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

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> JINR Dubna April 2016

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Summary

Introduction

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
 - D Two sublattice degrees of freedom (pseudospin)
 - D Two valley degrees of freedom (2 Dirac points)
 - \Rightarrow reducible 4-spinor description in $D=2+1 \iff$ chiral γ^5

- Chiral "valley-sublattice" symmetry $\mathit{U}(2)_{\rm vs}$
- Inclusion of Coulomb interaction and general four-fermion interactions \Rightarrow 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:

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

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

$$\begin{split} \mathcal{L}_{0} &= \overline{\psi} \left[i \gamma^{0} \partial_{0} + i v_{\mathrm{F}} \gamma^{1} \partial_{x} + i v_{\mathrm{F}} \gamma^{2} \partial_{y} \right] \psi = \overline{\psi} i \gamma^{\mu} \widetilde{\partial}_{\mu} \psi \\ \\ \tilde{\partial}_{\mu} &= (\partial_{0}, v_{\mathrm{F}} \vec{\nabla}), \ v_{\mathrm{F}} = \frac{3}{2} t a \\ \\ \psi^{t} &= (\psi^{Aa}_{K}, \psi^{Ba}_{K}, -i \psi^{Ba}_{K'}, i \psi^{Aa}_{K'}) \end{split}$$

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

$$\begin{split} \gamma^0 &= \begin{pmatrix} 0 & \mathrm{I}_2 \\ \mathrm{I}_2 & 0 \end{pmatrix}, \ \gamma^1 = \begin{pmatrix} 0 & -\tau^1 \\ \tau^1 & 0 \end{pmatrix}, \ \gamma^2 = \begin{pmatrix} 0 & -\tau^2 \\ \tau^2 & 0 \end{pmatrix} \\ \gamma^3 &= \begin{pmatrix} 0 & -\tau^3 \\ \tau^3 & 0 \end{pmatrix}, \ \gamma^5 = \begin{pmatrix} \mathrm{I}_2 & 0 \\ 0 & -\mathrm{I}_2 \end{pmatrix}, \ \gamma^{35} = \frac{1}{2} \begin{bmatrix} \gamma^3, \gamma^5 \end{bmatrix} = \begin{pmatrix} 0 & \tau^3 \\ \tau^3 & 0 \end{pmatrix}. \end{split}$$

"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 $U(2)_{vs}$ -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 \mathcal{P} , \mathcal{C} , \mathcal{T} :

$$\begin{split} \psi(x^{0}, x, y) &\xrightarrow{\mathcal{P}} i\gamma^{1}\gamma^{5}\psi(x^{0}, -x, y), \\ \psi(x^{0}, \vec{r}) &\xrightarrow{\mathcal{C}} \gamma^{1}\overline{\psi}^{t}(x^{0}, \vec{r}), \\ \psi(x^{0}, \vec{r}) &\xrightarrow{\mathcal{T}} i\sigma^{2}\gamma^{1}\gamma^{5}\psi(-x^{0}, \vec{r}) \end{split}$$

Four-fermion interactions

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

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

$$\widetilde{D}_{\mu} = (\partial_0 - i e A_0, v_{\mathrm{F}} (ec{
abla} + i e ec{\mathcal{A}}))$$

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

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

Instantaneous Coulomb potential

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

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 $U(2N_{\rm f})$ -invariant four-fermion interaction Lagrangian:

$$\mathcal{L}_{ ext{int}}^{C} = -rac{\mathcal{G}_{c} v_{ ext{F}}}{2} \left[\overline{\psi}(x) \gamma^{0} \psi(x)
ight]^{2}$$

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

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

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

$$\mathcal{L}_{\mathrm{int}} = -\frac{1}{2} G_{c} v_{\mathrm{F}} (\overline{\psi} \gamma^{0} \psi)^{2} + \frac{\widetilde{G} v_{\mathrm{F}}}{2} (\overline{\psi} \psi)^{2}, \quad \widetilde{G} = G + g$$

