Phase transitions in hexagonal, graphen-like lattice sheets and nanotubes

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Introduction

 $Figure: a.)$ Hexagonal honeycomb lattice with two interpenetrating triangular lattices of A and B sites. $\vec{\delta}_i$, $i = 1, 2, 3$ are the nearest neighbor vectors

- b.) Corresponding Brillouin zone: the Dirac cones of the fermion spectrum are located at the K and K' points
	- \triangleright Two sublattice degrees of freedom (pseudospin)
	- \triangleright Two valley degrees of freedom (2 Dirac points)
	- \Rightarrow reducible 4-spinor description in $D=2+1$ $\;\Leftrightarrow$ chiral γ^5
- $-$ Chiral "valley-sublattice" symmetry $U(2)_{\text{vs}}$
- $−$ Inclusion of Coulomb interaction and general four-fermion interactions $⇒$ extended schematic graphen-like model
- − Chiral symmetry breaking: fermion mass and exciton spectrum
- − Construction of the effective potential. Phase transitions under external conditions: temperature, chemical potential, and Zeeman effect
- − Compactification of one dimension: nanotubes, Aharonov–Bohm effect

Effective free low-energy model

Tight-binding Hamiltonian:

$$
H_0 = -t \sum_{\vec{r} \in B} \sum_{i=1,2,3} \left[\psi^{+Aa}(\vec{r} + \vec{\delta}_i) \psi^{Ba}(\vec{r}) + h.c. \right]
$$

 \bullet t — hopping constant; ψ^{+Aa} , ψ^{Ba} — fermion field operators belonging to triangular sublattices with A and B sites; $\vec{\delta}$ nearest neighbor vectors. "Multilayer" case of $N_f = 2N$ degenerate fermion species (flavors) of real spin \uparrow and \downarrow , living on N hexagonal monolayers; flavor index $a = (1, ..., N_f = 2N)$. \bullet Low energy expansion around 2 Dirac points K, K' and continuous limit \Rightarrow effective free low-energy Lagrangian:

$$
\mathcal{L}_0 = \overline{\psi} \left[i\gamma^0 \partial_0 + i v_{\rm F} \gamma^1 \partial_{\rm x} + i v_{\rm F} \gamma^2 \partial_{\rm y} \right] \psi = \overline{\psi} i \gamma^\mu \tilde{\partial}_\mu \psi
$$

$$
\tilde{\partial}_\mu = \left(\partial_0, v_{\rm F} \vec{\nabla} \right), \ v_{\rm F} = \frac{3}{2} t a
$$

$$
\psi^t = \left(\psi_K^{Aa}, \psi_K^{Ba}, -i \psi_{K'}^{Ba}, i \psi_{K'}^{Aa} \right)
$$

• Reducible chiral (Weyl) 4×4 representation of Dirac matrices:

$$
\gamma^0 = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}, \ \gamma^1 = \begin{pmatrix} 0 & -\tau^1 \\ \tau^1 & 0 \end{pmatrix}, \ \gamma^2 = \begin{pmatrix} 0 & -\tau^2 \\ \tau^2 & 0 \end{pmatrix}
$$

$$
\gamma^3 = \begin{pmatrix} 0 & -\tau^3 \\ \tau^3 & 0 \end{pmatrix}, \ \gamma^5 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \ \gamma^{35} = \frac{1}{2} \begin{bmatrix} \gamma^3, \gamma^5 \end{bmatrix} = \begin{pmatrix} 0 & \tau^3 \\ \tau^3 & 0 \end{pmatrix}.
$$

"Right" and "left" spinors:

$$
\psi_{\pm} = \mathcal{P}_{\pm}\psi, \ \ \mathcal{P}_{\pm} = \frac{1}{2}(1 \pm \gamma^5)
$$

$$
\gamma^5 \psi_{\pm} = \pm \psi_{\pm}
$$

Chirality eigenvalues ± 1 corresponding to valley indices for K, K'.

