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Carbon-Related Systems and Nanomaterials

Frequency-Dependent Conductivity of Graphene Subjected to Modulation

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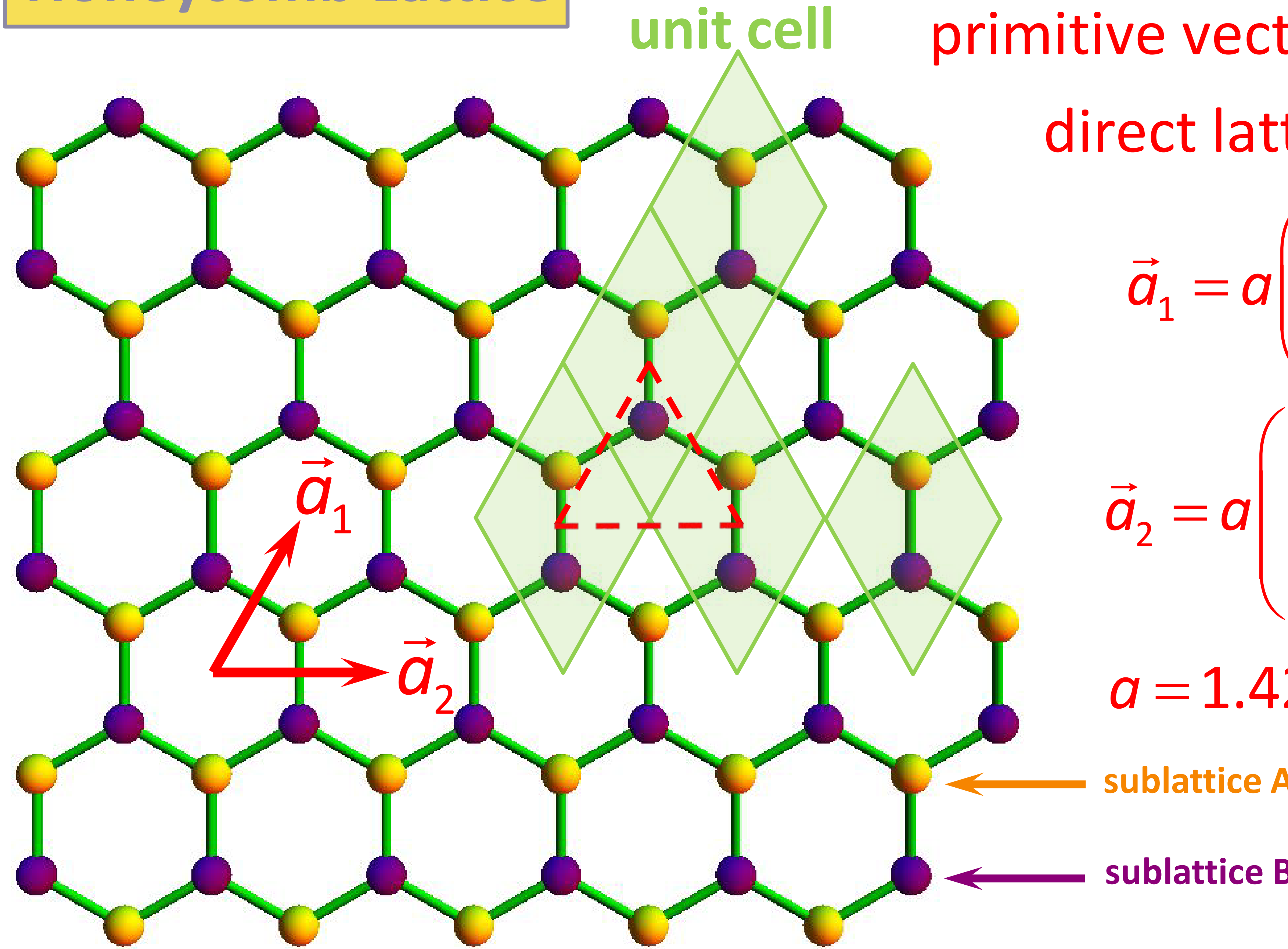
Honeycomb Lattice



primitive vectors

direct lattice

$$\vec{a}_1 = a\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\vec{a}_2 = a\begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}$$

$$a = 1.42\ \text{Å}$$

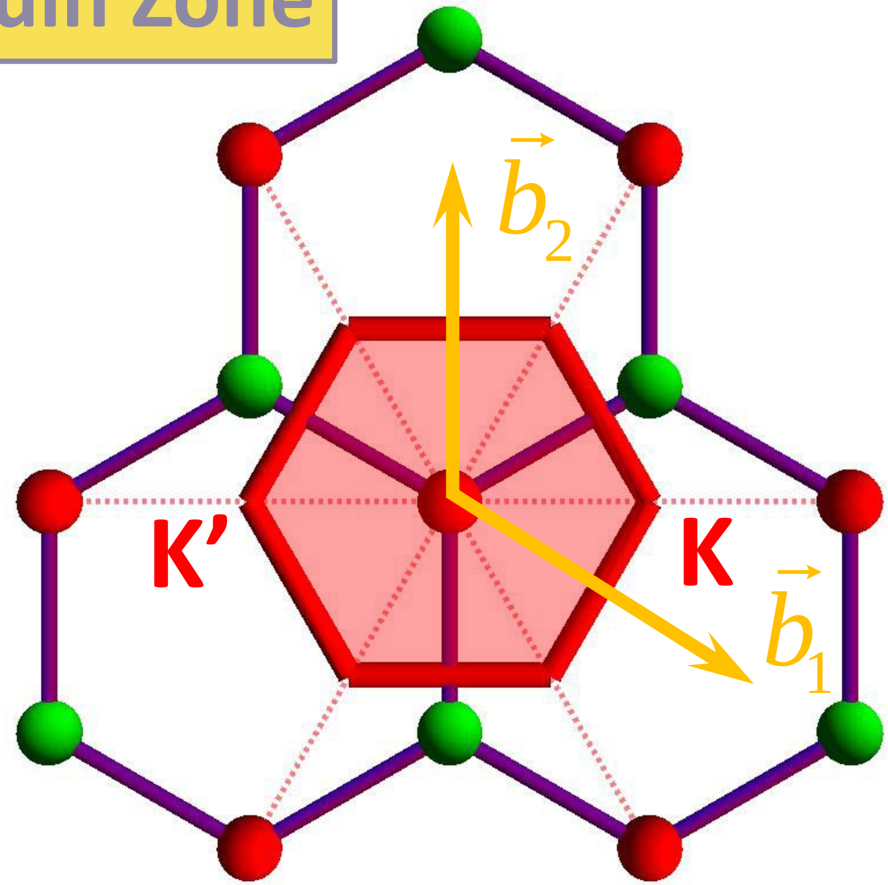
Reciprocal Lattice, Brillouin Zone

primitive vectors

reciprocal lattice

$$\vec{b}_1 = \frac{4\pi}{\sqrt{3}a}\begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix}$$

$$\vec{b}_2 = \frac{4\pi}{\sqrt{3}a}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