• Fierz-transformation:

$$\begin{split} \mathcal{L} &= \mathcal{L}_{0} + \mathcal{L}_{\text{int}} = \overline{\psi} i \widetilde{\partial} \psi \\ &+ \Big\{ \frac{1}{2N_{\text{f}}} G_{1} v_{\text{F}} (\overline{\psi} \psi)^{2} + \frac{1}{2N_{\text{f}}} G_{2} v_{\text{F}} (\overline{\psi} \gamma^{35} \psi)^{2} \\ &+ \frac{1}{2N_{\text{f}}} H_{1} v_{\text{F}} (\overline{\psi} i \gamma^{5} \psi)^{2} + \frac{1}{2N_{\text{f}}} H_{2} v_{\text{F}} (\overline{\psi} \gamma^{3} \psi)^{2} \Big\} \end{split}$$

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

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Effective potential; gap equation and exciton spectrum

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

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

• Field equations for exciton fields

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

• Gap equations:

$$\begin{split} \langle \sigma_1 \rangle &= -2 \frac{G_1 v_{\rm F}}{N_{\rm f}} \langle \overline{\psi} \psi \rangle = 2 \frac{G_1 v_{\rm F}}{N_{\rm f}} {\rm Tr}_{\rm sf} \left[iG(x, x) \right], \\ \langle \sigma_2 \rangle &= -2 \frac{G_2 v_{\rm F}}{N_{\rm f}} \langle \overline{\psi} \gamma^{35} \psi \rangle = 2 \frac{G_2 v_{\rm F}}{N_{\rm f}} {\rm Tr}_{\rm sf} \left[\gamma^{35} iG(x, x) \right], \\ \langle \varphi_1 \rangle &= -2 \frac{H_1 v_{\rm F}}{N_{\rm f}} \langle \overline{\psi} i \gamma^5 \psi \rangle = 2 \frac{H_1 v_{\rm F}}{N_{\rm f}} {\rm Tr}_{\rm sf} \left[i \gamma^5 iG(x, x) \right], \\ \langle \varphi_2 \rangle &= -2 \frac{H_2 v_{\rm F}}{N_{\rm f}} \langle \overline{\psi} \gamma^3 \psi \rangle = 2 \frac{H_2 v_{\rm F}}{N_{\rm f}} {\rm Tr}_{\rm sf} \left[\gamma^3 iG(x, x) \right], \end{split}$$

Inverse fermion propagator

$$\left[G^{-1}(x,x')\right]^{ab}_{\alpha\beta} = \left[i\widetilde{\not} - \langle \sigma_1 \rangle - \langle \sigma_2 \rangle \gamma^{35} - \langle \varphi_1 \rangle i\gamma^5 - \langle \varphi_2 \rangle \gamma^3\right]_{\alpha\beta} \delta^{ab} \delta^{(3)}(x-x').$$

• Transformation properties of condensates

$\langle \overline{\psi} \Gamma_i \psi \rangle$	$\langle \overline{\psi}\psi \rangle$	$\langle \overline{\psi} \gamma^{35} \psi \rangle$	$\langle \overline{\psi} i \gamma^5 \psi \rangle$	$\left<\overline{\psi}\gamma^{3}\psi\right>$
\mathcal{P}	1	-1	-1	1
\mathcal{C}	1	1	$^{-1}$	1
\mathcal{T}	1	-1	1	1
γ^5	-1	1	-1	1
γ^3	-1	1	1	-1

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 \mathcal{P} , \mathcal{C} , \mathcal{T} and γ^5 , γ^3 transformations (here we consider $\mathcal{P} : (x^0, x, y) \to (x^0, -x, y)$).

- i $\langle \overline{\psi}\psi
 angle$ breaks $U(2N_{
 m f})$ and discrete γ^5 , γ^3 , but preserves ${\cal P}$, ${\cal C}$, ${\cal T}$
- ii $\langle \overline{\psi} \gamma^{35} \psi \rangle$ preserves $U(2N_{\rm f})$, C, γ^5 , γ^3 , but breaks \mathcal{P} , \mathcal{T} . ,,Haldane mass" $m_2 = \langle \sigma_2 \rangle / v_{\rm F}^2$ 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 \mathcal{P} , \mathcal{C} , γ^5 , but preserves \mathcal{T} and γ^3
- iv $\langle \overline{\psi} i \gamma^3 \psi \rangle$ breaks $U(2N_{
 m f})$ and γ^3 , but preserves ${\cal P}$, ${\cal C}$, ${\cal T}$ and γ^5

• Partition function of semi-bosonized Lagrangian:

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

Fermion determinant of Dirac operator $\hat{D}(x, y) = D(x, y)I_{N_f}$ (being the inverse propagator) rewritten by using $\text{Det}(\hat{D}) = (\text{Det }D)^{N_f} = \exp(N_f \text{Tr}_{sx} \ln D)$:

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

$$S_{\rm eff}(\sigma_i,\varphi_i) = -\int dx^0 d^2 x \sum_{k=1}^2 \left(\frac{\sigma_k^2}{4v_{\rm F}G_k} + \frac{\varphi_k^2}{4v_{\rm F}H_k}\right)$$
$$-i \operatorname{Tr}_{sx} \ln(i\widetilde{\partial} - \sigma_1 - \sigma_2 \gamma^{35} - \varphi_1 i \gamma^5 - \varphi_2 \gamma^3)$$

• Effective potential (large- $N_{\rm f}$ saddle point $\Rightarrow \sigma_i, \varphi_i = {\rm const}$)

$$\begin{split} V_{\text{eff}}(\sigma_i,\varphi_i) \int dx^0 d^2 x &= -S_{\text{eff}}(\sigma_i,\varphi_i) \Big|_{\sigma_i,\varphi_i=\text{const}},\\ V_{\text{eff}}(\sigma_i,\varphi_i) &= \sum_{k=1}^2 \left(\frac{\sigma_k^2}{4\nu_{\text{F}}G_k} + \frac{\varphi_k^2}{4\nu_{\text{F}}H_k} \right) + i \int \frac{dp_0 d^2 \vec{p}}{(2\pi)^3} \text{Tr}_s \ln D(p),\\ D(p) &= p_0 \gamma^0 - \nu_{\text{F}} \vec{p} \vec{\gamma} - \sigma_1 - \sigma_2 \gamma^{35} - \varphi_1 i \gamma^5 - \varphi_2 \gamma^3 \end{split}$$

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

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

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

where $g_k = \frac{1}{G_k} - \frac{1}{G_{
m cr}}$, $h_k = \frac{1}{H_k} - \frac{1}{H_{
m cr}}$, $(G_{
m cr}^{-1} = H_{
m cr}^{-1} = \frac{2\Lambda}{\pi})$

• Gap equations

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

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

$$\begin{array}{l} \mathsf{i} \ \langle \sigma_1 \rangle = -\pi g v_{\mathrm{F}}/2, \ \langle \sigma_2 \rangle = \langle \varphi_1 \rangle = \langle \varphi_2 \rangle = 0 \\ \\ \mathsf{ii} \ \langle \sigma_2 \rangle = -\pi g v_{\mathrm{F}}/2, \ \langle \sigma_1 \rangle = \langle \varphi_1 \rangle = \langle \varphi_2 \rangle = 0 \\ \\ \\ \mathsf{iii} \ \langle \varphi_1 \rangle = -\pi g v_{\mathrm{F}}/2, \ \langle \sigma_1 \rangle = \langle \sigma_2 \rangle = \langle \varphi_2 \rangle = 0 \\ \\ \\ \\ \mathsf{iv} \ \langle \varphi_2 \rangle = -\pi g v_{\mathrm{F}}/2, \ \langle \sigma_1 \rangle = \langle \sigma_2 \rangle = \langle \varphi_1 \rangle = 0 \end{array}$$

• Exciton Spectrum:

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

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

$$\begin{split} \mathsf{\Gamma}_{\phi_k \phi_k}(x-y) &= \frac{\delta^2 \mathcal{S}_{\text{eff}}}{\delta \phi_k(x) \delta \phi_k(y)} \Big|_{\sigma_i, \varphi_i = 0} \ , \ \phi_k = \{\sigma_1, \sigma_2, \varphi_1, \varphi_2\}, \\ \mathsf{\Gamma}_{\phi_k \phi_k}(x-y) &= -\frac{1}{2 v_{\text{F}} \mathcal{G}_{\phi_k}} \delta^{(3)}(x-y) + i \text{Tr}_s \left[\hat{t}_k \mathcal{G}_0(x-y) \hat{t}_k \mathcal{G}_0(y-x) \right]. \end{split}$$

Notations:

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

$$G_0(x-y)_{\alpha\beta} = \int \frac{d^3p}{(2\pi)^3} \left(\frac{1}{\vec{p} - m_1 v_{\rm F}^2}\right)_{\alpha\beta} e^{-ip(x-y)} \qquad (\vec{p} = (p^0, v_{\rm F}\vec{p}))$$

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

$$\begin{split} \Gamma_{\sigma_1 \sigma_1}(p) &= \frac{\widetilde{p}^2 - (2m_1 v_{\rm F}^2)^2}{2\pi v_{\rm F}^2 \sqrt{-\widetilde{p}^2}} \Gamma(p), \\ \Gamma(p) &= \tan^{-1} \left(\frac{\sqrt{-\widetilde{p}^2}}{2m_1 v_{\rm F}^2} \right), \\ \Gamma_{\sigma_2 \sigma_2}(p) &= -\frac{1}{2v_{\rm F}} (g_2 - g_1) + \frac{\widetilde{p}^2 - (2m_1 v_{\rm F}^2)^2}{2\pi v_{\rm F}^2 \sqrt{-\widetilde{p}^2}} \Gamma(p), \\ \Gamma_{\varphi_k \varphi_k}(p) &= -\frac{1}{2v_{\rm F}} (h_k - g_1) - \frac{\sqrt{-\widetilde{p}^2}}{2\pi v_{\rm F}^2} \Gamma(p). \end{split}$$

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:

$$U_{\gamma^5}(1) : \psi o \exp(ilpha\gamma^5)\psi,$$

 \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 $\partial_2 \rightarrow D_2 = \partial_2 + ieA_2$. 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:

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

Fourier decomposition of spinors:

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

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

• Azimuthal component of the *p*₂ momentum:

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

 $\nu \neq \mathbf{0} \Rightarrow$ "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

$$\Delta \mathcal{E}(n=p_1=\phi=0)=2\sqrt{v_{\mathrm{F}}^2\left(rac{2\pi}{L}
ight)^2\left(rac{
u}{3}
ight)^2+(mv_{\mathrm{F}}^2)^2}.$$

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

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:

$$\int_{-\infty}^{\infty} rac{dp_0}{2\pi} f(p_0)
ightarrow rac{i}{eta} \sum_{\ell=-\infty}^{\infty} f(i\omega_\ell),$$
 $\omega_\ell = rac{2\pi}{eta} \left(\ell + rac{1}{2}
ight), \quad \ell = 0, \pm 1, \pm 2, ...$
 $eta = rac{1}{T}$, inverse temperature.

Standard shift

$$\omega_{\ell} \to \omega_{\ell} - i\hat{\mu}, \quad \hat{\mu} = \mu - \frac{g}{2} s\mu_{\rm B} B_{\parallel}$$
 (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 $p_2 \rightarrow p_{\nu\phi}(n) = \frac{2\pi}{L}(n + \phi - \frac{\nu}{3})$; ϕ expressed by magnetic AB flux.

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• Thermodynamic potential

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

Phase transitions: Aharonov-Bohm effect

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



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 $L < L_c (L_c = v_F \beta_c)$. Painted area: symmetrical phase Unpainted area: broken symmetry

Phase transitions: Zeeman effect



Figure: Phase diagram of the model in the plane ($\delta\mu$, *T*) Area I: broken symmetry, only one minimum at $\sigma \neq 0$ Area II: symmetrical phase, only one minimum at $\sigma = 0$ Area III: broken symmetry, global minimum at $\sigma \neq 0$, local minimum at $\sigma \neq 0$ Area IV: symmetrical phase, global minimum at $\sigma = 0$, local minimum at $\sigma \neq 0$ Line AB: phase transition of second kind Lines BC and BD: no phase transition, local minima appear/vanish

Summary

Summary

- Tight binding Hamiltonian \longrightarrow effective low energy Dirac-like model of massless electrons
 - ▷ (reducible) 4-spinors
 - 2 sublattice (A, B pseudospin)
 - 2 valley (Dirac points) d.o.f.
 - \triangleright Chirality operator γ^5 (pseudohelicity)
- $U(2N_{\rm f})$ chiral symmetry
- Four-fermion contact Coulomb, one-site scalar, and phonon-mediated interactions $\to \mathcal{X}SB$ 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 ${\cal T}$ with Zeeman effect