• Emergent continuous $U(2)_{\text{vs}}$ -symmetry:

$$
t^{1} = \frac{1}{2}i\gamma^{3}, \ t^{2} = \frac{1}{2}\gamma^{5}, \ t^{3} = \frac{1}{2}\gamma^{35}
$$

$$
[t^{i}, t^{j}] = i\varepsilon_{ijk}t^{k}
$$

- Invariance under larger group $U(2N_{\rm f})$, Generators $t^i\otimes \frac{\lambda^{\alpha}}{2}\otimes \sigma^m$.
- Discrete symmetries P , C , T :

$$
\psi(x^0, x, y) \xrightarrow{\mathcal{P}} i\gamma^1 \gamma^5 \psi(x^0, -x, y),
$$

$$
\psi(x^0, \vec{r}) \xrightarrow{\mathcal{C}} \gamma^1 \overline{\psi}^t(x^0, \vec{r}),
$$

$$
\psi(x^0, \vec{r}) \xrightarrow{\mathcal{T}} i\sigma^2 \gamma^1 \gamma^5 \psi(-x^0, \vec{r})
$$

Four-fermion interactions

• "Reduced" QED scenario with Dirac-Maxwell interaction:

$$
S = \int d^3x \overline{\psi} i\gamma^{\mu} \widetilde{D}_{\mu} \psi - \frac{\varepsilon_0}{4} \sum_{\mu,\nu=(0,\dots,3)} \int d^4x F_{\mu\nu} F^{\mu\nu}
$$

$$
\widetilde{D}_{\mu}=(\partial_0 - ieA_0, v_{\rm F}(\vec{\nabla} + ie\vec{A}))
$$

Fermion quasiparticles run in $(2 + 1)$ -dim. space-time $x^{(3)} = (x^0, x^1, x^2)$ with Fermi velocity v_F ; $U(1)$ gauge field propagates in $(3 + 1)$ -dim. bulk space-time $x^{(4)}=(x^0,x^1,x^2,x^3)$ with speed of light $c\,(=1).$

• Partition function

$$
Z=\int D\psi D\overline{\psi}D_{\mu}[A_{\mu}]\exp[iS],
$$

• Integration over gauge field yields Coulomb interaction

$$
S = S_0 - \frac{v_{\rm F}}{2c} \int d^{(3)}x' \int d^{(3)}x \left[\overline{\psi}(x^0, \vec{r}) \gamma^0 \psi(x^0, \vec{r}) \right] U_0^C(x^0 - x'^0, |\vec{r} - \vec{r}'|) \times \\ \times \left[\overline{\psi}(x'^0, \vec{r}') \gamma^0 \psi(x'^0, \vec{r}') \right]
$$

Instantaneous Coulomb potential

$$
U_0^C(x^0,|\vec{r}|) = \frac{e^2 \delta(x^0)}{\varepsilon_0 v_{\rm F}} \int \frac{d^2 k}{(2\pi)} \exp(i\vec{k}\vec{r}) \frac{1}{|\vec{k}|} = \frac{\alpha}{\varepsilon_0} \left(\frac{c}{v_{\rm F}}\right) \frac{\delta(x^0)}{|\vec{r}|}
$$

with $v_{\rm F}/c \sim 1/300$ and $\alpha_{\rm eff} = \alpha \frac{c}{v_{\rm F}} \sim 2 \Rightarrow$ strong interaction!

• Low-energy contact approximation:

Local $U(2N_f)$ -invariant four-fermion interaction Lagrangian:

$$
\mathcal{L}_{\text{int}}^{\text{C}} = -\frac{\mathcal{G}_{c} \nu_{\text{F}}}{2} \left[\overline{\psi}(x) \gamma^{0} \psi(x) \right]^{2}
$$

• Coulomb interaction on the lattice contains additionally a small on-site scalar repulsive interaction term:

$$
\Delta L_{\rm int} = \frac{G_{V_{\rm F}}}{2} (\overline{\psi}\psi)^2 \ \ \Rightarrow \ \ \mathcal{X} {\rm SB}: \ \mathcal{U}(2N_{\rm f}) \longrightarrow \mathcal{U}(N_{\rm f})_{t^0} \otimes \mathcal{U}(N_{\rm f})_{t^3}
$$

Inclusion of phonon-mediated interaction with coupling strength g yields symmetry breaking interaction Lagrangian:

$$
\mathcal{L}_{\rm int}=-\frac{1}{2}\mathcal{G}_c\nu_F(\overline{\psi}\gamma^0\psi)^2+\frac{\widetilde{G}\nu_F}{2}(\overline{\psi}\psi)^2,\quad \widetilde{\mathcal{G}}=\mathcal{G}+\mathcal{g}
$$