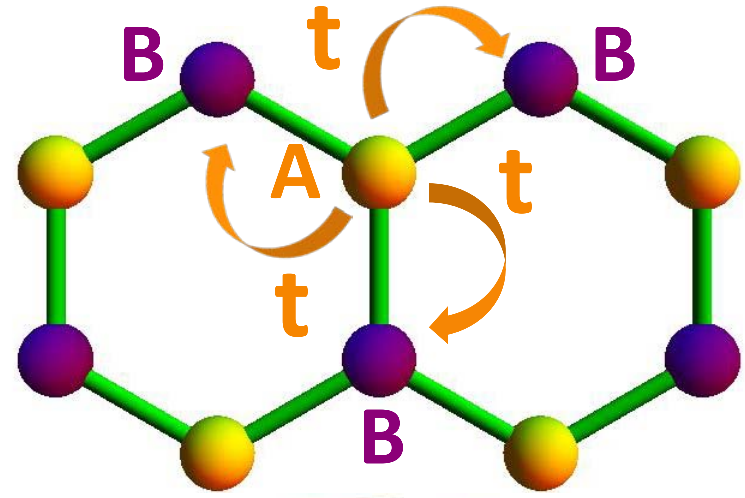
area of Brillouin zone

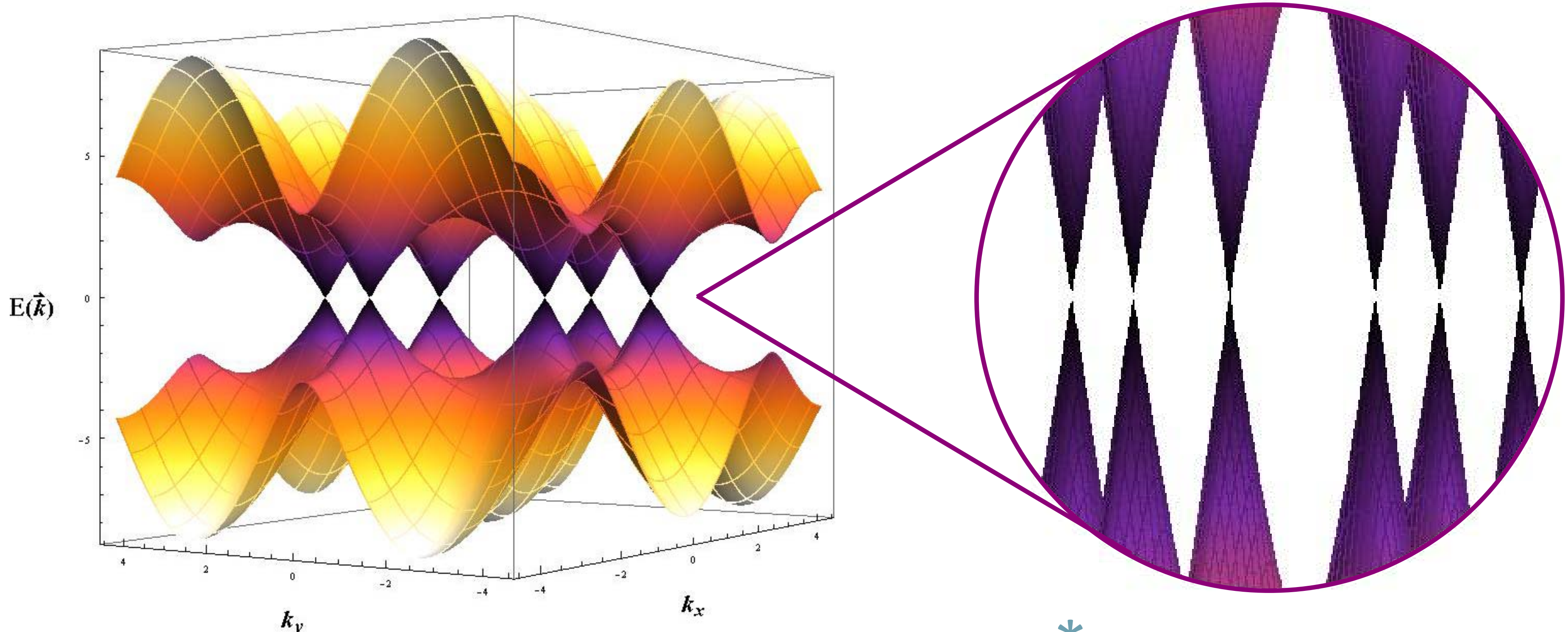
$$\frac{8\pi^2}{\sqrt{3}a^2} = 7.53\ \text{Å}^{-2}$$

Energy dispersion with nearest-neighbor hopping

$$H_{\vec{k}} = -t \begin{bmatrix} 0 & \varepsilon(\vec{k}) \\ \varepsilon^*(\vec{k}) & 0 \end{bmatrix}$$

$t = 2.7 eV$ *

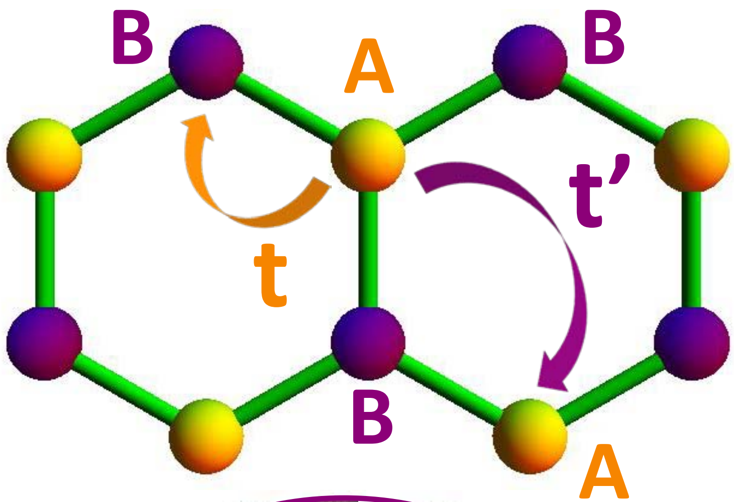




$$\varepsilon(\vec{k}) = \pm t \sqrt{3 + 2\cos(a k_x) + 4\cos\left(\frac{a}{2} k_x\right)\cos\left(\frac{\sqrt{3}a}{2} k_y\right)}$$

* A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. **81**, 109 (2009).

