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SUMMER SCHOOL
on
LOW-DIMENSIONAL QUANTUM SYSTEMS:
Theory and Experiment
(16 - 27 JULY 2001)

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PRE-TUTORIAL SESSIONS
(11 - 13 JULY 2001)

ELECTRON EDGE STATES IN QUASI-ONE-DIMENSIONAL ORGANIC CONDUCTORS

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Electron Edge States in Quasi-One-Dimensional Organic Conductors

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Outline

I. Localized electron state at the end of a 1D system with a periodic potential

II. The structure of the Q1D organic conductors $(TMTTF)_2X$ and $(TMTSF)_2X$

III. Holon edge states in the charge-gap regime of $(TMTTF)_2X$

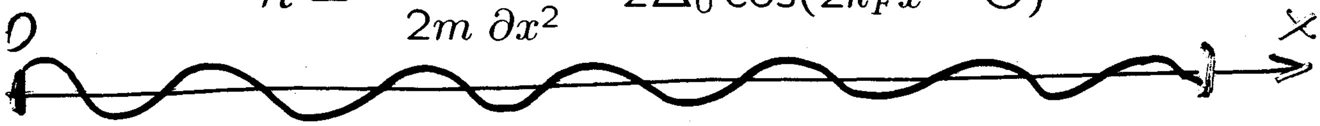
IV. Midgap Andreev bound states in the triplet superconducting state of $(TMTSF)_2X$

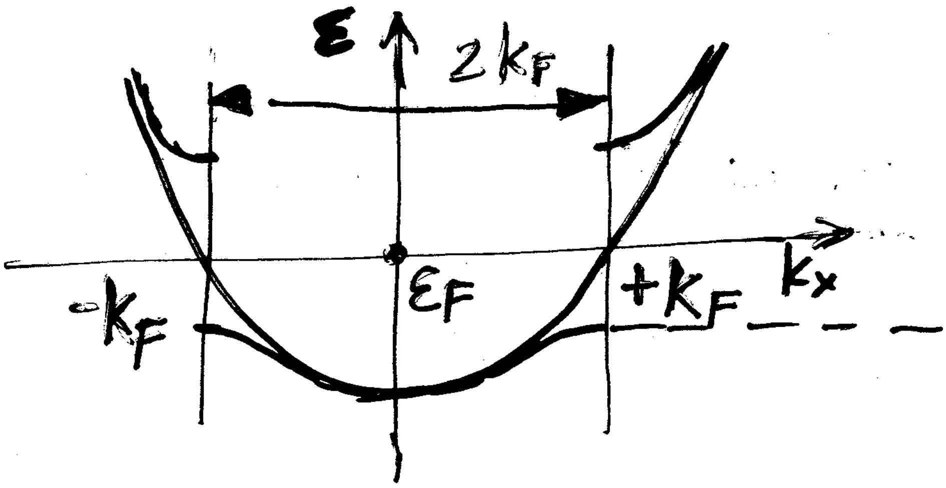
V. Chiral edge states in the quantum Hall regime of $(TMTSF)_2X$

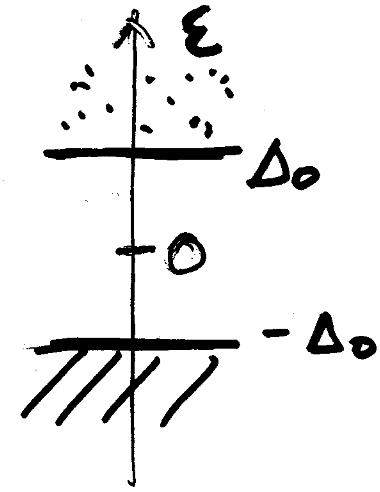
VI. Conclusions

Semi-infinite one-dimensional system with a periodic potential (CDW, SDW)

$$\hat{\mathcal{H}} = -\frac{1}{2m}\frac{\partial^2}{\partial x^2} - 2\Delta_0 \cos(2k_F x - \Theta)$$







$$\psi(x) = \psi_+(x)\, e^{ik_F x} + \psi_-(x)\, e^{-ik_F x}$$

$$\begin{pmatrix} -iv_F\partial_x & -\Delta_0 e^{-i\Theta} \\ -\Delta_0 e^{i\Theta} & iv_F\partial_x \end{pmatrix} \begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix}$$

Delocalized bulk states

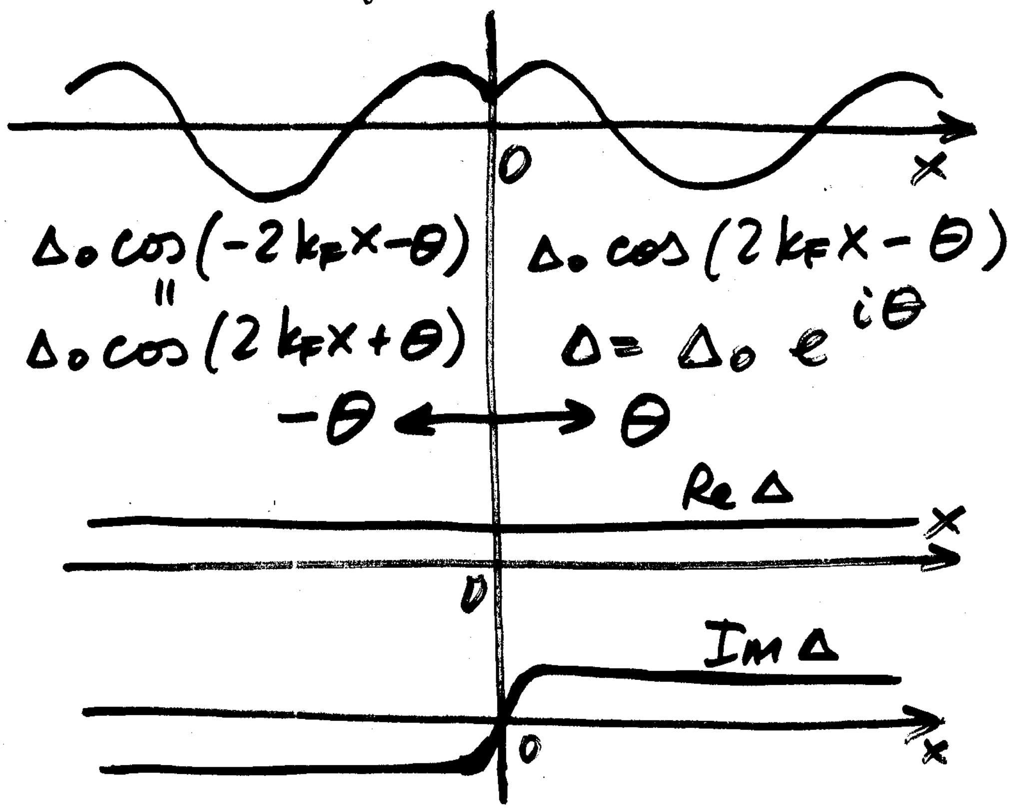
$$\begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix} \propto e^{ikx} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}, \qquad \varepsilon = \pm\sqrt{(v_F k)^2 + \Delta_0^2}$$