• Fierz-transformation:

$$
\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\text{int}} = \overline{\psi}i\widetilde{\theta}\psi \n+ \Big\{ \frac{1}{2N_f} G_1 v_F (\overline{\psi}\psi)^2 + \frac{1}{2N_f} G_2 v_F (\overline{\psi}\gamma^{35}\psi)^2 \n+ \frac{1}{2N_f} H_1 v_F (\overline{\psi}i\gamma^5\psi)^2 + \frac{1}{2N_f} H_2 v_F (\overline{\psi}\gamma^3\psi)^2 \Big\}
$$

Here we omitted any constrains between coupling constants \Rightarrow extended schematic Gross–Neveu model

Effective potential; gap equation and exciton spectrum

• Introduce (auxiliary) excitonic fields σ_1 , σ_2 , φ_1 , φ_2 via the Hubbard–Stratonovich transformation

$$
\mathcal{L}[\overline{\psi}, \psi, \sigma_i, \varphi_i] = \overline{\psi} \Big[i \widetilde{\partial} - \sigma_1 - \sigma_2 \gamma^{35} - \varphi_1 i \gamma^5 - \varphi_2 \gamma^3 \Big] \psi
$$
\n
$$
- N_f \sum_{k=1}^2 \left(\frac{\sigma_k^2}{4 \nu_F G_k} + \frac{\varphi_k^2}{4 \nu_F H_k} \right)
$$
\n(1)

• Field equations for exciton fields

$$
\begin{aligned} \sigma_1 &= -2 \frac{G_1 v_\text{F}}{N_\text{f}} \overline{\psi} \psi, & \sigma_2 &= -2 \frac{G_2 v_\text{F}}{N_\text{f}} \overline{\psi} \gamma^{35} \psi, \\ \varphi_1 &= -2 \frac{H_1 v_\text{F}}{N_\text{f}} \overline{\psi} i \gamma^5 \psi, & \varphi_2 &= -2 \frac{H_2 v_\text{F}}{N_\text{f}} \overline{\psi} \gamma^3 \psi \end{aligned}
$$

• Gap equations:

$$
\langle \sigma_1 \rangle = -2 \frac{G_1 v_F}{N_f} \langle \overline{\psi} \psi \rangle = 2 \frac{G_1 v_F}{N_f} \text{Tr}_{\text{sf}} \left[i G(x, x) \right],
$$

\n
$$
\langle \sigma_2 \rangle = -2 \frac{G_2 v_F}{N_f} \langle \overline{\psi} \gamma^{35} \psi \rangle = 2 \frac{G_2 v_F}{N_f} \text{Tr}_{\text{sf}} \left[\gamma^{35} i G(x, x) \right],
$$

\n
$$
\langle \varphi_1 \rangle = -2 \frac{H_1 v_F}{N_f} \langle \overline{\psi} i \gamma^5 \psi \rangle = 2 \frac{H_1 v_F}{N_f} \text{Tr}_{\text{sf}} \left[i \gamma^5 i G(x, x) \right],
$$

\n
$$
\langle \varphi_2 \rangle = -2 \frac{H_2 v_F}{N_f} \langle \overline{\psi} \gamma^3 \psi \rangle = 2 \frac{H_2 v_F}{N_f} \text{Tr}_{\text{sf}} \left[\gamma^3 i G(x, x) \right],
$$

Inverse fermion propagator

$$
\left[G^{-1}(x,x')\right]_{\alpha\beta}^{ab} = \left[i\widetilde{\emptyset} - \langle \sigma_1 \rangle - \langle \sigma_2 \rangle \gamma^{35} - \langle \varphi_1 \rangle i\gamma^5 - \langle \varphi_2 \rangle \gamma^3\right]_{\alpha\beta} \delta^{ab} \delta^{(3)}(x-x').
$$

• Transformation properties of condensates

$\langle \overline{\psi} \mathsf{\Gamma}_i \psi \rangle$	$\langle \overline{\psi} \psi \rangle$	$\langle \overline{\psi} \gamma^{35} \psi \rangle$	$\langle \overline{\psi} i \gamma^5 \psi \rangle$	$\langle \overline{\psi} \gamma^3 \psi \rangle$

 ${\sf Table:}$ Transformation properties of various condensates $\langle \overline{\psi} \Gamma_i \psi \rangle$, where now $\Gamma_i=\{I_4, \gamma^{35}, i\gamma^5, \gamma^3\}$, under discrete ${\cal P}$, C, $\mathcal T$ and γ^5 , γ^3 transformations (here we consider $\mathcal P$: $(x^0, x, y) \to (x^0, -x, y)$).