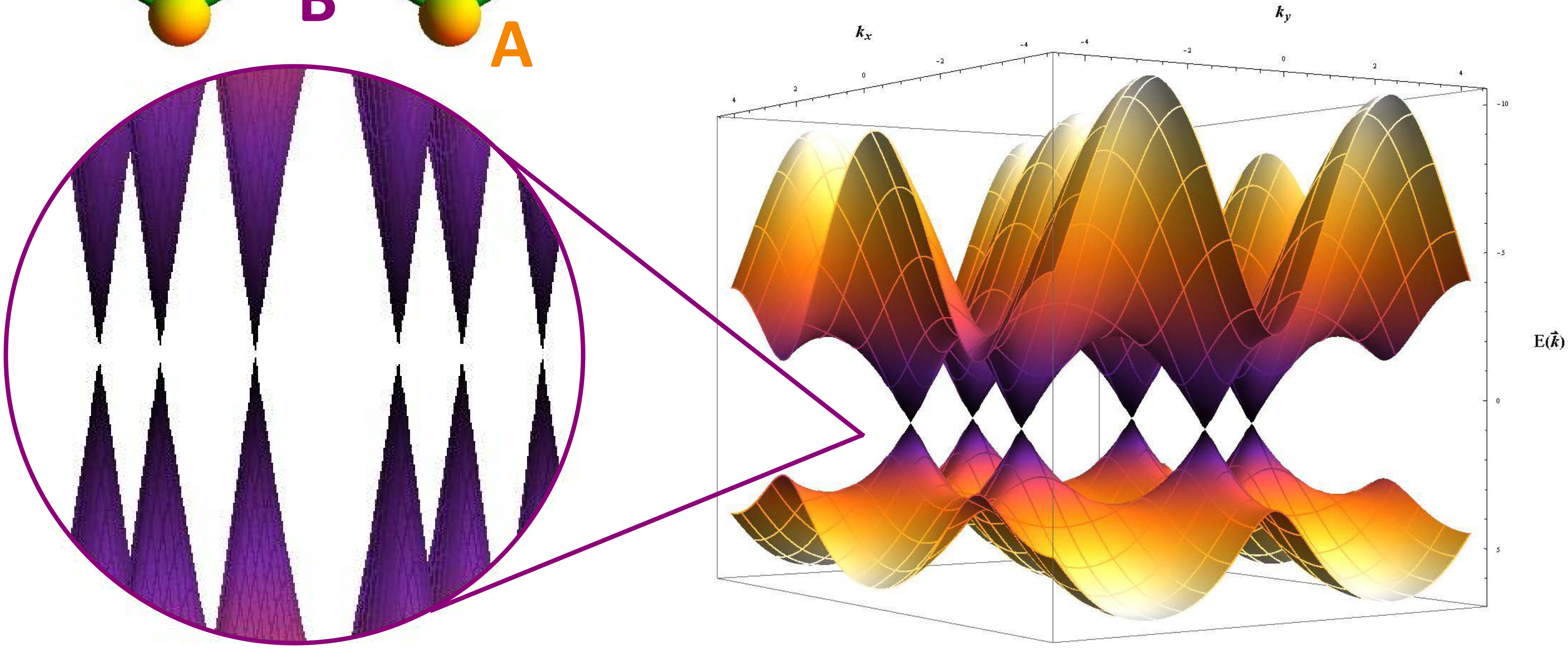
Energy dispersion with next nearest-neighbor hopping



$$H = -\begin{bmatrix} t'\kappa(\vec{k}) & t\varepsilon(\vec{k}) \\ t\varepsilon^*(\vec{k}) & t'\kappa(\vec{k}) \end{bmatrix}$$

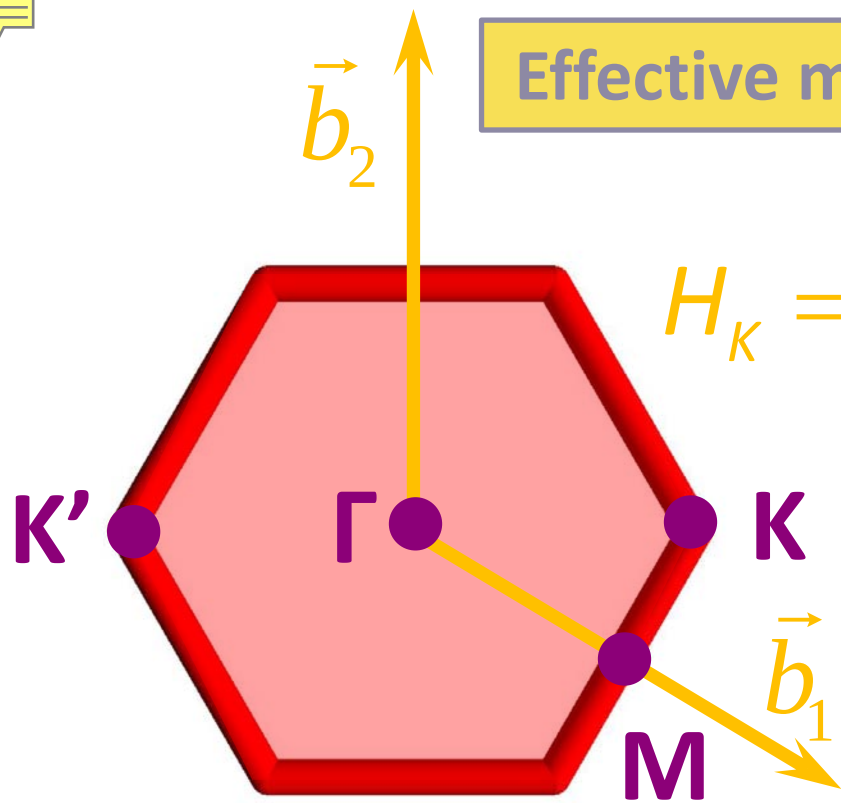
$t' = -0.2t$ *

* A. H. Castro Neto, et.al., Rev. Mod. Phys. **81**, 109 (2009).



$$E(\vec{k}) = \pm t\sqrt{3 + 2\cos(ak_x) + 4\cos\left(\tfrac{a}{2}k_x\right)\cos\left(\tfrac{\sqrt{3}a}{2}k_y\right)} - t'\left[2\cos(ak_x) + 4\cos\left(\tfrac{a}{2}k_x\right)\cos\left(\tfrac{\sqrt{3}a}{2}k_y\right)\right]$$