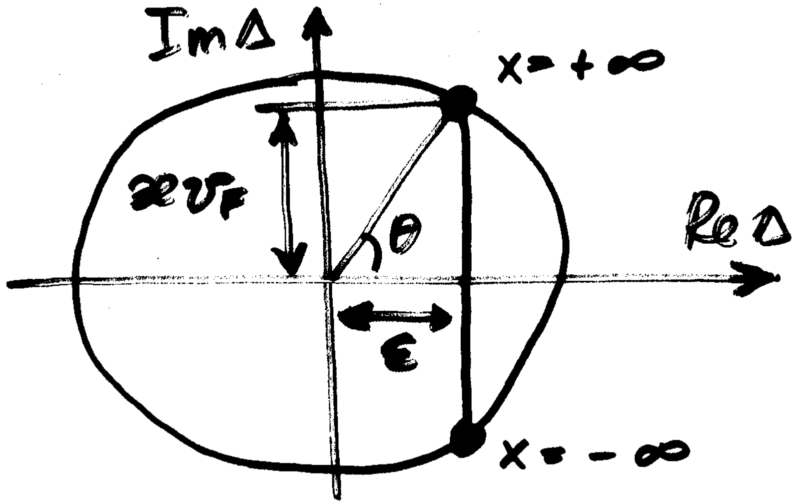
Localized edge state

Boundary condition: $\psi(x=0) = 0 \;\Rightarrow\; \psi_+ = -\psi_-$

$$\begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix} \propto e^{-\kappa x} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \qquad \varepsilon = \Delta_0 \cos\Theta, \qquad \kappa = \frac{\Delta_0}{v_F}\sin\Theta$$

$\Psi(-x) = -\Psi(x)$ Reflection around $x=0$ and kink-soliton states

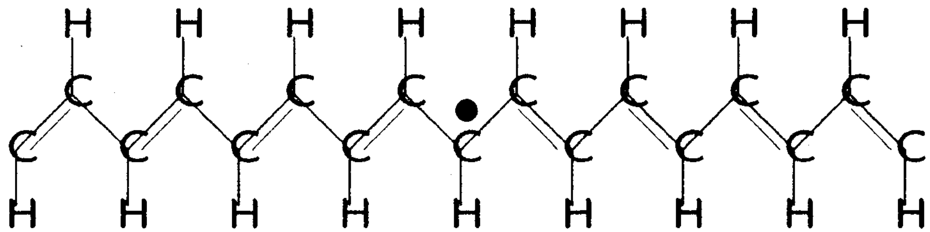




Bound state

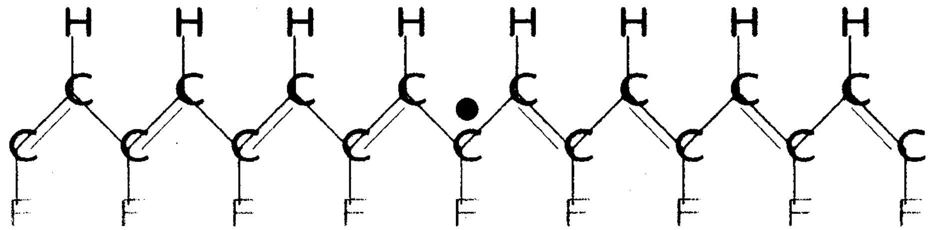
$$\varkappa = \mathrm{Im}\,\Delta / v_F$$

$$\varepsilon = \mathrm{Re}\,\Delta$$



Polyacetylene $(CH)_n$

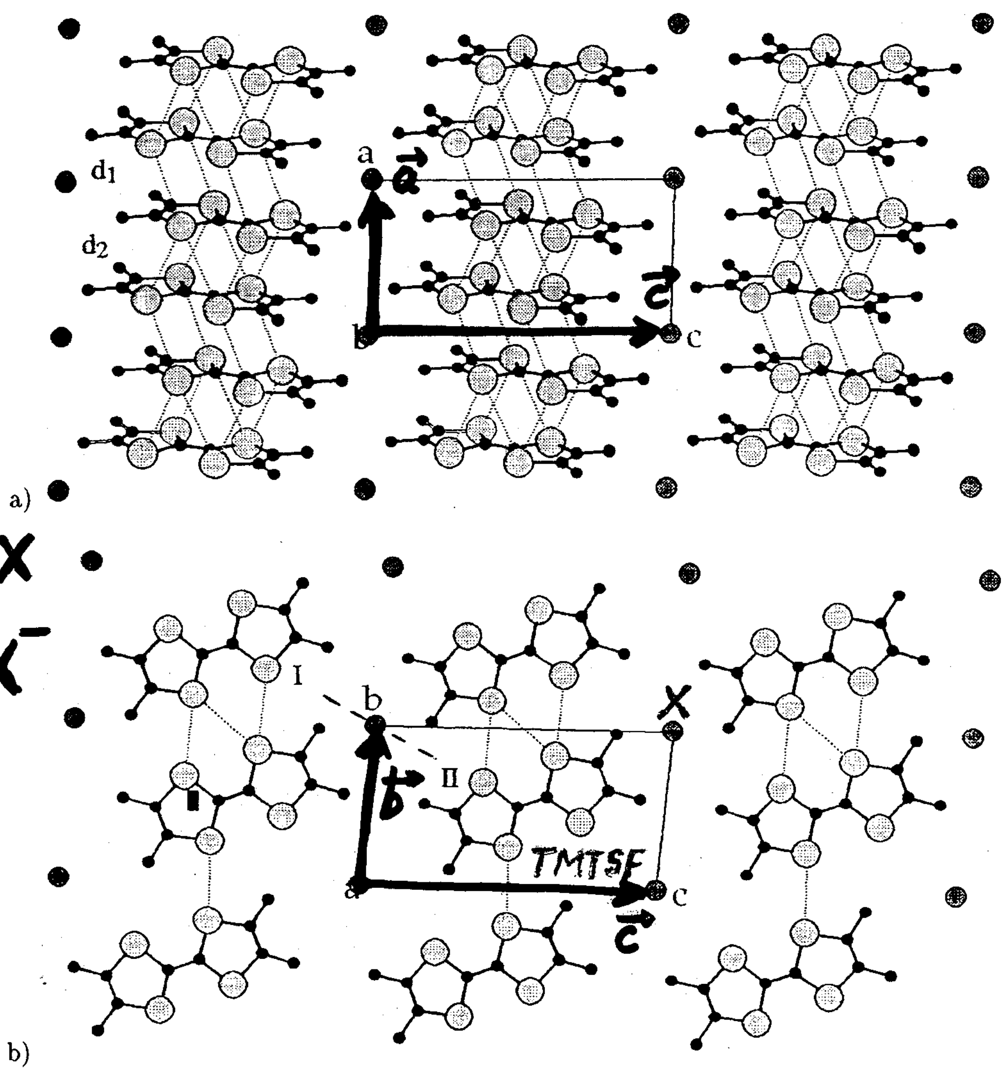
$\mathrm{Re}\Delta = 0 \Rightarrow$ midgap state $\varepsilon = 0$



$(CHCF)_n$ $\quad \varepsilon = \mathrm{Re}\Delta \neq 0$

Brazovskii (1980)
Brazovskii, Kirova, Matveenko (1984)

J.P. Pouget and S. Ravy J. Phys. I France $\underline{6}$, 1501 (1996)