- i $\langle \overline{\psi}\psi\rangle$ breaks $U(2N_{\rm f})$ and discrete γ^5 , γ^3 , but preserves ${\cal P}$, ${\cal C}$, ${\cal T}$
- ii $\langle \overline{\psi}\gamma^{35}\psi\rangle$ preserves $U(2N_{\rm f}),$ ${\cal C},$ γ^5 , γ^3 , but breaks ${\cal P},$ ${\cal T}.$,,Haldane mass" $m_2 = \langle \sigma_2 \rangle / {\sf v_{\rm F}}^2$ related to parity anomaly in $D = (2 + 1)$ dimension
- iii $\langle \overline{\psi} i\gamma^5 \psi\rangle$ breaks $U(2N_{\rm f})$ and discrete ${\cal P}$, ${\cal C}$, γ^5 , but preserves ${\cal T}$ and γ^3
- iv $\langle \overline{\psi} i\gamma^3 \psi \rangle$ breaks $U(2N_{\rm f})$ and γ^3 , but preserves ${\cal P}$, ${\cal C}$, ${\cal T}$ and γ^5

• Partition function of semi-bosonized Lagrangian:

$$
Z = \int D\overline{\psi}D\psi \int D\sigma_1 D\sigma_2 D\varphi_1 D\varphi_2 \exp\left\{i \int dx^0 d^2x \mathcal{L}[\overline{\psi}, \psi, \sigma_i, \varphi_i]\right\}
$$
 (2)

Fermion determinant of Dirac operator $\hat{D}(x,y)=D(x,y)I_{N_{\mathrm{f}}}\,$ (being the inverse propagator) rewritten by using $\mathsf{Det}(\hat{D}) = (\mathsf{Det}\,D)^{\mathsf{N}_\mathrm{f}} = \mathsf{exp}(\mathsf{N}_\mathrm{f} \text{Tr}_{\mathsf{s}\mathsf{x}} \mathsf{In}\,D)$:

$$
Z = \int D\sigma_1 D\sigma_2 D\varphi_1 D\varphi_2 \exp \{iN_f S_{\text{eff}}(\sigma_i, \varphi_i)\},
$$

$$
S_{\text{eff}}(\sigma_i, \varphi_i) = -\int dx^0 d^2x \sum_{k=1}^2 \left(\frac{\sigma_k^2}{4v_{\text{F}} G_k} + \frac{\varphi_k^2}{4v_{\text{F}} H_k}\right)
$$

$$
-i \text{Tr}_{\text{sx}} \ln(i\tilde{\phi} - \sigma_1 - \sigma_2 \gamma^{35} - \varphi_1 i \gamma^5 - \varphi_2 \gamma^3)
$$

 \bullet Effective potential (large- \mathcal{N}_{f} saddle point \Rightarrow $\sigma_i, \varphi_i = \mathrm{const})$

$$
V_{\text{eff}}(\sigma_i, \varphi_i) \int d x^0 d^2 x = -S_{\text{eff}}(\sigma_i, \varphi_i) \Big|_{\sigma_i, \varphi_i = \text{const}},
$$

$$
V_{\text{eff}}(\sigma_i, \varphi_i) = \sum_{k=1}^2 \left(\frac{\sigma_k^2}{4v_{\text{F}} G_k} + \frac{\varphi_k^2}{4v_{\text{F}} H_k} \right) + i \int \frac{d\rho_0 d^2 \vec{p}}{(2\pi)^3} \text{Tr}_s \ln D(p),
$$

$$
D(p) = p_0 \gamma^0 - v_{\text{F}} \vec{p} \vec{\gamma} - \sigma_1 - \sigma_2 \gamma^{35} - \varphi_1 i \gamma^5 - \varphi_2 \gamma^3
$$