Effective mass Hamiltonian around point K



First Brillouin zone and some special points of symmetry

$$H_K = \hbar v_F \begin{bmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{bmatrix}$$

Fermi speed*

$$v_F = \frac{\sqrt{3}at}{2\hbar} \approx 9 \cdot 10^5 \frac{m}{s}$$

* A. H. Castro Neto, et.al., Rev. Mod. Phys. **81**, 109 (2009).

with $\vec{k} = \vec{K} - \delta\vec{k}$

Expand around $\vec{K}$

Substitute $\vec{k} \rightarrow -i\hbar\left(\partial_x, \partial_y\right) = \left(p_x, p_y\right)$

Complete, low-energy Hamiltonian

$$H = \begin{bmatrix} H_K & 0 \\ 0 & H_{K'} \end{bmatrix} \longleftrightarrow H_{Dirac} = \begin{bmatrix} -c\sigma \cdot p & 1mc^2 \\ 1mc^2 & c\sigma \cdot p \end{bmatrix}$$

$1 \equiv 2 \times 2$ identity matrix

$\sigma \equiv$ Pauli spin matrices

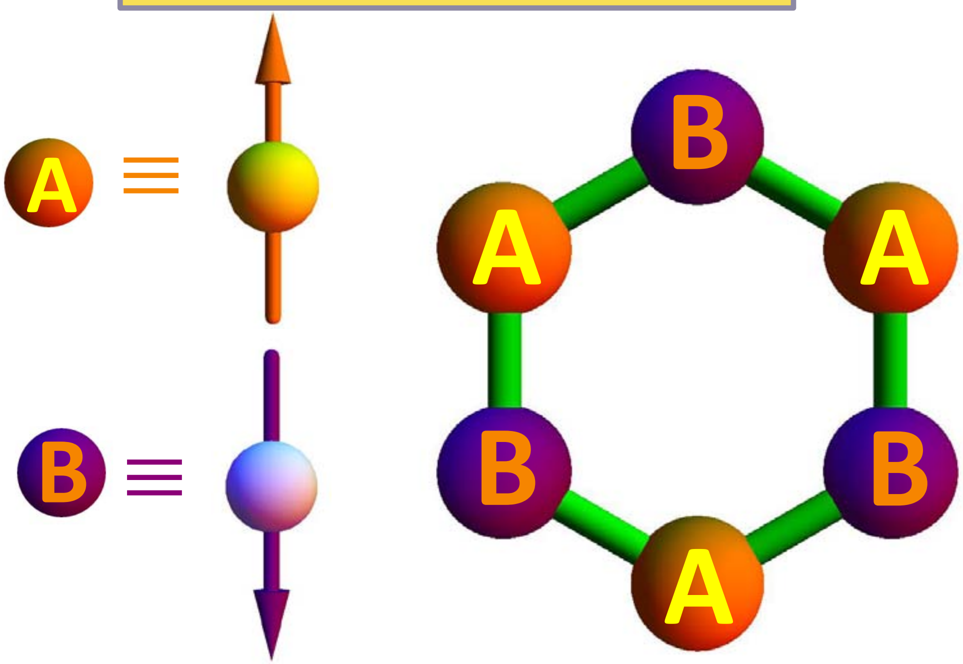
4-component spinor wavefunction

sublattice index "isospin"

$$\Psi = \begin{bmatrix} \psi_{K,A} \\ \psi_{K,B} \\ \psi_{K',A} \\ \psi_{K',B} \end{bmatrix}$$

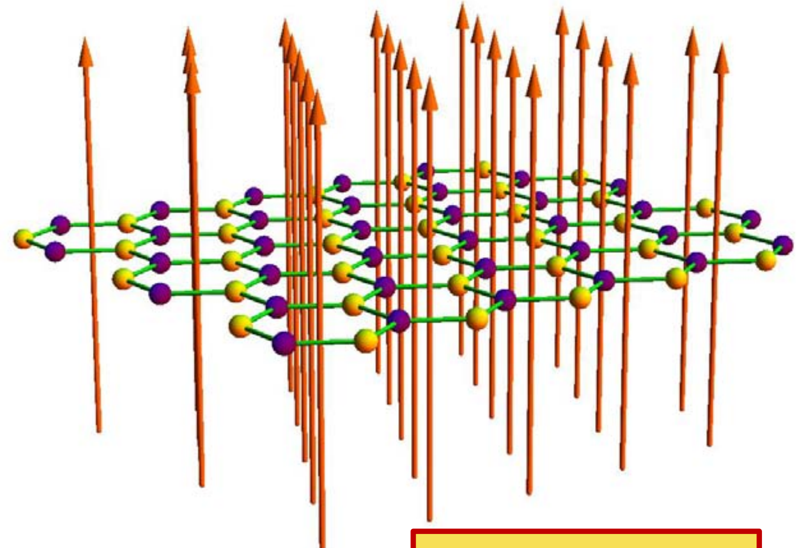
valley index

Interpretation of isospin for graphene



4×4 effective Hamiltonian

graphene in uniform, perpendicular B-field



K, A — K, B — K', A — K', B

$$H = v_F \begin{pmatrix} 0 & p_x - ip_y & 0 & 0 \\ p_x + ip_y & 0 & 0 & 0 \\ 0 & 0 & 0 & p_x + ip_y \\ 0 & 0 & p_x - ip_y & 0 \end{pmatrix}$$

Peierls substitution

$$p \rightarrow \hat{\pi} = p + q\vec{A}$$

valid when $L_B = \sqrt{\frac{\hbar}{Be}} >> a$

Landau gauge

$$\vec{A} = \left(-yB, 0, 0\right)$$

translation invariance in the x-direction

$$H_K = v_F \begin{bmatrix} 0 & \frac{\hbar}{i}\partial_x + Bey - \hbar\partial_y \\ \frac{\hbar}{i}\partial_x + Bey + \hbar\partial_y & 0 \end{bmatrix}$$

$$H_{K'} = v_F \begin{bmatrix} 0 & \frac{\hbar}{i}\partial_x + Bey + \hbar\partial_y \\ \frac{\hbar}{i}\partial_x + Bey - \hbar\partial_y & 0 \end{bmatrix}$$