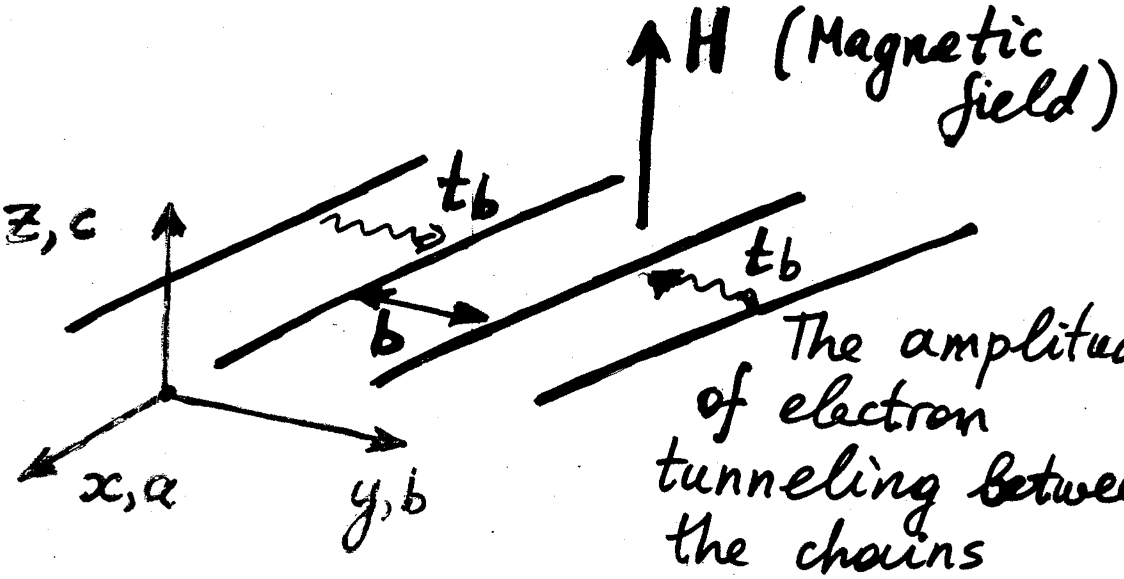
$(TMTTF)_2X$

$(TMTSF)_2^+X^-$

$X = PF_6$,

ClO_4

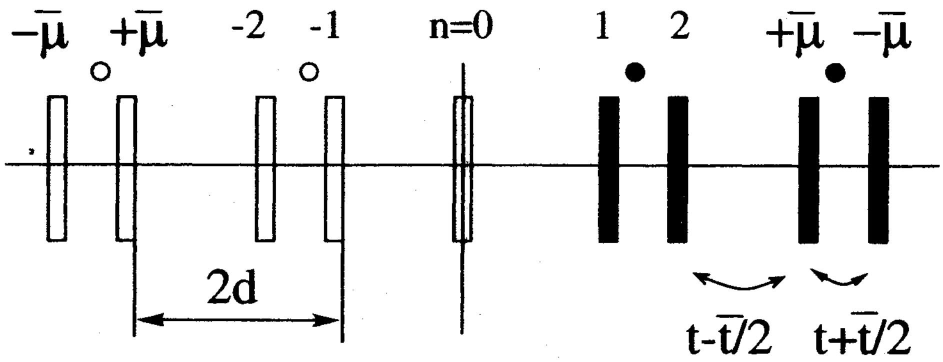
Fig. 1. — Projections of the crystallographic structure of $(TMTSF)_2X$ in the $(\mathbf{a}, \mathbf{c})$ plane (a) and the $(\mathbf{b}, \mathbf{c})$ plane (b). Only the Se (large grey dots) and C (small black dots) atoms of the TMTSF molecule are represented. The grey dots of medium size between the molecules symbolizes the location of the anions X.



The amplitude of electron tunneling between the chains

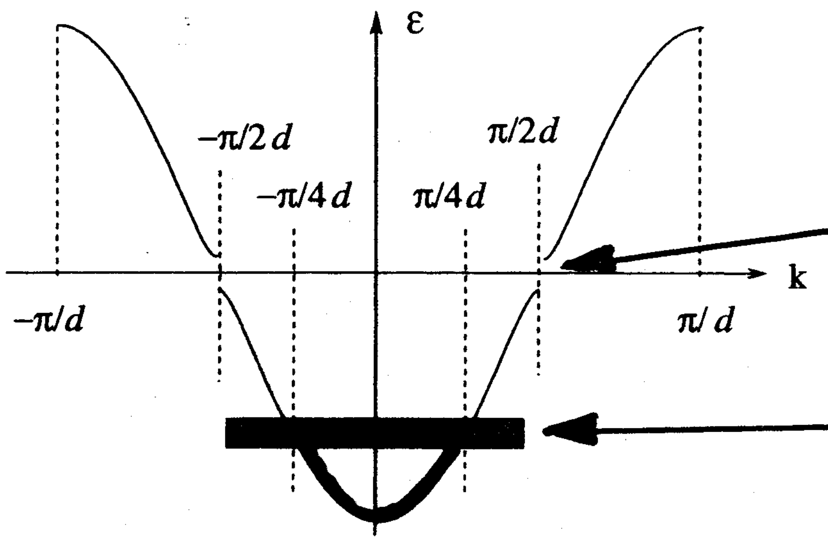
The structure of $(TMTTF)_2X$

Bonds are always dimerized, but the sites dimerize only below the ferroelectric transition, where the anions X displace to asymmetric positions [Nad', Monceau et al. (2000), S. Brown et al. (2000), Brazovskii et al. (2001)].



$$\hat{H} = -\sum_{n=1,\,s}^{\infty}\left[t_n(\hat{\psi}^{\dagger}_{n,s}\hat{\psi}_{n+1,s} + \text{H.c.}) + \mu_n\hat{\psi}^{\dagger}_{n,s}\hat{\psi}_{n,s}\right],$$

$$t_n = t - (-1)^n\bar{t}/2, \qquad \mu_n = \mu - (-1)^n\bar{\mu}.$$



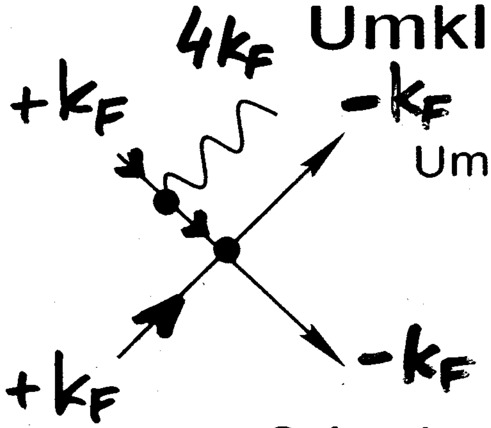
Single-particle gap around $\varepsilon = 0$ at 1/2 filling

Correlation gap due to umklapp at 1/4 filling

For the single-particle gap around $\varepsilon = 0$ (at 1/2 filling):

$$\Delta = -\bar{\mu} - i\bar{t}, \qquad \kappa u_F = \mathrm{Im}\Delta = -\bar{t}, \qquad \varepsilon_c = \mathrm{Re}\Delta = -\bar{\mu}$$