Using $\text{Tr}_{\bm{s}}$ In $D(\bm{p}) = \sum_i \text{ln } \epsilon_i$ with ϵ_i the four eigenvalues of the 4 \times 4 matrix $D(p)$, one can calculate the momentum integral and obtain (for $M_k/\Lambda \ll 1$):

$$
V_{\text{eff}}(\sigma_i, \varphi_i) = \sum_{k=1}^2 \left\{ \frac{g_k \sigma_k^2}{4v_F} + \frac{h_k \varphi_k^2}{4v_F} + \frac{M_k^3}{6\pi v_F^2} \right\},
$$

$$
M_{1,2} = |\sigma_2 \pm \rho|, \ \rho = \sqrt{\sigma_1^2 + \varphi_1^2 + \varphi_2^2},
$$

where $g_k = \frac{1}{\mathsf{G}_k} - \frac{1}{\mathsf{G}_{\mathrm{cr}}},\ h_k = \frac{1}{\mathsf{H}_k} - \frac{1}{\mathsf{H}_{\mathrm{cr}}},\ (\mathsf{G}_{\mathrm{cr}}^{-1} = \mathsf{H}_{\mathrm{cr}}^{-1} = \frac{2\Lambda}{\pi})$

• Gap equations

$$
\frac{\partial V_{\text{eff}}(\sigma_i, \varphi_i)}{\partial \sigma_i} = 0, \quad \frac{\partial V_{\text{eff}}(\sigma_i, \varphi_i)}{\partial \varphi_i} = 0, \quad i = 1, 2 \tag{3}
$$

Illustration: $g_1 = g_2 = h_1 = h_2 = g$ **Solutions**

i
$$
\langle \sigma_1 \rangle = -\pi g v_F/2
$$
, $\langle \sigma_2 \rangle = \langle \varphi_1 \rangle = \langle \varphi_2 \rangle = 0$
\nii $\langle \sigma_2 \rangle = -\pi g v_F/2$, $\langle \sigma_1 \rangle = \langle \varphi_1 \rangle = \langle \varphi_2 \rangle = 0$
\niii $\langle \varphi_1 \rangle = -\pi g v_F/2$, $\langle \sigma_1 \rangle = \langle \sigma_2 \rangle = \langle \varphi_2 \rangle = 0$
\niv $\langle \varphi_2 \rangle = -\pi g v_F/2$, $\langle \sigma_1 \rangle = \langle \sigma_2 \rangle = \langle \varphi_1 \rangle = 0$

• Exciton Spectrum:

$$
\sigma_k(x) \to \langle \sigma_k \rangle + \sigma_k(x), \ \varphi_k(x) \to \langle \varphi_k \rangle + \varphi_k(x)
$$

Consider now the phase with $\langle \sigma_1 \rangle = m_1 v_{\rm F}^2$, $\langle \sigma_2 \rangle = \langle \varphi_1 \rangle = \langle \varphi_2 \rangle = 0$. Two point 1PI Green function (inverse propagators) of fluctuating fields:

$$
\Gamma_{\phi_k\phi_k}(x-y) = \frac{\delta^2 S_{\text{eff}}}{\delta\phi_k(x)\delta\phi_k(y)}\Big|_{\sigma_i,\varphi_i=0} , \phi_k = \{\sigma_1,\sigma_2,\varphi_1,\varphi_2\},
$$

$$
\Gamma_{\phi_k\phi_k}(x-y) = -\frac{1}{2v_{\text{F}}G_{\phi_k}}\delta^{(3)}(x-y) + i\text{Tr}_s \left[\hat{t}_k G_0(x-y)\hat{t}_k G_0(y-x)\right].
$$

Notations:

$$
G_{\phi_k} = \{ G_1, G_2, H_1, H_2 \}, \qquad \hat{t}_k = \{ I_4, \gamma^{35}, i\gamma^5, \gamma^3 \}, \qquad k = (1, ..., 4),
$$

$$
G_0(x-y)_{\alpha\beta}=\int \frac{d^3p}{(2\pi)^3}\left(\frac{1}{\widetilde{p}-m_1v_{\rm F}^2}\right)_{\alpha\beta}e^{-ip(x-y)}\qquad (\widetilde{p}=(p^0,v_{\rm F}\vec{p}))
$$

• The straightforward loop calculations yields in momentum space (Minkowski metric):

$$
\Gamma_{\sigma_1 \sigma_1}(p) = \frac{\tilde{p}^2 - (2m_1v_F^2)^2}{2\pi v_F^2 \sqrt{-\tilde{p}^2}} \Gamma(p),
$$

\n
$$
\Gamma(p) = \tan^{-1}\left(\frac{\sqrt{-\tilde{p}^2}}{2m_1v_F^2}\right),
$$

