Physics of quasi one dimensional conductors

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1D systems

• Allow to obtain exact solutions of N body problem
  – AF chain (Ising, Hülten, Bethe, Griffiths, De Cloizeau & Pearson, Haldane…)
  – 1D interacting electron gas (Lieb & Wu, Mattis, Tomonaga & Luttinger (TL), Luther & Emery (LE)…)

• In 1D: enhanced quantum and thermal fluctuations
  – in 1D no long range order at finite T
    Ising chain (Landau)
    XY and Heisenberg chains (Mermin and Wagner)
  – 1D interacting electron gas: Collective (non Fermi liquid) behavior; quasi–order at T=0°K (TL and LE liquids)
  – Exact treatment of thermal fluctuations
    (matrix transfer method)

• Since ~1970 experimental results allow to test exact calculations
1D experimental systems

- magnetic (AF) chains and ladders
- 1D inorganic and organic electronic conductors
- edge states in 2D conductors
- quantum wires
- carbon nanotubes

Real materials made of weakly coupled chains
1D behavior for: $\pi k_B T > J_\perp$ inter-chain coupling
outlook

• One dimensional conductors

• Peierls/charge density wave (CDW) instability
  – Inorganic conductors: Mo blue bronze
  – Organic charge transfer salts

• Effect of electron-electron interactions
  (organic conductors: charge transfer salts, Fabre and Bechgaard salts)
  – $4k_F$ CDW instability/charge ordering
  – spin Peierls instability
  – Spin density waves and generalized density waves
  – Unconventional superconductivity
ONE DIMENSIONAL CONDUCTORS

Structural anisotropy: \( d_{//} < d_{\perp} \)

\( d_{//} \)

\( d_{\perp} \)

Anisotropy of overlap of wave functions

Organics: \( p\pi \)

Inorganics: \( dz^2 \)

Charge transport: \( \sigma_{//}(\omega) \gg \sigma_{\perp}(\omega) \)

Real 1D conductor: no coherent interchain electronic transfer

Imply: \( t_{\perp} \ll \pi k_B T \) (Fermi surface thermal broadening)
**Inorganics**

K$_2$Pt(CN)$_4$·0.3Br·xH$_2$O

1D overlap of dz$^2$ orbitals

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**Organics**

(TMTSF)$_2$PF$_6$

1D overlap of p$_\pi$ orbitals
Blue Bronze

$A_0.3\text{MoO}_3$

$A$: K, Rb, Tl

1D
Anisotropic optical conductivity $\sigma(\omega)$

B.P. Gorshunov et al PRL 73, 308 (1994)
1D non interacting electron gas

No orbital degree of freedom

\( \rho \) electrons per atom (per unit cell of length \( d_{//} \))

\[ \rho = 2 \times 2k_F \]

Spin degree of freedom

For a free electron gas in D dimensions: \( k_F \approx (n)^{1/D} \)

\( n = \rho / d_{//} \) is the electron density

in 1D: \( n = (2/\pi)k_F \) (with \( k_F \) expressed in Å\(^{-1}\))
1D metal coupled to the lattice: unstable at 0\(^\circ\)K towards a Periodic Lattice Distortion which provides a new \((2k_F)^{-1}\) lattice periodicity

PLD opens a gap \(2\Delta\) at the Fermi level: insulating ground state
Peierls’ instability (basic)

- **In the static (adiabatic) limit:**
  
  Set a $2k_F$ static PLD: $u(x) = u_0 \sin (2k_F x + \varphi)$ at $T=0^\circ K$

  A gap $2\Delta$ is open at $\pm k_F$  

  ($\Delta = gu \ g$: electron-phonon coupling)

  Gain of electronic energy:
  
  $E_{el} \approx \Delta^2 N(E_F) \ln (\Delta/\varepsilon_F)$

  Cost of elastic distortion energy
  
  $E_{dis} = 1/2K u_0^2 = 1/2K(\Delta/g)^2$

  Because of $\ln (\Delta/\varepsilon_F)$: $E_{el} + E_{dis} < 0$ whatever $\Delta$

  Long range PLD always energetically favorable

  **1D metallic state not stable at $0^\circ K$**

  (Peierls « theorem » 1955)
Peierls ground state

- Gap at 0°K (in the adiabatic limit)
  \[ \Delta_0 = 2\varepsilon_F \exp(-1/\lambda) \]
  with the reduced electron-phonon coupling:
  \[ \lambda = n(2s+1)N(E_F)g^2/K^* \]
  \(N(E_F)\) density of states per spin direction

- Complex order parameter (\(\rho\) incommensurate)
  \[ u_0/\Delta_0 \exp(i\varphi) \quad (\exp \pm 2ik_F) \]
  amplitude phase new spatial periodicity

* \(s=0\) for spinless fermions
  \(s=1/2\) for fermions with spin
  \(n=1\) for incommensurate band filling \(\rho\)
  \(n=2\) for half-band filling \((\rho=1)\): real order parameter
Electron-phonon coupling (basic)

- **PLD displacement of site** \( l \): \( u_l \)
  
  [in the continuum limit: \( u_l \rightarrow u(x) = u_0 \sin(2k_F x + \phi) \)]
  
  for the bond \((l, l+1)\): \( d_0 \rightarrow d = d_0 + u_{l+1} - u_l \)

