Elementary Electronic Excitations in Graphene Nanoribbons.

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- Electronic structure of nanoribbons.

  Armchair

  Zigzag

- Random Phase Approximation.

  Armchair

- Comments on Zigzag.

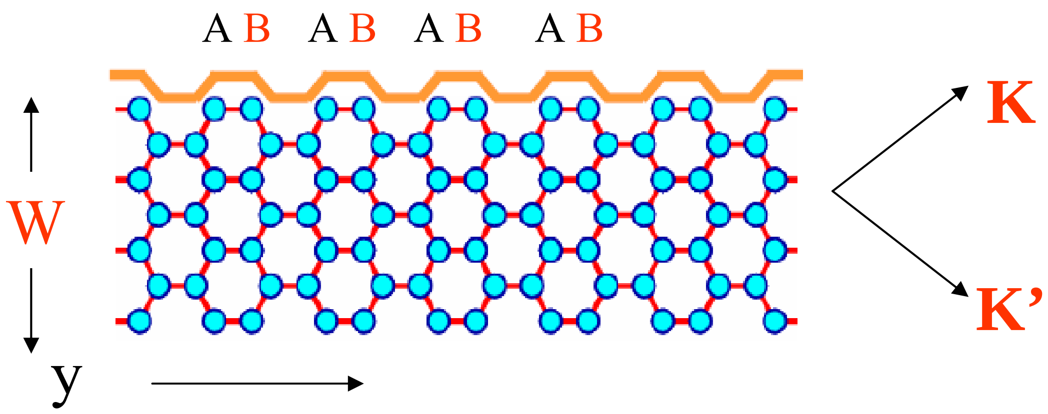
Graphene. Electronic Structure.

$$
\begin{array}{cccccc}
 & \text{K,A} & \text{K,B} & \text{K',A} & \text{K',B} \\
H = \gamma a_0 & \multicolumn{4}{c}{\begin{pmatrix} 0 & k_x - ik_y & 0 & 0 \\ k_x + ik_y & 0 & 0 & 0 \\ 0 & 0 & 0 & -k_x - ik_y \\ 0 & 0 & -k_x + ik_y & 0 \end{pmatrix}}
\end{array}
$$

$$\varepsilon = s\gamma a_0 \,|\vec{k}| \quad \text{with} \qquad s = \pm 1$$

$$\psi_{s,K} = \begin{pmatrix} e^{-i\theta_{\vec{k}}} \\ s \\ 0 \\ 0 \end{pmatrix} e^{i\vec{k}\vec{r}} \qquad \psi_{s,K'} = \begin{pmatrix} 0 \\ 0 \\ e^{i\theta_{\vec{k}}} \\ s \end{pmatrix} e^{i\vec{k}\vec{r}} \qquad \theta_{\vec{k}} = \arctan \frac{k_x}{k_y}$$