\n
$$
\Gamma_{\sigma_2 \sigma_2}(p) = -\frac{1}{2v_F}(g_2 - g_1) + \frac{\tilde{p}^2 - (2m_1v_F^2)^2}{2\pi v_F^2 \sqrt{-\tilde{p}^2}} \Gamma(p),
$$

\n
$$
\Gamma_{\varphi_k \varphi_k}(p) = -\frac{1}{2v_F}(h_k - g_1) - \frac{\sqrt{-\tilde{p}^2}}{2\pi v_F^2} \Gamma(p).
$$

The inverse expressions are just the exciton propagators, the singularities of which determine their mass spectrum and dispersion laws. Scalar excitation σ_1 corresponds to a stable particle with a mass $m_{\sigma} = 2m_1$. Quasiparticle σ_2 is scalar resonance

• Under certain restrictions of coupling constants, the model Lagrangian acquires additional continuous symmetry. Illustration: $g_1 = h_1 = g < 0$, $g_2 = h_2 > g \Rightarrow \langle \sigma_1 \rangle \sim \langle \overline{\psi} \psi \rangle \neq 0$

Lagrangian is invariant under continuous chiral symmetry:

$$
U_{\gamma^5}(1) \; : \; \psi \to \exp(i\alpha \gamma^5) \psi,
$$

 \Rightarrow massless GB: φ_1 .

• Compactification:

One spatial dimension compactified and lattice sheet is rolled up to a cylinder. Compactification of coordinate $x^2=R\varphi$ with a length $L=2\pi R$ (R cylinder radius) and x^1 pointing in *z*-direction, parallel to cylinder axis.

There exists a constant gauge field A_2 (not to be gauged away) to be included by $\partial_2 \rightarrow D_2 = \partial_2 + i e \mathcal{A}_2$. Alternatively, keep ∂_2 and include an effective magnetic phase ϕ into the boundary condition:

$$
\phi = \frac{e\mathcal{A}_2 L}{2\pi} = \frac{\Phi_m}{\Phi_m^0}
$$

 Φ_m — the magnetic flux passing through the tube cross section, $\Phi_m^0=2\pi/e$ is magnetic flux quantum.

Boundary condition:

$$
\psi_{\mathsf{K}}(x^0, \vec{r} + \vec{L}) = e^{2\pi i (\phi - \frac{1}{3}\nu)} \psi_{\mathsf{K}}(x^0, \vec{r}), \quad \nu = (0, \pm 1), \psi_{\mathsf{K}'}(x^0, \vec{r} + \vec{L}) = e^{2\pi i (\phi + \frac{1}{3}\nu)} \psi_{\mathsf{K}'}(x^0, \vec{r}).
$$

Fourier decomposition of spinors:

$$
\psi = \frac{1}{L} \sum_{n=-\infty}^{\infty} e^{i \left[\frac{x^2}{R} (n+\phi) + p_1 x^1 + p_0 x^0 \right]} \begin{pmatrix} \psi_{Nn}^{(1)} \\ \psi_{K'n}^{(2)} \end{pmatrix},
$$

$$
\psi_{Kn}^{(1)} = \begin{pmatrix} \psi_{Kn}^A \\ \psi_{Kn}^B \end{pmatrix} e^{-i\frac{x^2}{R} \left(\frac{u}{3}\right)},
$$

$$
\psi_{K'n}^{(2)} = \begin{pmatrix} -i\psi_{K'n}^B \\ i\psi_{K'n}^A \end{pmatrix} e^{i\frac{x^2}{R} \left(\frac{u}{3}\right)}.
$$

• Azimuthal component of the p_2 momentum:

$$
p_{\nu\phi}(n)=\frac{2\pi}{L}(n+\phi-\frac{\nu}{3}),
$$

 $\nu \neq 0 \Rightarrow$ "semiconductor" energy gap between conduction/valence bands

$$
\Delta \mathcal{E}(n=\phi=p_1=0)=v_{\rm F}\frac{4\pi}{L}\frac{|\nu|}{3}\neq 0.
$$

 $\nu = 0 \Rightarrow$ "metallic" behavior.

