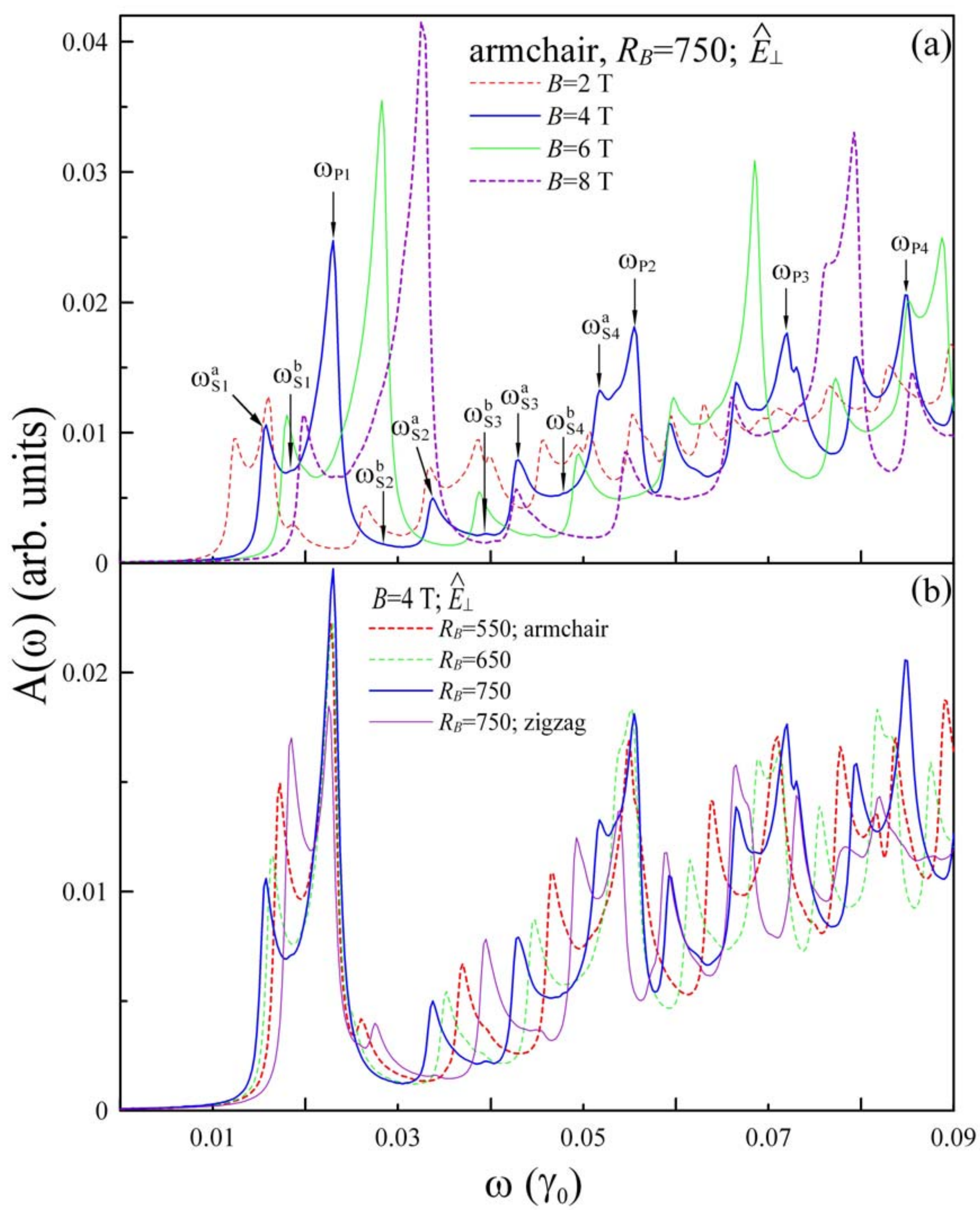
A_o^c k_y=k_1; n^c=1
(a)
B_o^c
(i)
k_y=k_2
(b)
(j)
k_y=k_3
(c)
(k)
k_y=k_4
(d)
(l)
k_y=k_1; n^c=2
(e)
(m)
k_y=k_2
(f)
(n)
k_y=k_3
(g)
(o)
k_y=k_4
(h)
(p)
0.08
0
-0.08
Wave functions (arb. units)
0.1
0.3
0.5
0.7
0.9
a_m (b_m) / $2R_B$