Armchair nanoribbons



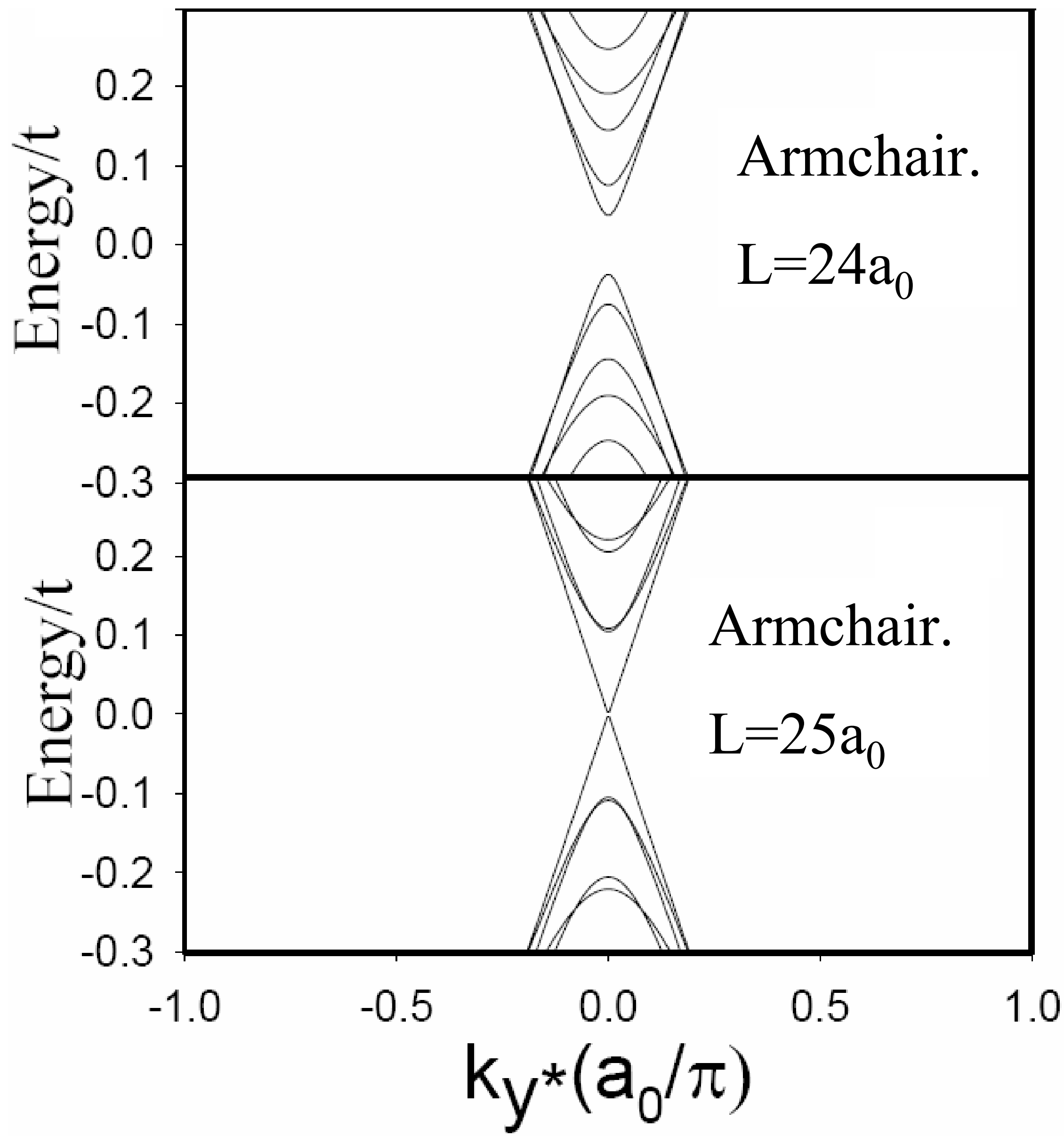
Boundary conditions:
$\varphi_B(x=0)+\varphi'_B(x=0)=0$
$\varphi_A(x=0)+\varphi'_A(x=0)=0$
Admixes valleys

$$\psi_{n,s} = \begin{pmatrix} e^{-i\theta_{k_n,k_y}} e^{ik_n x} \\ s e^{ik_n x} \\ e^{-i\theta_{k_n,k_y}} e^{-ik_n x} \\ -s e^{-ik_n x} \end{pmatrix} e^{ik_y y}$$

$$\varepsilon_{n,s}(k_y) = s\gamma a_0 \sqrt{k_n^2 + k_y^2}$$

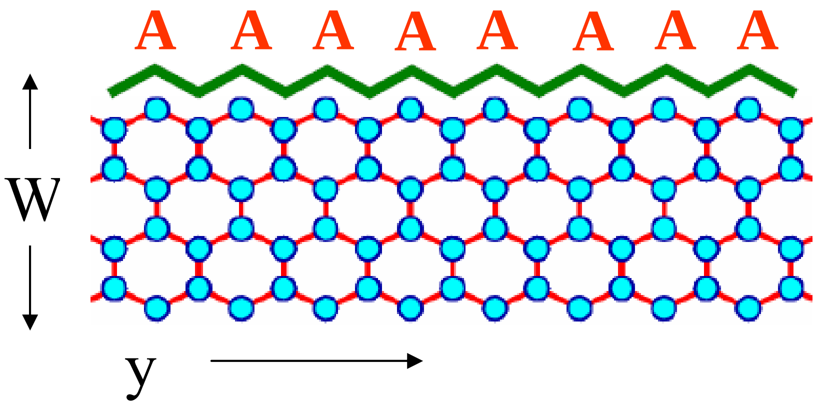
$$k_n = \frac{2\pi n}{2W + a_0} + \frac{2\pi}{3a_0}$$

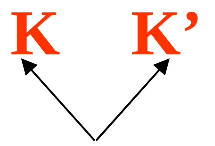
$W=(3M+1)a_0$ metallic, $k_n=0$
otherwise semiconductor.