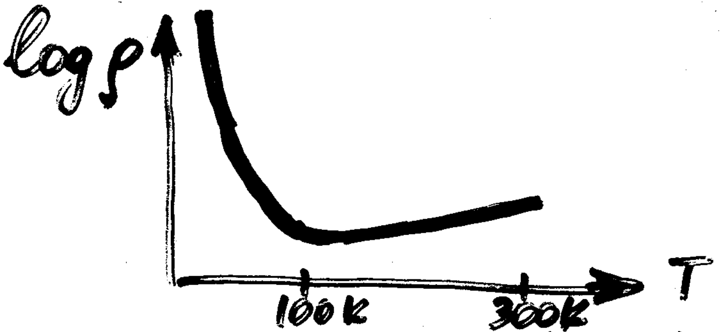
Umklapp and charge gap



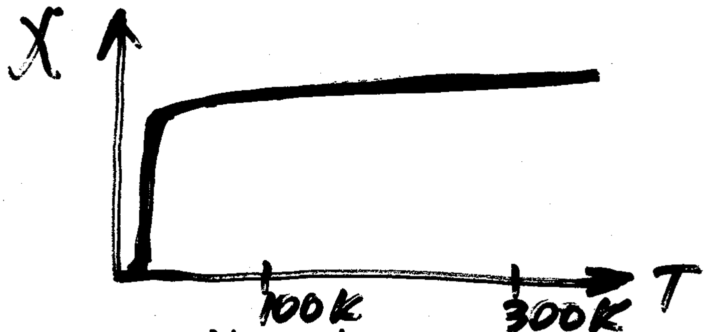
Umklapp scattering amplitude $g_3 = g_3^a + i g_3^b$,

$$g_3^a = -\sqrt{2}\, U d \frac{\bar{\mu}}{t}, \quad g_3^b = U d \frac{\bar{t}}{t}$$

Spin-charge separation in (TMTTF)$_2$X



Charge gap: $\rho \propto \exp(\Delta_\rho / T)$



No spin gap

Bosonization

$\psi_{\pm,\sigma} \to \dfrac{e^{i\phi_{\pm,\sigma}}}{\sqrt{2\pi\zeta}}$, separation into charge and spin channels.

At $K_\rho = 1/2$, Luther-Emery fermionization: $\dfrac{e^{i\varphi_\rho}}{\sqrt{2\pi\zeta}} \to \psi_\rho$.

Charge gap $\Delta_\rho = \dfrac{-g_3^b - i g_3^a}{2\pi\zeta}$ for the holons ψ_ρ.

Holon edge state

$$\varepsilon_{\rho e} = -\frac{g_3^b}{2\pi\zeta} = -|\Delta_\rho| \frac{\bar{t}}{\sqrt{\bar{t}^2 + 2\bar{\mu}^2}}, \quad v_{\rho\kappa} = -\frac{g_3^a}{2\pi\zeta} = |\Delta_\rho| \frac{\bar{\mu}\sqrt{2}}{\sqrt{\bar{t}^2 + 2\bar{\mu}^2}}$$

Prediction: The holon edge state should appear below the ferroelectric transition, which causes site dimerization.

For spin channel: Fabrizio & Gogolin (1995), Gogolin (1996).
For two legs: Maslov, Glazman et al. (1999), Le Hur (2000).

cond-mat/0010206   PRB. 63, 144531 (2001)

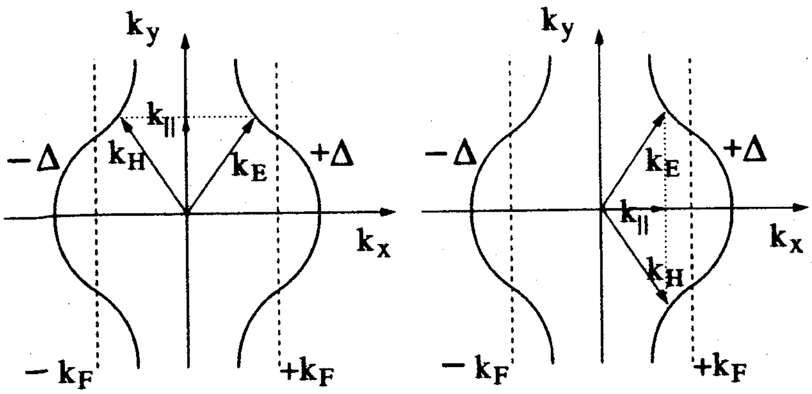
Edge states in the triplet superconducting state of Q1D conductor $(TMTSF)_2X$

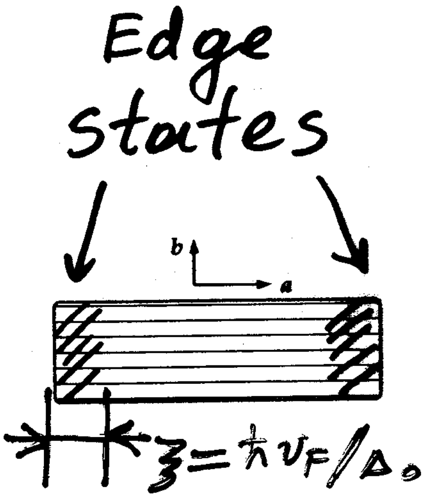
Singlet pairing: *s*-wave: common; *d*-wave: high-T_c cuprates

$$\langle \hat{\psi}_\alpha(k_F)\hat{\psi}_\beta(-k_F)\rangle = \epsilon_{\alpha\beta}\Delta(k_F) = i\sigma_y\Delta(k_F), \quad \Delta(+k_F)=\Delta(-k_F)$$

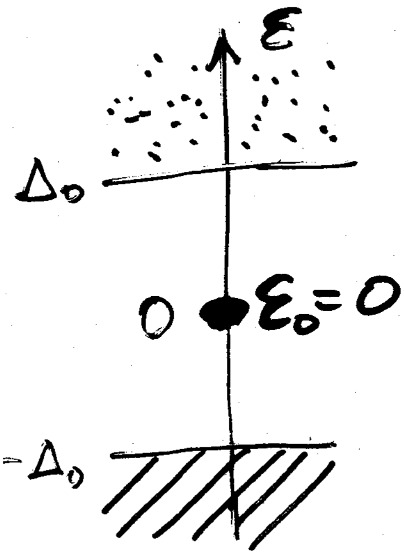
Triplet pairing: $(TMTSF)_2X$, *p*-wave: ^3He, Sr_2RuO_4