Dirac fermion ladder operators

raising operator

$$\hat{a}^{\dagger} = \frac{1}{\sqrt{2}}\left(\mathrm{Y} - \partial_{\mathrm{Y}}\right)$$

lowering operator

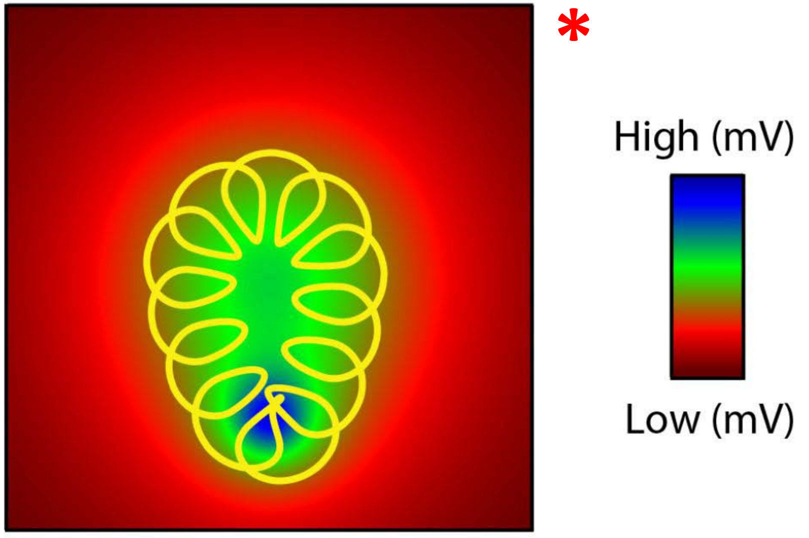
$$\hat{a} = \frac{1}{\sqrt{2}}\left(\mathrm{Y} + \partial_{\mathrm{Y}}\right)$$

with

$$\mathrm{Y} = \frac{y}{L_B} - L_B k_x$$

coordinate of guiding center

$$y_0 = L_B^2 k_x$$



Hamiltonian in B-field

$$H_{\vec{B}} = \mathrm{sgn}(n)\frac{\sqrt{2}v_F}{L_B}\begin{bmatrix} 0 & \hat{a} \\ \hat{a}^{\dagger} & 0 \end{bmatrix}$$

$$\mathrm{sgn}(n) = \begin{cases} 0, & n = 0 \\ \dfrac{n}{|n|}, & n \neq 0 \end{cases}$$

$$\omega_c^{SLG} = \frac{\sqrt{2}v_F}{L_B}$$

* Image from PhD thesis of Kevin Dean Kubista, "Local measurements of cyclotron states in graphene", GIT 2011

Solution

$$H_{\vec{B}}\psi_n = E_n\psi_n$$

2-component spinor eigenfunction

$$\psi_n = \exp(-ik_x x)\begin{pmatrix} c_n^A\phi_n^A \\ c_n^B\phi_n^B \end{pmatrix}$$

coupled DE

$$\begin{cases} \hbar\omega_c^D \operatorname{sgn}(n)\hat{a}c_n^B\phi_n^B = E_n c_n^A\phi_n^A \\ \hbar\omega_c^D \operatorname{sgn}(n)\hat{a}^\dagger c_n^A\phi_n^A = E_n c_n^B\phi_n^B \end{cases}$$

equation for 2nd spinor

$$\hat{a}^\dagger a\phi_n^B = \left(\frac{E_n}{\hbar\omega_c^D}\right)^2 \phi_n^B$$

2nd spinor

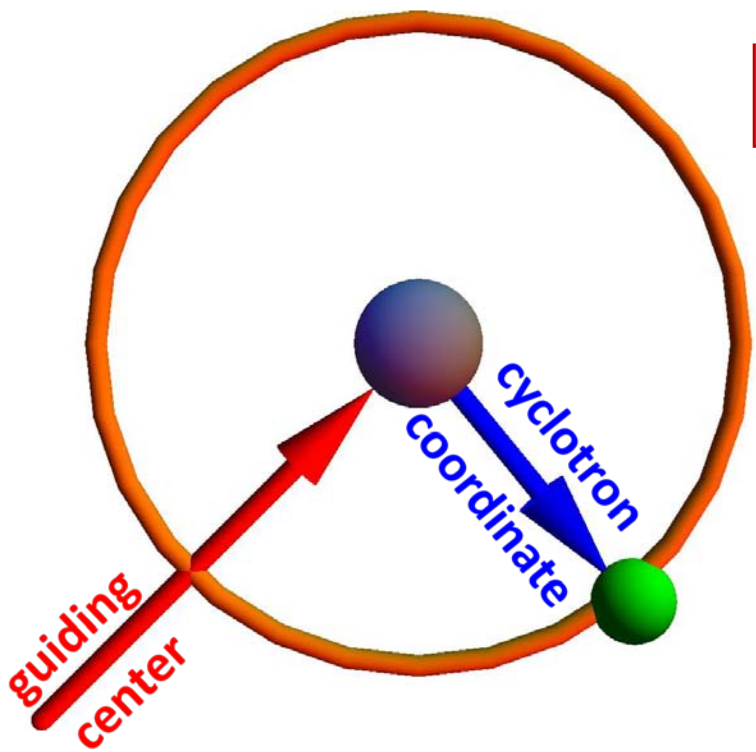
$$\hat{a}^\dagger a|n\rangle = n|n\rangle \qquad c_n^B\phi_n^B \rightarrow c_n^B|n\rangle$$

Solution, continued

Energy $E_n^2 = n\left(\hbar\omega_c^D\right)^2$

equation for 2nd spinor $\hbar\omega_c^D \hat{a}^\dagger c_n^A \phi_n^A = \sqrt{n}\hbar\omega_c^D c_n^B |n\rangle$

1st spinor $\hat{a}^\dagger |n-1\rangle = \sqrt{n}|n\rangle \qquad c_n^A \phi_n^A \rightarrow c_n^A |n-1\rangle$



$\vec{B}$ **magnetic field out of the page**

$$\phi_{n,m}^{A,B} = \phi_n^{A,B} \otimes |m\rangle$$

$m \geq 0$, integer

Eigenvalues and eigenvectors

$$E_n = \mathrm{sgn}(n)\hbar\omega_c^{Dirac}\sqrt{|n|}$$

or $$E_n = \mathrm{sgn}(n)\sqrt{2\hbar e|n|B}$$

cyclotron frequency

$$\omega_c^{Dirac} = \frac{\sqrt{2}v_F}{L_B}$$

magnetic length

$$L_B = \sqrt{\frac{\hbar}{Be}}$$

$n = 0, \pm 1, \pm 2, \ldots$ **Landau level index**

$$\psi_{n,m}^{K,\pm}(x,y) = \frac{C_n}{\sqrt{L_x}} e^{-i(k_x - K)x} \begin{bmatrix} \mathrm{sgn}(n)\phi_{|n|-1,m}^{A}(\Upsilon) \\ \phi_{|n|,m}^{B}(\Upsilon) \\ 0 \\ 0 \end{bmatrix}$$

$$\psi_{n,m}^{K',\pm}(x,y) = \frac{C_n}{\sqrt{L_x}} e^{-i(k_x + K')x} \begin{bmatrix} 0 \\ 0 \\ \phi_{|n|,m}^{A}(\Upsilon) \\ \mathrm{sgn}(n)\phi_{|n|-1,m}^{B}(\Upsilon) \end{bmatrix}$$