Energy/t
0.2
0.1
0.0
-0.1
-0.2
-0.3
Armchair.
L=24a0
Energy/t
0.2
0.1
0.0
-0.1
-0.2
-0.3
Armchair.
L=25a0
-1.0
-0.5
0.0
0.5
1.0
ky*(a0/π)

Zigzag nanoribbons.





$K_y \neq K_y'$

Boundary conditions:

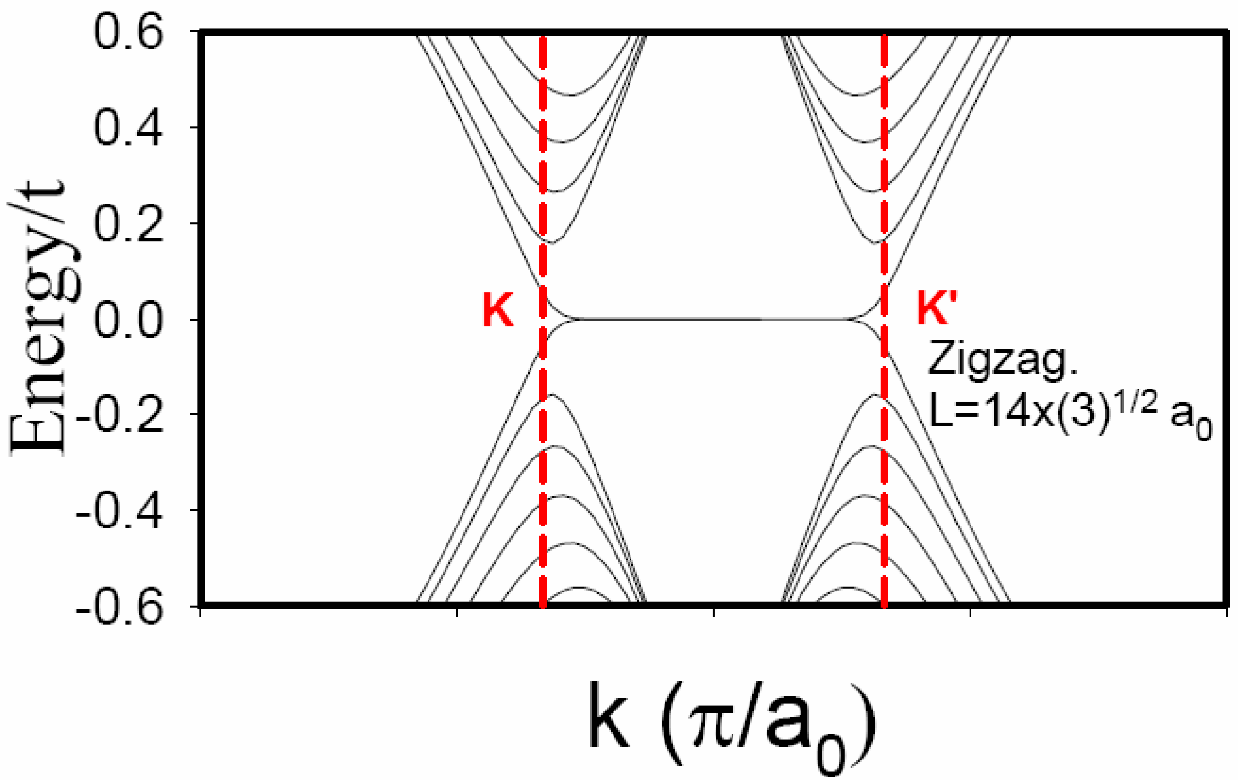
$\varphi_A(x=0)=0$

$\varphi_B(x=W)=0$

$$\psi_{n,s} = \begin{pmatrix} is\sinh(z_n x) \\ \sinh((W-x)z_n) \end{pmatrix} e^{ik_y y}$$