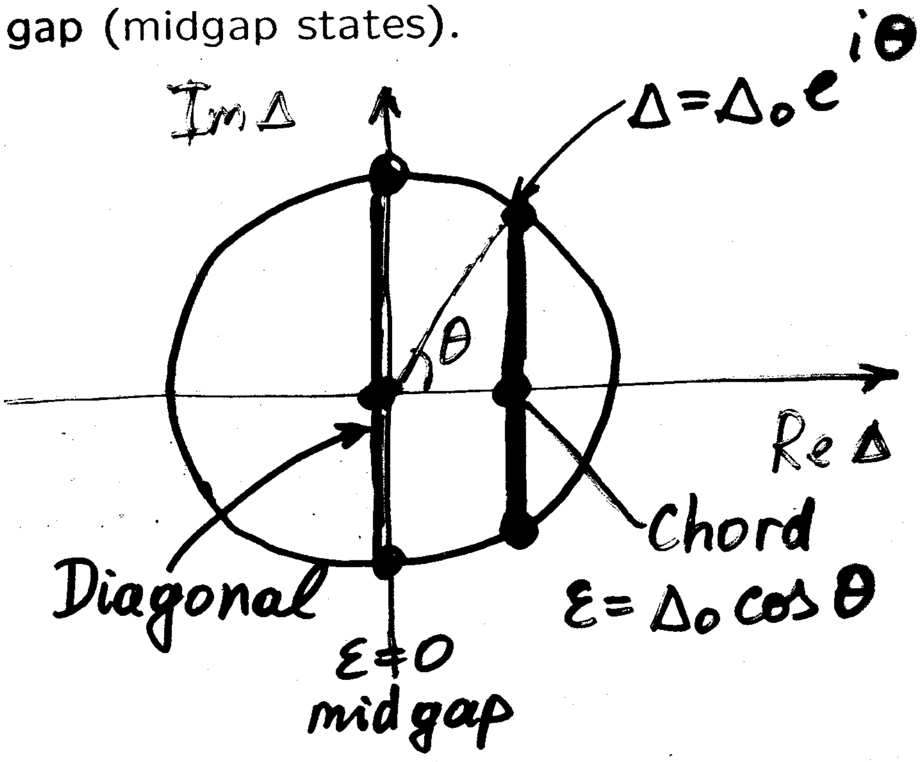
$$\langle \hat{\psi}_\alpha(k_F)\hat{\psi}_\beta(-k_F)\rangle = i\sigma_y(\mathbf{d}\cdot\boldsymbol{\sigma})\Delta(k_F), \quad \Delta(+k_F) = -\Delta(-k_F)$$





Because $\Delta(\pm k_F)$ changes sign, Andreev bound states form at the ends of the chains with the energy exactly in the middle of the energy gap (midgap states).





Midgap Andreev edge states

The wave function of a Bogolyubov quasiparticle in a Q1D superconductor:

$$\Psi(x,y) = e^{ik_y y}\left[Ae^{ik_F x}\begin{pmatrix}u_+(x)\\ v_+(x)\end{pmatrix} + Be^{-ik_F x}\begin{pmatrix}u_-(x)\\ v_-(x)\end{pmatrix}\right]$$

$[u_\pm(x), v_\pm(x)]$ obey the Bogolyubov-de Gennes equations:

$$\begin{pmatrix}\mp i v_F \partial_x & \pm\Delta \\ \pm\Delta & \pm i v_F \partial_x\end{pmatrix}\begin{pmatrix}u_\pm(x)\\ v_\pm(x)\end{pmatrix} = \varepsilon\begin{pmatrix}u_\pm(x)\\ v_\pm(x)\end{pmatrix}$$

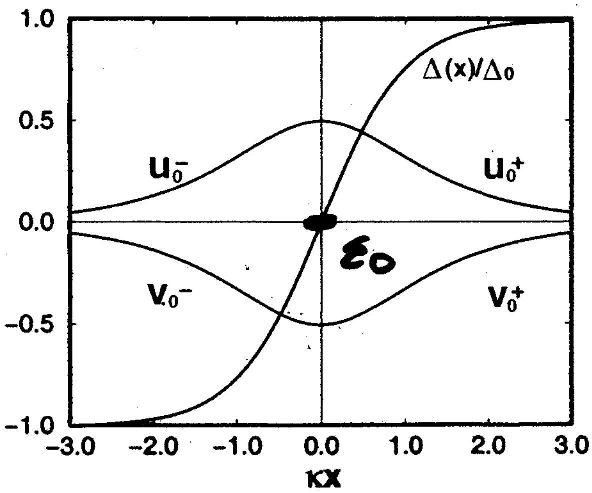
To satisfy the boundary condition $\Psi(0) = 0$, we choose $A = -B$ and $[u_+(0), v_+(0)] = [u_-(0), v_-(0)]$. Then we extend the problem to $-\infty < x < +\infty$:

$$\Psi(x) = \begin{cases}[u_+(x), v_+(x)], & x > 0\\ [u_-(-x), v_-(-x)], & x < 0\end{cases}$$

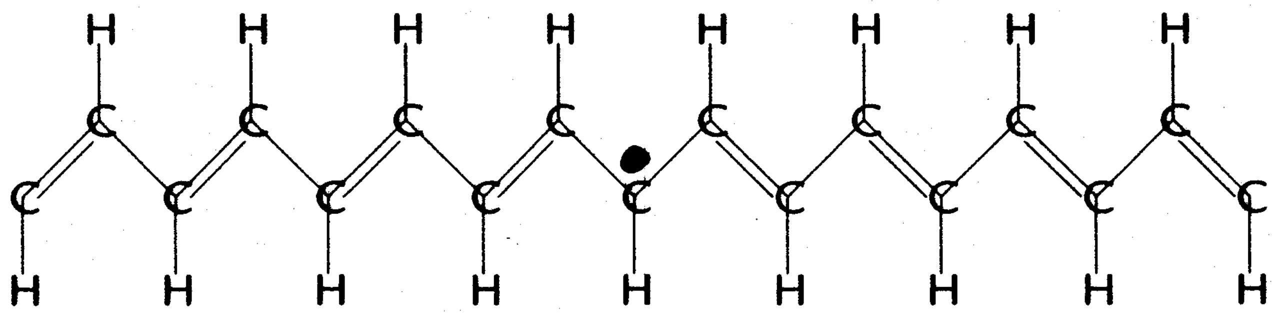
Self-consistent pair potential:
$\Delta(x) = i\Delta_0 \tanh(\kappa x)$, $\kappa = \Delta_0/v_F$

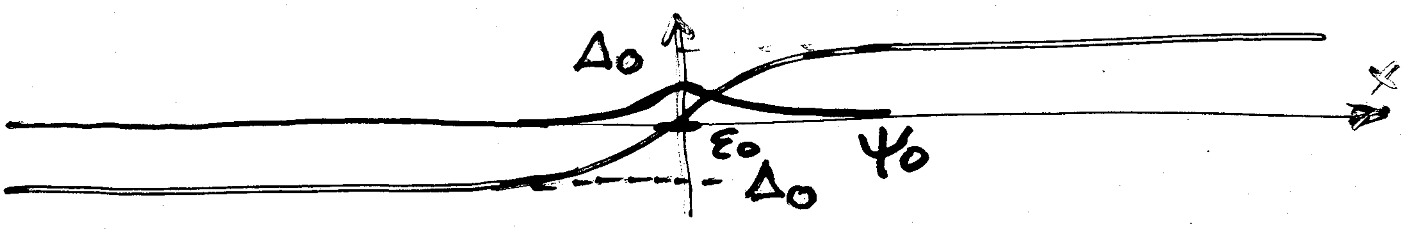
Localized zero-energy state:

$$\varepsilon_0 = 0,\quad \begin{pmatrix}u_0(x)\\ v_0(x)\end{pmatrix} = \frac{\sqrt{\kappa}}{2\cosh(\kappa x)}\begin{pmatrix}1\\ -1\end{pmatrix}$$