L_x = sample length in x direction

$$\Upsilon = \frac{y}{L_B} - L_B k_x = \frac{y - y_0}{L_B}$$

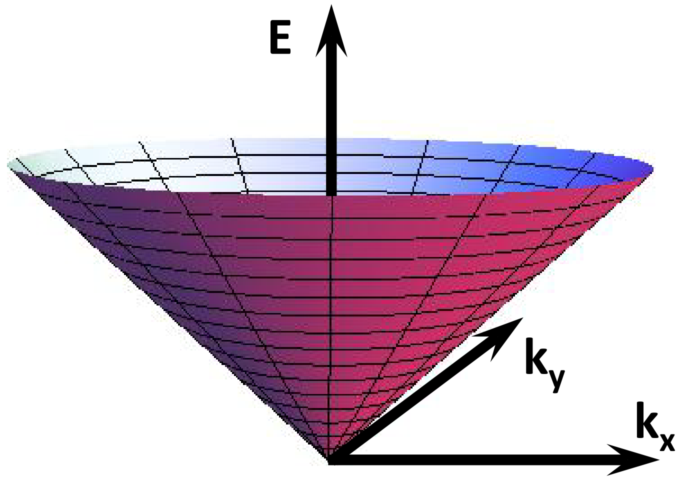
$$C_n = \delta_{n,0} + \left(1 - \delta_{n,0}\right)\sqrt{2}^{-1}$$

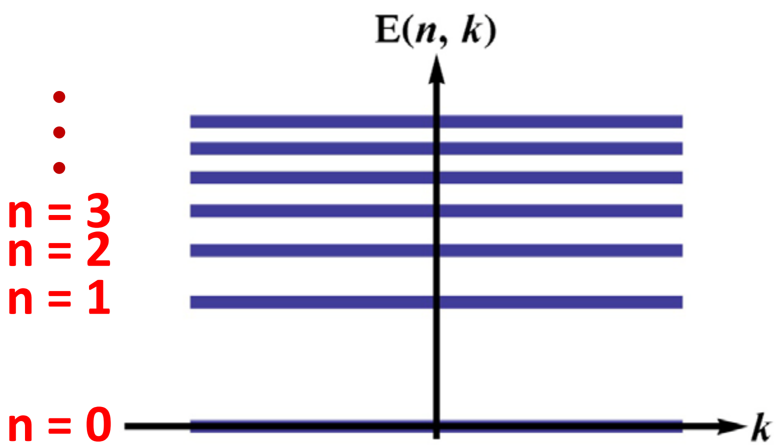
normalization constant

$$\phi_{n,m}(Y) = \frac{1}{(\pi)^{1/4}} \frac{1}{\sqrt{2^n n!}} \exp\left[-\frac{(y - y_0)^2}{2L_B^2}\right] H_n\left(\frac{y - y_0}{L_B}\right)$$

Landau levels

single layer graphene

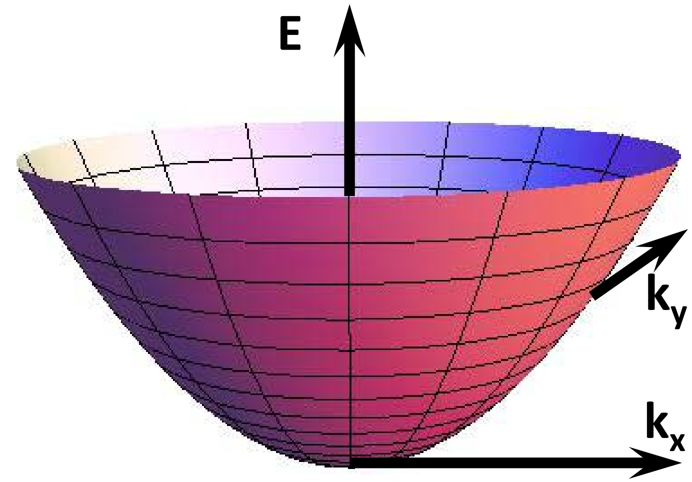


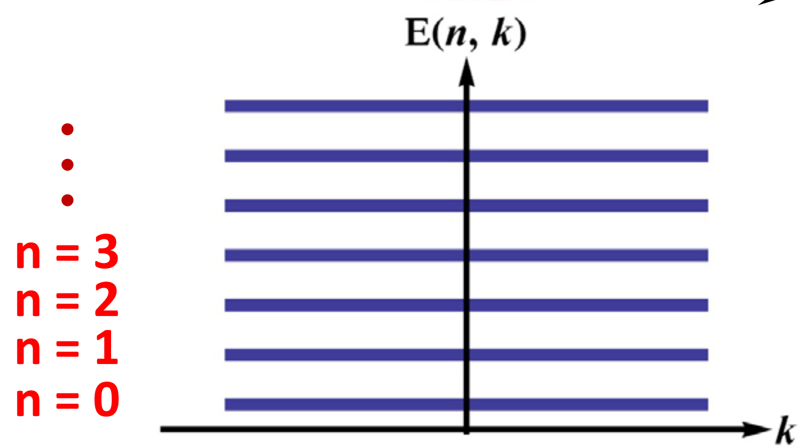


$$E_n^{SLG} = \hbar\omega_C^{Dirac}\sqrt{n}$$

$$\omega_c^{SLG} = \frac{\sqrt{2}v_F}{L_B} \qquad L_B = \sqrt{\frac{\hbar}{Be}}$$