(a)
armchair; R_B=750
B=2 T
B=4 T
B=6 T
B=8 T
(b)
B=4 T
R_B=550; armchair
R_B=650; armchair
R_B=750; armchair
R_B=750; zigzag
D_J (ω)
ω (γ_0)
0
0.2
0.4
0.6
0.01
0.03
0.05
0.07
0.09



armchair, R_B=750; $\hat{E}_{//}$
(a)
B=2 T
B=4 T
B=6 T
B=8 T
ω_{P1}
ω_{P2}
ω_{P3}
ω_{P4}
ω^b_{S1}
ω^a_{S1}
ω^b_{S2}
ω^a_{S2}
ω^b_{S3}
ω^a_{S3}
ω^b_{S4}
ω^a_{S4}
(b)
B=4 T; $\hat{E}_{//}$
R_B=550; armchair
R_B=650
R_B=750
R_B=750; zigzag
A(ω) (arb. units)
ω (γ_0)
0
0.01
0.02
0.03
0.04
0.05
0.07
0.09



armchair, R_B=750; $\hat{E}_\perp$
(a)
B=2 T
B=4 T
B=6 T
B=8 T
ω_{P1}
ω_{P2}
ω_{P3}
ω_{P4}
ω_{S1}^a
ω_{S1}^b
ω_{S2}^a
ω_{S2}^b
ω_{S3}^a
ω_{S3}^b
ω_{S4}^a
ω_{S4}^b
B=4 T; $\hat{E}_\perp$
(b)
R_B=550; armchair
R_B=650
R_B=750
R_B=750; zigzag
A(ω) (arb. units)
ω (γ_0)
0
0.01
0.02
0.03
0.04
0.05
0.07
0.09

Optical selection rule:

For ω_{P} **:** $|\Delta n| = |n^c - n^v| = 1$

For ω_{SP} **:** $|\Delta n| = |n^c - n^v| = 1,\ \mathbf{0}$

Velocity matrix element:

$$M^{cv}=\left\langle \Psi^{c}\left(\mathbf{k},\tilde{n}\right)\right|\frac{\hat{\mathbf{E}}\bullet\mathbf{P}}{m_e}\left|\Psi^{v}\left(\mathbf{k},\tilde{n}'\right)\right\rangle$$