Insulator phase for dynamical mass

$$
\Delta \mathcal{E}(n=p_1=\phi=0)=2\sqrt{v_{\rm F}^2\left(\frac{2\pi}{L}\right)^2\left(\frac{\nu}{3}\right)^2+(mv_{\rm F}^2)^2}.
$$

• Thermodynamic potential $\Omega_T (\rightarrow V_{\text{eff}})$:

Inclusion of temperature T and extended "chemical" potential $\hat{\mu} = \mu - \frac{g}{2} s \mu_{\rm B} B_{\parallel}$ describing Zeeman interaction.

Replace p_0 -integration in effective potential by summation over Matsubara frequencies ω_{ℓ} using rule:

$$
\int_{-\infty}^{\infty} \frac{dp_0}{2\pi} f(p_0) \to \frac{i}{\beta} \sum_{\ell=-\infty}^{\infty} f(i\omega_{\ell}),
$$

$$
\omega_{\ell} = \frac{2\pi}{\beta} \left(\ell + \frac{1}{2}\right), \quad \ell = 0, \pm 1, \pm 2, ...
$$

$$
\beta = \frac{1}{\mathcal{T}}, \text{ inverse temperature.}
$$

Standard shift

$$
\omega_{\ell} \to \omega_{\ell} - i\hat{\mu}, \quad \hat{\mu} = \mu - \frac{g}{2} s \mu_{\rm B} B_{\parallel} \tag{4}
$$

where $s = \pm 1$ for up/down spin, g Landé factor, $\mu_B = e/(2m)$ the Bohr magneton and B_{\parallel} longitudinal in-plane magnetic field. Boundary condition for nanotubes gives $p_2 \to p_{\nu\phi}(n) = \frac{2\pi}{L}(n + \phi - \frac{\nu}{3});$ ϕ expressed by magnetic AB flux.

• Thermodynamic potential

$$
V_{\text{eff}}(\sigma_i, \varphi_i, \mathcal{T}, \hat{\mu}, \phi) = \sum_{k=1}^{2} \left\{ \left(\frac{\sigma_k^2}{4v_{\text{F}} G_k} + \frac{\varphi_k^2}{4v_{\text{F}} H_k} \right) - \frac{1}{\beta L \sum_{s=\pm 1}^{2} \sum_{\ell=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \int \frac{dp_1}{2\pi} \ln \left[\left(\frac{2\pi}{\beta} \left(\ell + \frac{1}{2} \right) - i\hat{\mu} \right)^2 + v_{\text{F}}^2 \left(\frac{2\pi}{L} \right)^2 \left(n + \phi - \frac{\nu}{3} \right)^2 + v_{\text{F}}^2 p_1^2 + M_k^2 \right] \right\}.
$$

Phase transitions: Aharonov–Bohm effect

• Numerical investigation of the global minima of the thermodynamic potential $V_{\text{eff}}(\sigma, \phi, T)$.

Figure: Phase diagrams of the model in the plane (L, β) with different values of the magnetic phase ϕ and in the plane (ϕ, β) with fixed $L < L_c$ ($L_c = v_{\rm F} \beta_c$). Painted area: symmetrical phase Unpainted area: broken symmetry

Phase transitions: Zeeman effect

Area II: symmetrical phase, only one minimum at $\sigma = 0$

Area III: broken symmetry, global minimum at $\sigma \neq 0$, local minimum at $\sigma = 0$

Area IV: symmetrical phase, global minimum at $\sigma = 0$, local minimum at $\sigma \neq 0$

Line AB: phase transition of second kind

Line BE: phase transition of first kind

Lines BC and BD: no phase transition, local minima appear/vanish

Summary

- Tight binding Hamiltonian \rightarrow effective low energy Dirac-like model of massless electrons
	- \triangleright (reducible) 4-spinors
		- $-$ 2 sublattice $(A, B \rightarrow)$ pseudospin)
		- − 2 valley (Dirac points) d.o.f.
	- \triangleright Chirality operator γ^5 (pseudohelicity)
- $U(2N_f)$ chiral symmetry
- Four-fermion contact Coulomb, one-site scalar, and phonon-mediated interactions \rightarrow XSB by condensates
- Fierz-transformation and generalization to extended schematic GN model
- Effective potential: gap eqs. and exciton spectrum
- • Nanotubes by compactification and boundary conditions
	- \triangleright Phase transitions at L, T, ϕ with AB effect
	- \triangleright Phase transitions at $\delta\mu$ and T with Zeeman effect