2-dimensional electron gas

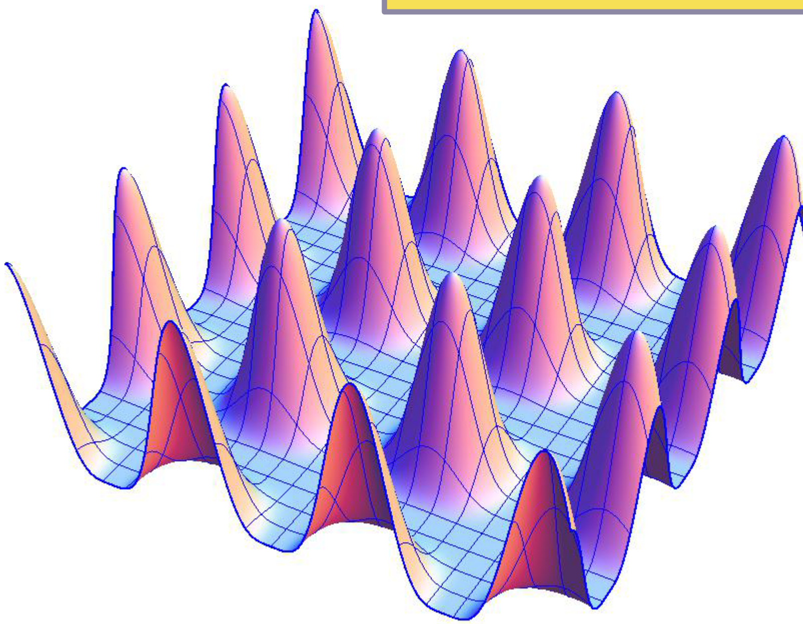




$$E_n^{2DEG} = \hbar\omega_C^{2DEG}\left(n + \frac{1}{2}\right)$$

$$\omega_c^{2DEG} = \frac{eB}{m}$$

Two-dimensional scatter potential



$$V(x,y) = V_0\left[\cos\left(\frac{\pi x}{d_x}\right)\cos\left(\frac{\pi y}{d_y}\right)\right]^{2N}$$

$N =$ integer

$V_0 =$ modulation amplitude

$d_x =$ modulation period in x direction

$d_y =$ modulation period in y direction

Hamiltonian including modulation

$$H = \mathrm{sgn}(n)v_F\begin{bmatrix} V(x,y) & p_x + Bey - ip_y & 0 & 0 \\ \hat{p}_x + Bey\hat{x}_0 + ip_y & V(x,y) & 0 & 0 \\ 0 & 0 & V(x,y) & \hat{p}_x + Bey\hat{x}_0 + ip_y \\ 0 & 0 & \hat{p}_x + Bey\hat{x}_0 - ip_y & V(x,y) \end{bmatrix}$$

Effect of 2D potential

flux quantum

$$\Phi_0 = \frac{h}{e}$$

flux ratio

$$\frac{p}{q} = \frac{\Phi_B}{\Phi_0} = \frac{Bd_x d_y}{\Phi_0}$$

$p, q =$ relative primes

Landau gauge

$$\vec{A} = \left(-yB, 0, 0\right)$$

magnetic translation

$$x \to x + ud_x$$

$$y \to y + qvd_y$$

$u, v =$ integers

magnetic Brillouin zone (MBZ)

$$\left|k_x\right| \geq \frac{\pi}{d_x}; \qquad \left|k_y\right| \geq \frac{\pi}{qd_y}$$

generalized Bloch-Peierls condition

$$\psi\left(x, y\right) = \psi\left(x + d_x, y + qd_y\right) e^{-ik_x d_x} e^{-ik_y qd_y} e^{-2\pi ip\frac{x}{d_x}}$$

Quantum number "accountability"

Bloch-Peierls condition

$$\psi_{k_x,k_y}(x,y)=\psi(x,y+qd_y)e^{-ik_y q d_y} \quad *$$

$$\frac{p}{q}=\frac{Bd_x d_y}{\frac{h}{e}}=\frac{d_y G_x}{L_B^2}$$

guiding center translation

$$\psi_n\left(x,\frac{y-y_0}{L_B}\right)\rightarrow\psi_{n,m}\left(x,\frac{y-y_0-mG_xL_B^2}{L_B}\right)$$

magnetic translation

$$\psi_{n,m}\left(x,\frac{y-y_0-mG_xL_B^2}{L_B}\right)\rightarrow\psi_{n,m,p}\left(x,\frac{y-y_0-(p+m)G_xL_B^2}{L_B}\right)$$

* *Quantized Hall Conductance in a Two-Dimensional Periodic Potential*, Thouless et. al. Phys. Rev. Lett. **49**, 405 (1982)

Modified eigenfunction

$$\psi^{K,\pm}_{n,m,p}(x,y)=\frac{1}{\sqrt{N_y L_x}}\sum_{s=-\infty}^{\infty} e^{i\left[k_x-(sp+m)G_x\right]x}\, e^{ik_y L_B^2(sp+m)G_x}\begin{bmatrix}\operatorname{sgn}(n)\,\phi^{A}_{|n|-1,k_x-(sp+m)G_x}(\Upsilon)\\ \phi^{B}_{|n|,k_x-(sp+m)G_x}(\Upsilon)\\ 0\\ 0\end{bmatrix}$$

$$N_y=\frac{L_y}{qd_y}=\text{number of unit cells in } y\text{-direction}$$

$$L_{x/y}=\text{sample length in } x/y\text{-direction}$$

$$G_x=\frac{2\pi}{d_x}=\text{a reciprocal lattice vector}$$

$$m=1,2,\ldots,p=\text{quantum number}$$

Potential matrix elements

$$V_{m,n,\mu}^{m',n',\mu'}\left(\vec{k}\right)=\sum_{\vec{k}}\iint dxdy\left[\phi_{m',n'}^{\mu'}(x,y)\right]^{\dagger}V(x,y)\phi_{m,n}^{\mu}(x,y)$$

$\mu,\mu'=\pm$

$$V_{m,n,\mu}^{m',n',\mu'}\left(\vec{k}\right)=\frac{V_0 C_{n'} C_n}{4^{2N}}\left\{e^{ik_yG_x(m-m')}\sum_{i=0}^{N-1}\sum_{j=0}^{N-1}\left[\mathcal{F}_{i,j}^{B}+\mathrm{sgn}(n')\mathrm{sgn}(n)\mathcal{F}_{i,j}^{A}\right]+\delta_{m,m'}\delta_{n,n'}\left[1+\mathrm{sgn}(n')\mathrm{sgn}(n)\right]\left[\frac{(2N)!}{(N!)^2}\right]^2\right\}$$

$$\mathcal{F}_{i,j}^{A,B}={}_{2N}C_i\,{}_{2N}C_N A_1^{A,B}(0,N-i)+{}_{2N}C_j\,{}_{2N}C_N A_2^{A,B}(N-j,0)+2\,{}_{2N}C_i\,{}_{2N}C_j A_3^{A,B}(N-j,N-i)$$

$${}_nC_k=\frac{n!}{k!(n-k)!}$$ binomial coefficient $n\geq k$

Other notation introduced on previous slide

$$A_1^{(A,B)}(r,s) = D_{n',n}^{r,s(A,B)} T_m^s \delta_{m,m'}$$

$$A_2^{(A,B)}(r,s) = D_{n',n}^{r,s(A,B)} \left\{ \delta_{m-m',r} \left[\operatorname{sgn}(n'-n)\right]^{\xi} + \delta_{m'-m,r} \left[\operatorname{sgn}(n-n')\right]^{\xi} \right\}$$