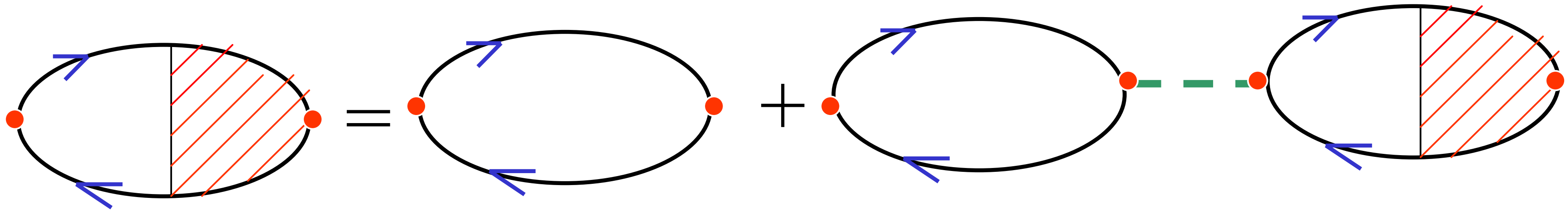
$$\varepsilon_{n,s}(k_y) = s\gamma a_0 \sqrt{k_n^{\,2} - z_n^{\,2}}$$

$$\frac{k_y - z_n}{k_y + z_n} = e^{-2Wz_n}$$



0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
Energy/t
K
K'
Zigzag.
L=14x(3)^{1/2} a_0
k (π/a_0)

Collective Excitations RPA



$$\Pi \quad = \quad \Pi^0 \quad + \quad \Pi^0 \; \mathrm{v}_q \; \Pi$$

$$\varepsilon(q,\omega) = 1 - \mathrm{v}_q \Pi^0(q,\omega)$$

Armchair nanoribbons

$$k_n = \frac{2\pi n}{2W + a_0} + \frac{2\pi}{3a_0}$$

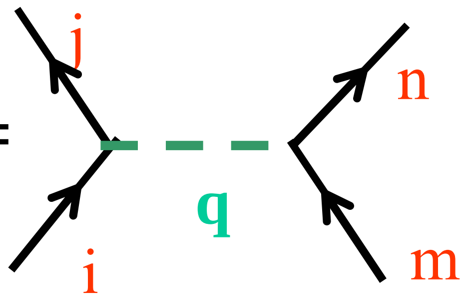
$$\boxed{\varepsilon_{ijmn}(q,\omega) = \delta_{i,m}\delta_{j,n} - \mathrm{v}_{ijmn}(k_y,q)\Pi_{mn}(q,\omega)}$$

$$\boxed{\Pi_{nn'}(q,\omega) = \frac{g_s}{L_y}\sum_{k_y}\frac{f(\varepsilon_{n'}(k_y+q)) - f(\varepsilon_n(k_y))}{\varepsilon_{n'}(k_y+q) - \varepsilon_n(k_y) - \hbar\omega}F_{nn'}(k_y,k_y,+q)}$$