Exact mapping to the solitons in polyacetylene $(CH)_x$

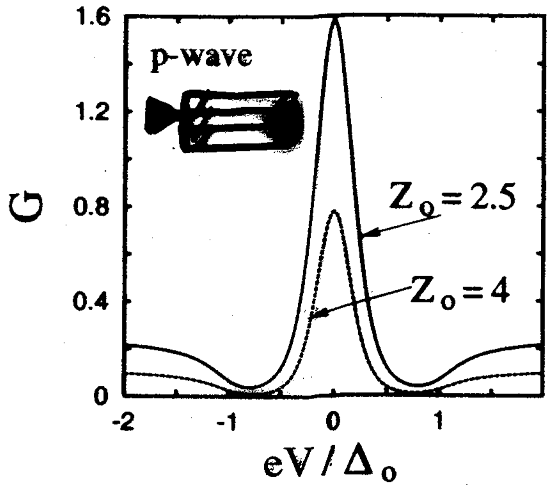


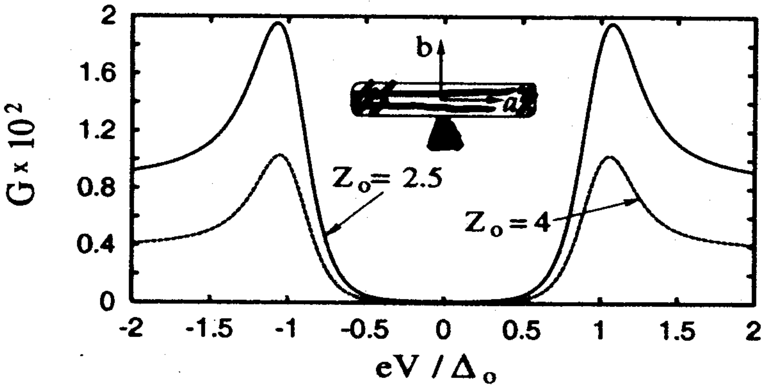


Tunneling into midgap Andreev edge states

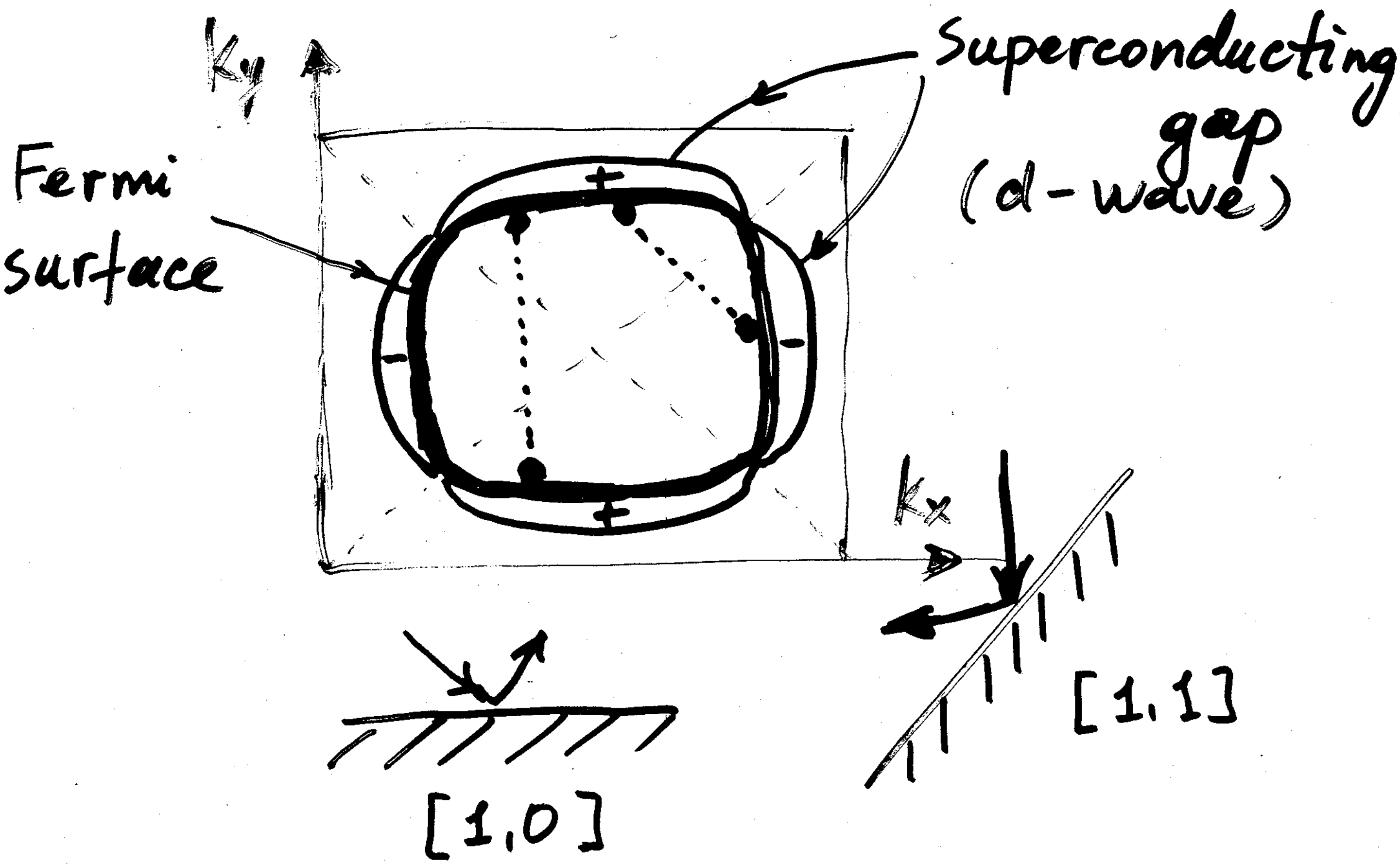
Tunneling along the chains:
Zero-bias conductance peak

Across the chains:
No zero-bias peak



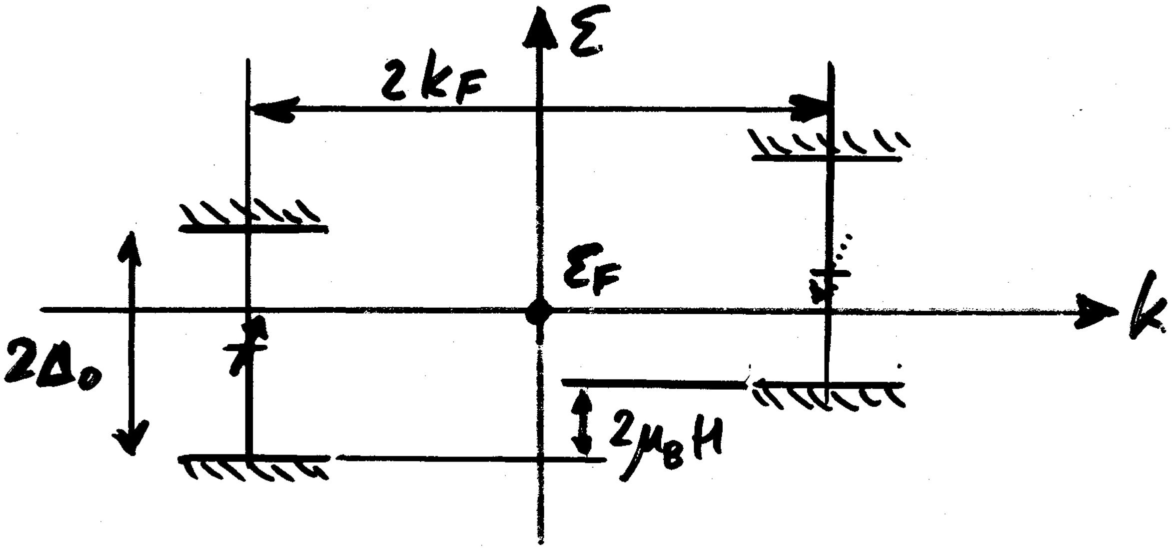


Similar to tunneling into the [1,1] and [1,0] edges for the d-wave superconductivity in high-T_c cuprates:

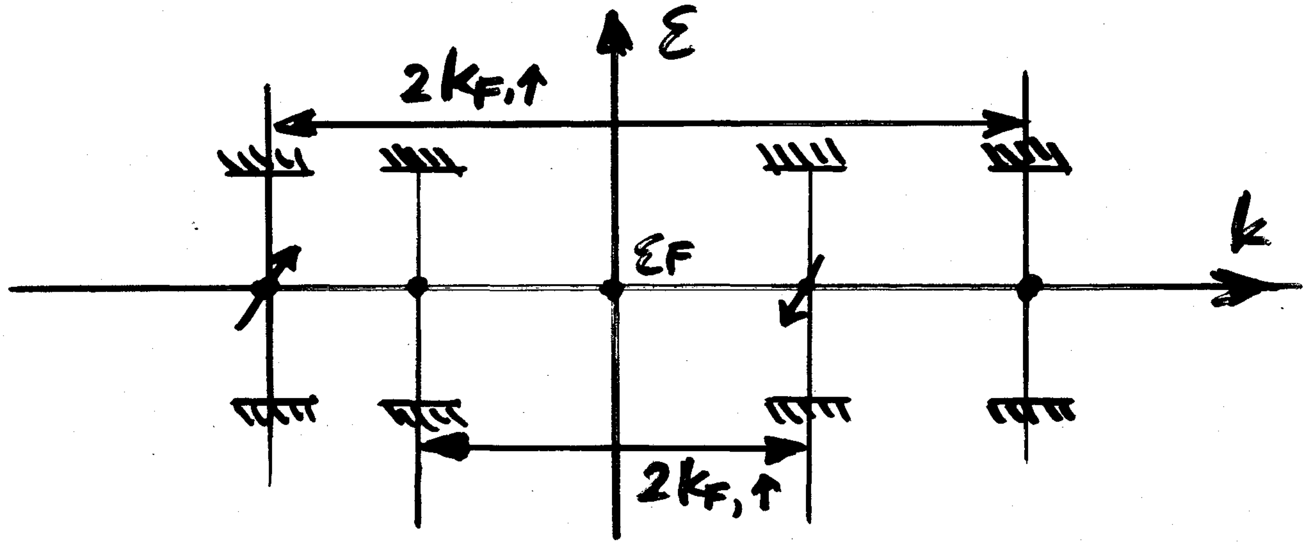


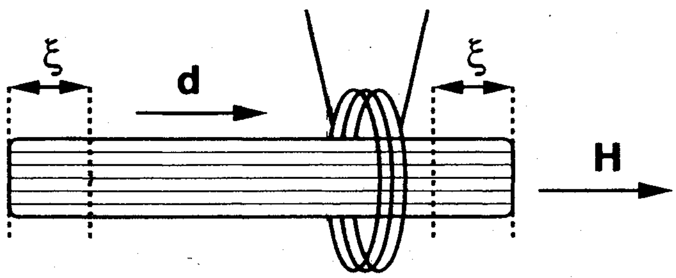
Spin response of the edge states

H || **d**: net spin and magnetic moment appear



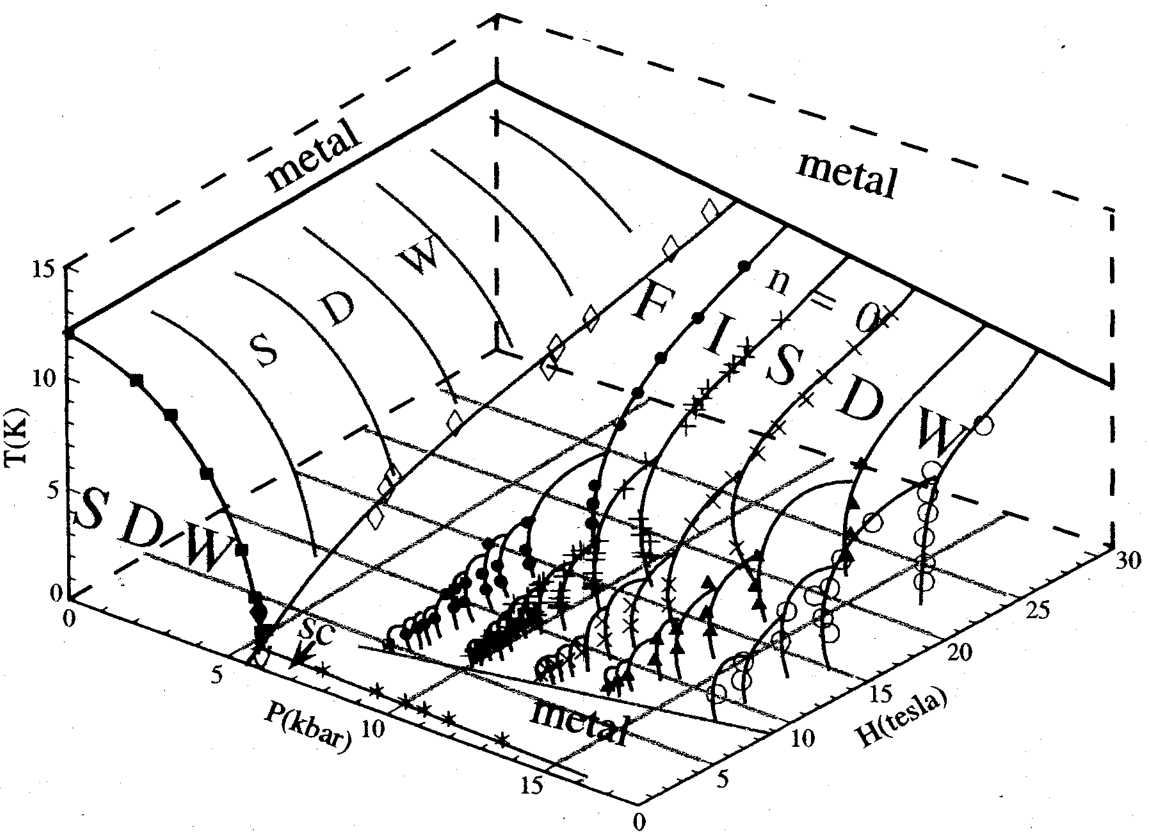
H ⊥ **d**: net spin and magnetic moment do not appear





Schematic experimental setup to measure magnetic susceptibility of the edge states localized at the ends of the chains.

Phase Diagram of $(TMTSF)_2PF_6$



W. Kang et al

SC = Superconductivity

SDW = Spin-Density Wave

FISDW = Magnetic-Field-Induced Spin-Density Wave

Quantum Hall effect in Q1D conductors

$$\hat{\mathcal{H}} = -\frac{1}{2m}\frac{\partial^2}{\partial x^2} - 2\Delta_0 \cos[(2k_F - NG)x] + 2t_b \cos(k_y b - Gx)$$

- Δ_0 - the FISDW order parameter
- N - an integer number characterizing FISDW
- $G = ebH/\hbar c$ - the magnetic wave vector
- H - the external magnetic field, use gauge $A_y = Hx$
- t_b - the interchain tunneling amplitude
- k_y - the electron momentum transverse to the chains
- b - the interchain distance

The effective Hamiltonian (after some transformations):

$$\begin{pmatrix} -iv_F\partial_x & -\Delta_N e^{-iNk_yb} \\ -\Delta_N e^{iNk_yb} & iv_F\partial_x \end{pmatrix} \begin{pmatrix} \psi_+(x,k_y) \\ \psi_-(x,k_y) \end{pmatrix} = \varepsilon(k_y) \begin{pmatrix} \psi_+(x,k_y) \\ \psi_-(x,k_y) \end{pmatrix}$$

The same as the Hamiltonian in part I with $\Theta \to Nk_yb$.