$$A_3^{(A,B)}(r,s) = D_{n',n}^{r,s(A,B)} \left\{ \delta_{m-m',r} \left[\operatorname{sgn}(n'-n)\right]^{\xi} \cos\left[\Theta_{r,s}^{m'}(n',n)\right] + \delta_{m'-m,r} \left[\operatorname{sgn}(n-n')\right]^{\xi} \cos\left[\Theta_{r,s}^{m}(n,n')\right] \right\}$$

$$D_{n',n}^{r,s(B)} = \sqrt{\frac{n_1!}{n_2!}} e^{-\frac{W_{r,s}}{2\beta}} \left(\frac{W_{r,s}}{\beta}\right)^{\xi} L_{n_1}^{(\xi)}\left(\frac{W_{r,s}}{\beta}\right)$$

$$\Theta_{r,s}^{m}(n',n) = s\frac{k_x d_x - 2\pi\left(m + \frac{r}{2}\right)}{\beta} - \operatorname{sgn}(n'-n)\,\xi \tan^{-1}\frac{s d_x}{r d_y}$$

$$n_1 = \min(n,n')$$

$$n_2 = \max(n,n')$$

$$\beta = \frac{p}{q}$$

$$\xi = |n-n'|$$

$L_n^{(m)}$ = associated Laguerre polynomial

$$W_{r,s} = \frac{\pi\left(s^2 G_y^2 + r^2 G_x^2\right)}{G_x G_y}$$

$$T_m^s = \begin{cases} \pm 2\cos\dfrac{s(k_x d_x - 2\pi m)}{\beta} & \begin{array}{l} + \text{ for } \xi = 4N \\ - \text{ for } \xi = 4N+2 \end{array} \\ \pm 2\sin\dfrac{s(k_x d_x - 2\pi m)}{\beta} & \begin{array}{l} + \text{ for } \xi = 4N+1 \\ - \text{ for } \xi = 4N+2 \end{array} \end{cases}$$

Magnetic band structure

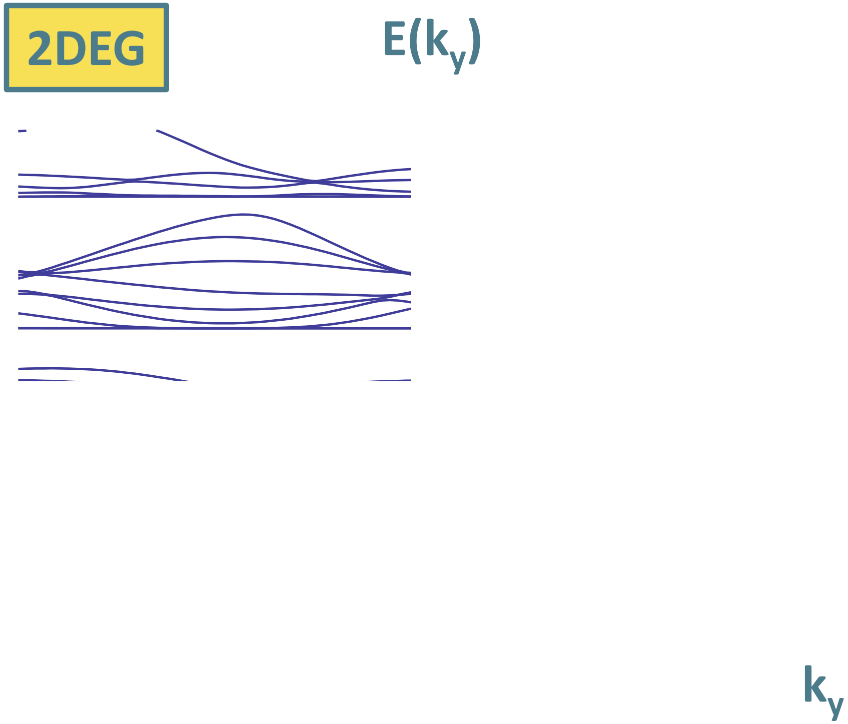
eigenvalue equation

$$\det\left\{\overleftrightarrow{\mathcal{M}}\right\} = 0$$

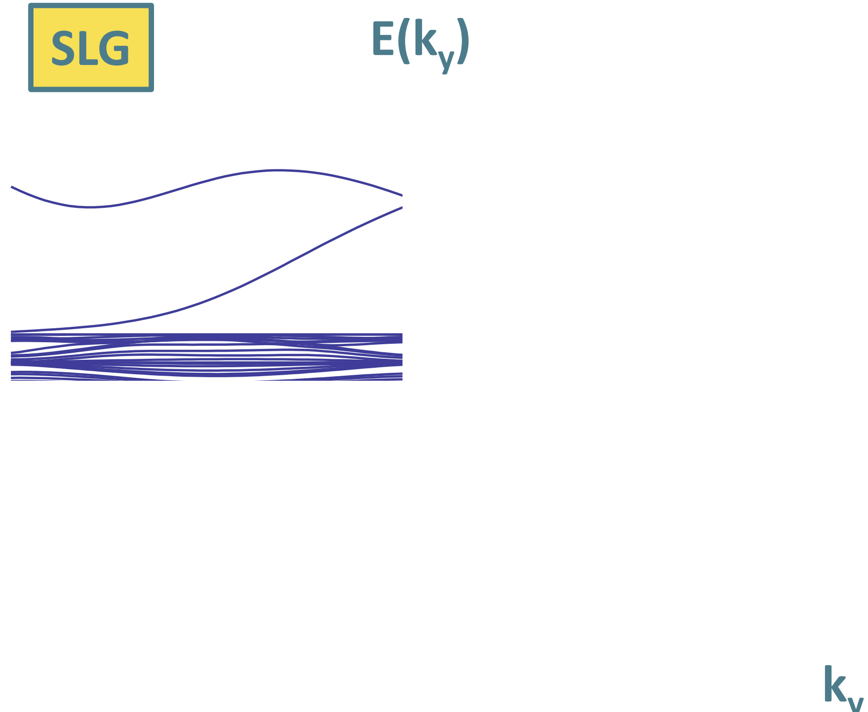
coefficient matrix

$$\left\{\overleftrightarrow{\mathcal{M}}\right\}_{i,j} = \left[E_n^{\mu} - \varepsilon\left(\vec{k}\right)\right]\delta_{n,n'}\delta_{m,m'}\delta_{\mu,\mu'}^{(n)} + V_{l,n,\mu}^{l',n',\mu'}$$

2DEG



SLG



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