$$\boxed{F_{nn'}(k_y,k_y,+q) = \frac{1}{2}(1 + ss'\cos\theta)}$$

$$\theta = \widehat{(k_n,k_y)(k_n,k_y+q)}$$

$$\mathrm{v}_{ijmn}(q) \quad =$$

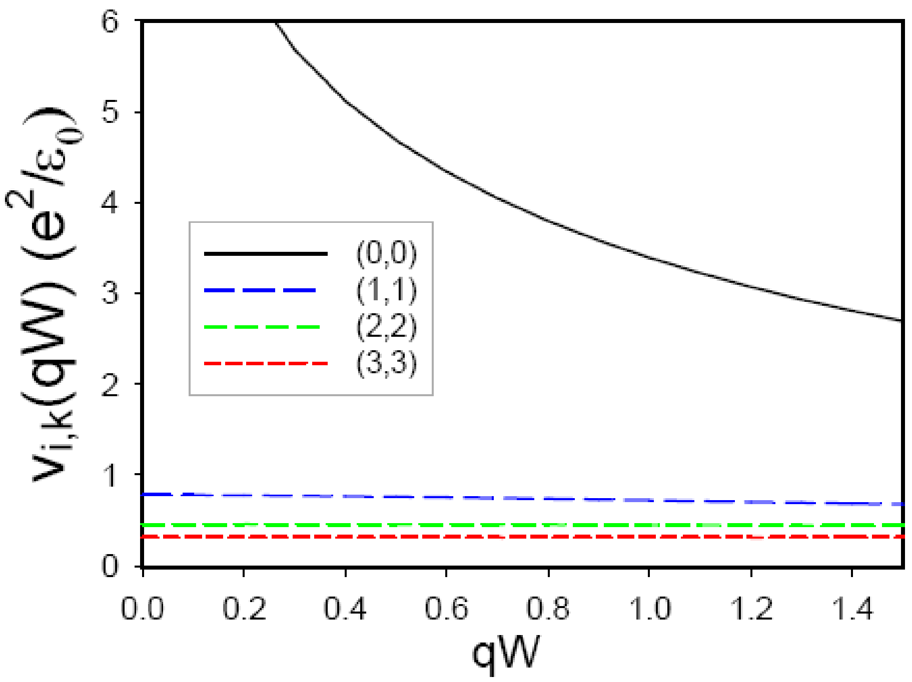


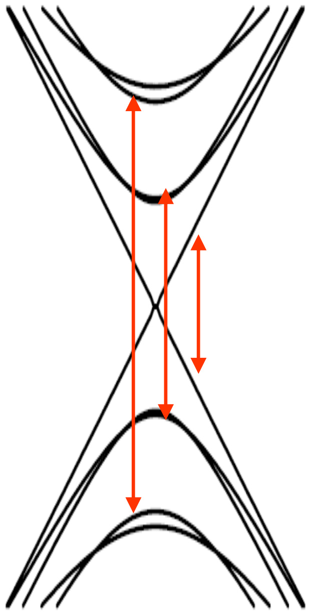
$$\mathrm{v}_{|i-j||m-n|}(q)$$

Coulomb interactions.

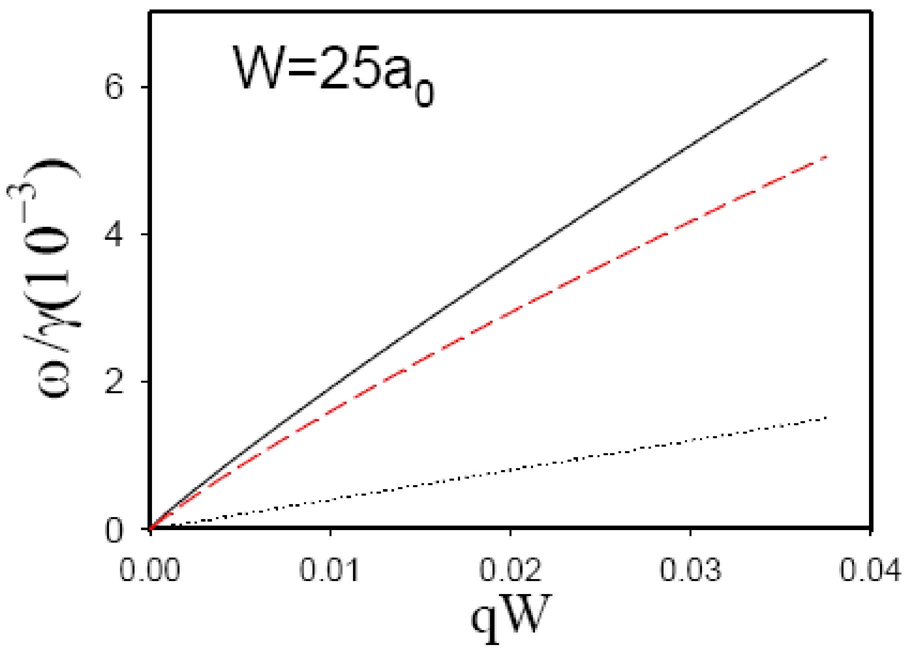
$$\mathrm{v}_{|i-j||m-n|}(q)=\int_0^1 du\int_0^1 du'\cos(\pi(i-j)u)\cos(\pi(m-n)u')\,\mathrm{v}_{\mathrm{q}}(W|u-u'|)$$

$$\mathrm{v}_{\mathrm{q}}(x)=\frac{2e^2}{\varepsilon_0}K_0(qx)\xrightarrow[q\to 0]{}-\frac{2e^2}{\varepsilon_0}\ln(qx)$$





Plasmons.