Topological winding number: **The phase of the gap changes by $2\pi N$ when k_y traverses the Brillouin zone from 0 to $2\pi/b$.**

The quantum Hall effect:

- **Apply electric field $\mathcal{E}_y$ transverse to the chains**
- **Use gauge $A_y = -\mathcal{E}_y ct$ and substitute $k_y \to k_y - eA_y/c$**
- **The phase $\Theta \to Nk_yb + Ne\mathcal{E}_y bt$ becomes time-dependent**
- **That results in the Fröhlich current along the chains:** $j_x = e\dot{\Theta}/\pi b$
- **After substitution, we find the (integer) quantum Hall effect:** $j_x = (2Ne^2/h)\,\mathcal{E}_y$

cond-mat/0006050 PRL 86, 1094 (2001)

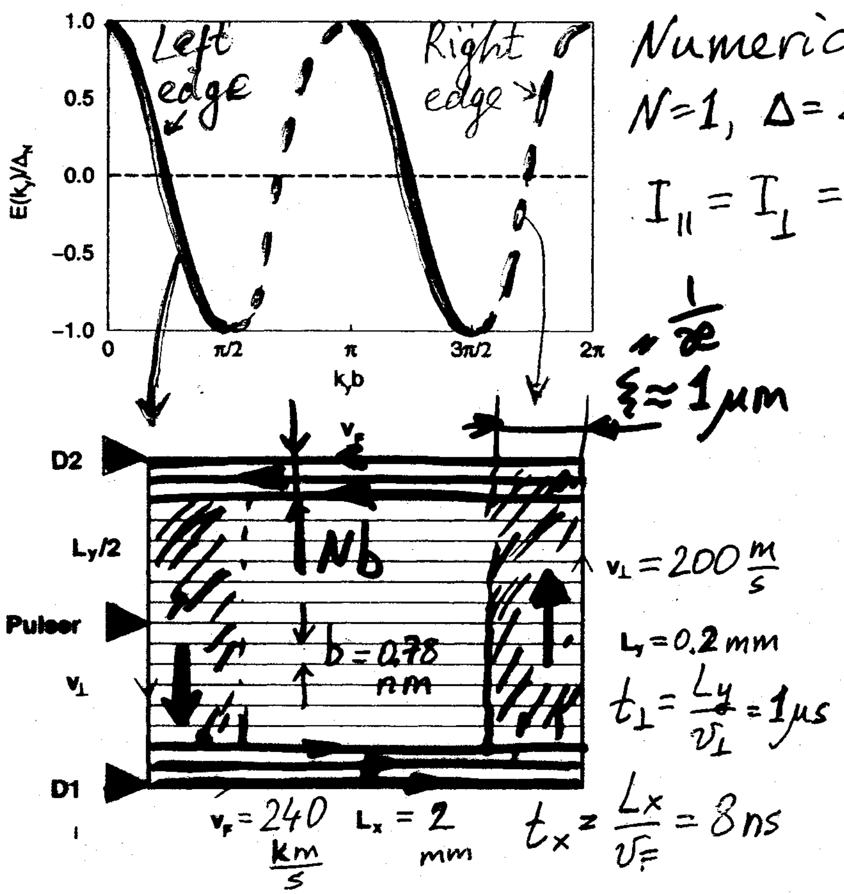
Chiral edge states in the quantum Hall regime of Q1D conductors

Use the results of part I with $\Theta \to N k_y b$.

N chiral branches of edges states at the ends of the chains

$$\begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix} \propto e^{ik_y y - \kappa x} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad \kappa = \frac{\Delta_N}{v_F} \sin(N k_y b) = \frac{1}{\xi}$$

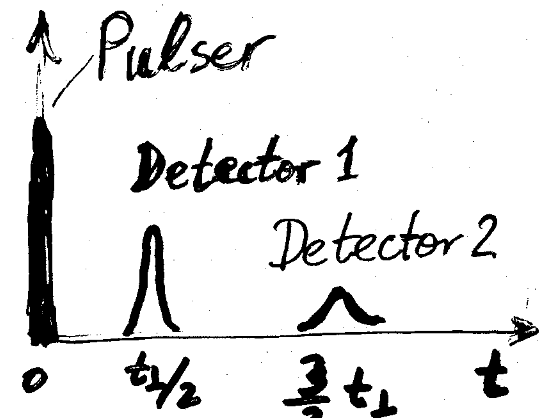
$$\varepsilon(k_y) = \Delta_N \cos(N k_y b), \quad v_\perp = \left.\frac{\partial \varepsilon(k_y)}{\partial k_y}\right|_{\varepsilon=0} = -N \Delta_N b$$



Numerical estimates for $N=1$, $\Delta = 2K$ ($2\Delta = 6K$ @ $25T$)

$$I_\parallel = I_\perp = \frac{e v_\perp}{\pi b} = 13\,\text{nA}$$

Proposed time-of-flight experiment



The edge contribution to the specific heat:

$$\frac{C_{\text{edge}}^{\text{FISDW}}}{T} = \frac{2N\pi k_B^2}{3\hbar}\left(\frac{L_y}{v_\perp} + \frac{L_x}{v_F}\right) \approx \frac{2\pi k_B^2 L_y}{3b\Delta_N}, \quad \frac{C_{\text{edge}}^{\text{FISDW}}}{C_{\text{bulk}}^{\text{normal}}} = \frac{2\xi_N}{L_x} \approx 10^{-3}$$

Conclusions

In the charge-gap state of $(TMTTF)_2X$:

- Holon edge states exist at the ends of the chains, at temperatures below the ferroelectric anion transition.
- They are similar to soliton states in 1D polymers.
- Reference: **cond-mat/0106516**.

In the triplet p-wave superconducting state of $(TMTSF)_2X$:

- Midgap edge states exist at the ends of the chains.
- These states should produce a zero-bias peak in electron tunneling.
- The spins of the edge states respond paramagnetically to a magnetic field parallel to the vector $\mathbf{d}$ that characterizes triplet pairing.
- They are similar to the midgap states in the singlet d-wave superconductors (high-T_c cuprates).
- Reference: PRB 63, 144531 (2001), cond-mat/0010206.

In the FISDW (QHE) state of $(TMTSF)_2X$:

- There exist N chiral electron edge states with the energies inside the gap.
- The velocities of the edge states are very anisotropic: 300 m/s perpendicular to the chains and 240 km/s parallel to the chains.
- We propose time-of-flight and specific-heat experiments to observe these edge states.
- Similar states should exist in the chiral p-wave superconductor Sr_2RuO_4, **cond-mat/0106198**.
- Reference: **PRL 86, 1094 (2001)**, **cond-mat**/0006050.