By gradient approximation

$$M^{cv}\approx$$

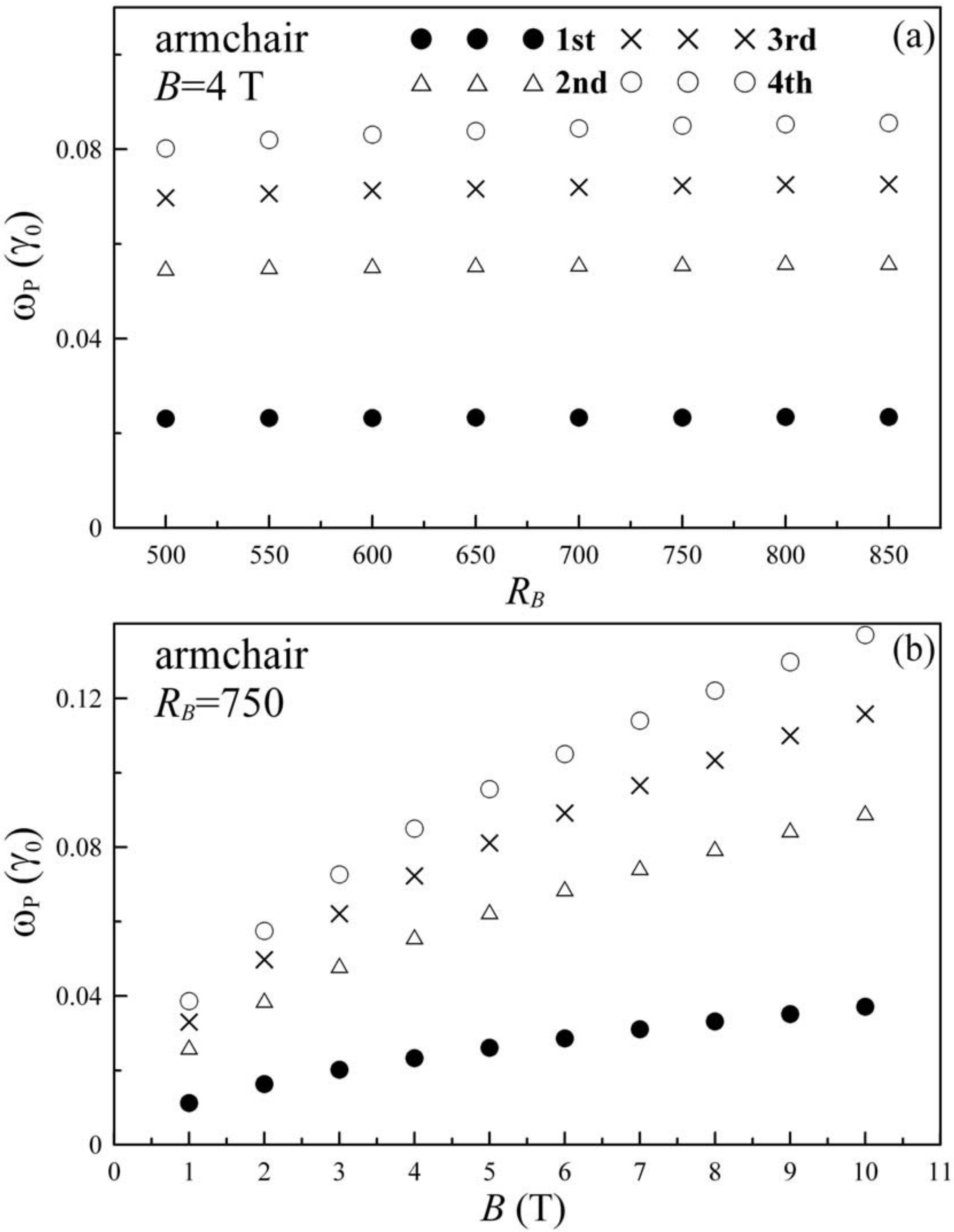
$$\sum_{m,m'=1}^{2R_B}\left[\left(A_o^c+A_e^c\right)^*\left(B_{o'}^v+B_{e'}^v\right)+\left(B_o^c+B_e^c\right)^*\left(A_{o'}^v+A_{e'}^v\right)\right]$$

$$\times\nabla_{\mathbf{k}}\left\langle a_{m\mathbf{k}}\right|H_B\left|b_{m'\mathbf{k}}\right\rangle \qquad \textbf{(22)}$$

$$M_{AB}^{cv}\equiv\left(A_o^c+A_e^c\right)^*\left(B_{o'}^v+B_{e'}^v\right)+\left(B_o^c+B_e^c\right)^*\left(A_{o'}^v+A_{e'}^v\right) \quad \textbf{(23)}$$

$$M_x^{cv}=\left|b'\gamma_0\left[\cos\left(\sqrt{3}b'k_y/2+G_m\right)-1\right]\right| \text{ for } \hat{\mathbf{E}}\parallel\hat{\mathbf{x}} \qquad \textbf{(24.a)}$$

$$M_y^{cv}=\left|\sqrt{3}b'\gamma_0\left[\sin\left(\sqrt{3}b'k_y/2+G_m\right)\right]\right| \text{ for } \hat{\mathbf{E}}\perp\hat{\mathbf{x}} \qquad \textbf{(24.b)}$$


armchair
B=4 T
1st
2nd
3rd
4th
(a)
ωP (γ0)
0.08
0.04
0
500
550
600
650
700
750
800
850
RB
armchair
RB=750
(b)
ωP (γ0)
0.12
0.08
0.04
0
0
1
2
3
4
5
6
7
8
9
10
11
B (T)

Conclusions:

1. The low-energy electronic properties of a graphene monolayer are strongly affected by a modulated magnetic field, i.e., the dimensionality, energy dispersions, extra band-edge states, asymmetry, state degeneracy, and anisotropy of energy bands.
2. The low-frequency optical absorption spectra exhibit many prominent absorption peaks resulting from the original and extra band-edge states. They reveal different optical selection rules because their wave functions present different features.
3. The anisotropic properties in the modulated directions and electric polarization direction could be reflected by the optical absorption spectra.

Thank You