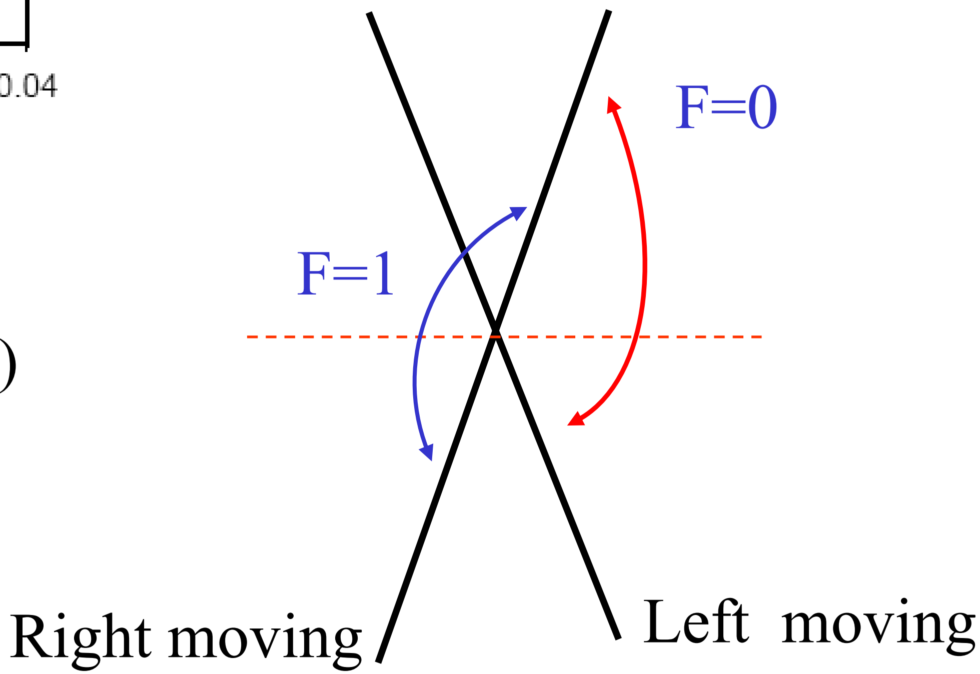


- No interband excitations (Damped).
- Intraband ,k_n=0,excitations no damped. Metallic.
- q(-lnq)1/2 plasmon.
- Single particle excitation is a line!!

$$F(k_y, k_{y'}+q) = \frac{1}{2}(1 + ss'\cos\theta)$$

$$\theta = \widehat{k_y, k_y + q}$$

k_n=0



Long wavelength limit. μ, T

$$\hbar\omega_p \approx \left(\frac{2g_s e^2}{\pi\varepsilon_0}\gamma a_0 q^2\right)^{1/2}\sqrt{-\ln(qw)}\sqrt{f_1(q,\beta,\mu)}$$

$$f_1(q,\beta,\mu) = -\frac{1}{\beta\gamma a_0 q}\left[-\beta\gamma a_0 q + 2\ln\frac{1-e^{-\beta\mu}}{1+e^{-\beta(\gamma a_0 q+\mu)}}\right]$$

- **Dispersion q(-lnq)$^{1/2}$**
- **At T=0 the plasmon frequency is independent of density.**
  In semiconductor QW has a dependence $n_{1D}^{1/2}$.
- Finite T does not produce extra thermo plasmon excitations.
- Strong dependence on the thickness W. Metallic armchair.

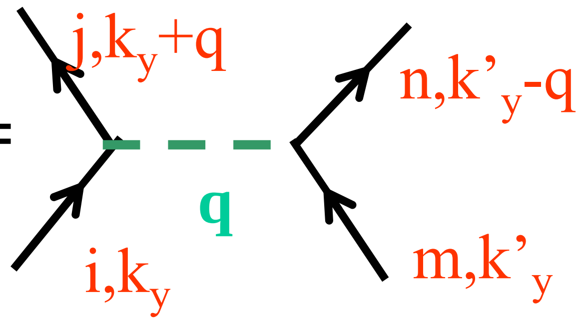
Zigzag nanoribbons.

$$\psi_{n,s} = \begin{pmatrix} i s \sinh(z_n x) \\ \sinh((W-x) z_n) \end{pmatrix} e^{i k_y y}$$

$$\frac{k_y - z_n}{k_y + z_n} = e^{-2W z_n}$$

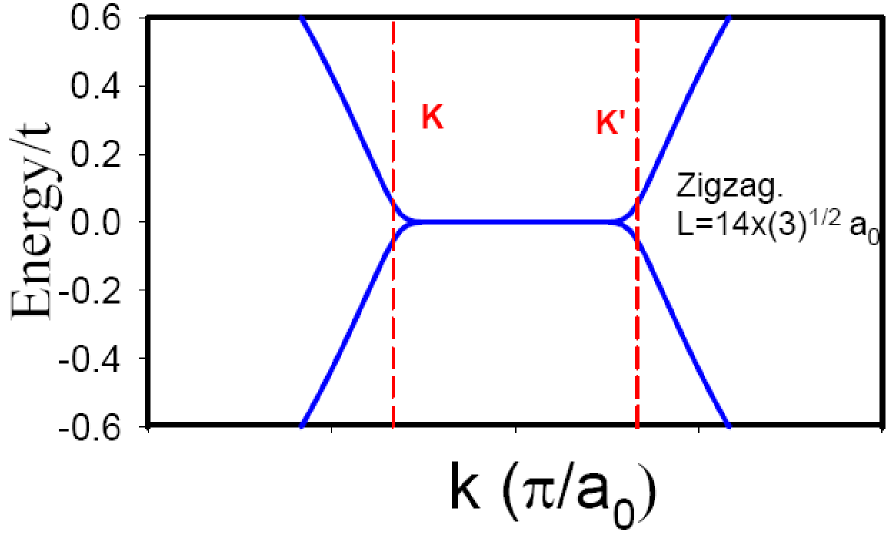
$$\boxed{\varepsilon_{ijmn}(k_y, k_y^{'}; q, \omega) = \delta_{i,m}\delta_{j,n}\delta_{k_y,k_y'} - \mathrm{v}_{ijmn}(k_y, k_y^{'}; q) \times g_s g_\mathrm{v} \frac{f(\varepsilon_m(k_y+q)) - f(\varepsilon_n(k_y))}{\varepsilon_m(k_y+q) - \varepsilon_n(k_y) - \hbar\omega}}$$

$$\mathrm{v}_{ijmn}(k_y, k_y^{'}; q) =$$

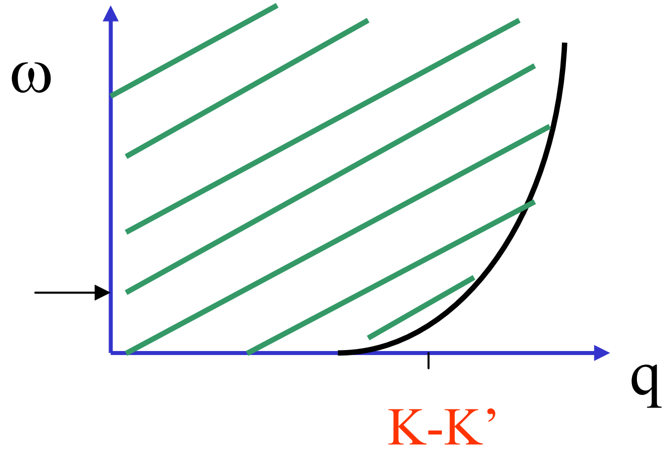


Zigzag nanoribbons.

Restrict to the lowest energy excitations.



•Ln(q) term cancells.
•No window for plasmons. Wide e-h region.



No low energy collective charge density excitations.

Conclusions.

- Collectice charge density excitations in graphene nanoribbons.
- Only low energy excitations in metallic armchair ribbons
- Plasmon disperse a $q(-\ln q)^{1/2}$. but density independent.