  This induces a modulation of the intersite transfer integral \( t^* \):
  
  \[
  t(d) = t(d_0) + \frac{\partial t}{\partial d} (u_{l+1} - u_l) \rightarrow t(d_0) - st \frac{\partial u(x)}{\partial x}
  \]

  which modulates the charge on the bonds:
  
  \[
  \rho(x) = \rho_0 + \delta \rho(x) \quad \text{with} \quad \delta \rho(x) \approx -\frac{\partial u(x)}{\partial x}
  \]

- **Electronic CDW**
  
  \[
  \delta \rho(x) = -[2N(E_F)g u_0/\lambda] \cos(2k_F x + \phi)
  \]

  \( \pi/2 \) phase shift between the PLD and the CDW

  \*\( t \) varies ~ exponentially with the intersite distance \( d \):
  
  \[
  \frac{\partial t}{\partial d} \approx -st
  \]
Charge density wave ground state

Charge density wave has two components:

- **Periodic Lattice Distortion** $u(x)$ (PLD):
  observed by diffraction (information in reciprocal space: $u(q)$)

- **Modulation of the electronic density** $\rho(x)$ (electronic CDW):
  observed by STM (information in direct space)

\[ \rho(x) = -\frac{\partial u(x)}{\partial x} \]

Coupled by the electron-phonon interaction ($g$)
Diffraction from a 2k_F modulated chain

**Direct space**

- amplitude diffracted:
  \[ A(Q) = \sum_n \exp(iQna) \]

**Reciprocal space**

- modulated lattice: atoms located in \( na + u_0 \sin(2k_F na + \phi) \)
  \[ A(Q) = \sum_n \exp(iQna) \exp[iQu_0\sin(2k_F na + \phi)]^* \]
  \[ \sum_r J_r(Qu_0) \sum_n \exp(iQna + r2k_F na + r\phi) \]
  \[ \sum_r J_r(Qu_0) \exp(ir\phi) \sum_q \delta(Q + r2k_F - h2\pi/a) \]

If \( Qu_0 << 1 \): \( J_r(Qu_0) \sim (Qu_0)^r \) only \( r = \pm 1 \) important

\[ I_{CDW}(Q) = |A(Q)|^2 \]

modulation of the phase of the scattered wave:

- side band satellite reflections in: \( Q = h2\pi/a - r2k_F \)

\[ \exp(iz\sin\theta) = \sum_r J_r(z) \exp(ir\theta) \textrm{ with } z = Qu_0 \textrm{ and } \theta = 2k_F na + \phi \]
2\(k_F\) modulated chain

Satellite lines: \(r = \pm 1\)

Fourier transform of a modulated chain: diffuse sheets in reciprocal space
Peierls instability of the blue bronze $\text{K}_0.3\text{MoO}_3$

$q_{\text{CDW}} = (1, 2k_F, 1/2)$

$2k_F = 1 - q_b \approx 3/4 \ b^*$

$(J. P. Pouget et al J. Physique Lettres 44, L113 (1983))$
STM observation of the CDW in the Rb blue bronze


Calculated image

E. Machado-Charry,¹ P. Ordejón,¹ E. Canadell,¹

$2k_F = 2\pi/\lambda_{CDW}$

FIG. 4: (Color online) (a) Constant current mode topographical image of $6.2 \times 6.2$ nm$^2$ on (201) plane of Rb$_{0.3}$MoO$_3$ at 63K (raw data image). The applied bias voltage is 420 mV and the set-up tunneling current is 110 pA. Molecular lattice and CDW superlattice coexist in the image. The three arrows indicate respectively the observed type I and II MoO$_6$ octahedra and the expected position of the Mo$_{III}$O$_6$ octahedra. Associated profile along Mo$_{I}$O$_6$ octahedra indicated by left arrow (from Ref. [3]). (b) (Color online) Calculated image and associated profile along the Mo$_{I}$O$_6$ octahedra for the modulated phase of Rb$_{0.3}$MoO$_3$. 
CDW instability: driven by the divergence of the electron-hole response function $\chi(q)$

$$\chi_e = \sum_k \frac{f(E_{k+q}) - f(E_k)}{E_{k+q} - E_k}$$

Divergence of $\chi(q)$ for $q$ such that $E_{k+q} \sim E_k$

$q$ best nesting wave vector of the Fermi surface

PLD fingerprint of $q$ wave vectors at which $\chi(q)$ diverges
Structural instability at $q$ wave vectors for which $\chi(q)$ diverges

screening of the force constant $K$ by setting $\rho_q$:

$$K_{\text{eff}} = K - 2g^2\chi(q)$$

max. screening for $q = 2k_F$ (in 1D)

set at $T = 0^\circ$K a $2k_F$ PLD (Peierls instability)

accompanied by a $2k_F$ modulation of the electron density $\rho(2k_F)$

vanishing of $K_{\text{eff}}$ induces a phonon softening (Kohn anomaly)
Thermal phase diagram

• Mean-field (BCS-like) theory (ignore fluctuations)

\[ 2\Delta_0 = 3.56k_B T_P^{MF} \]

• Isolated chain
(because of thermal fluctuations there is no Peierls LRO at finite \( T \))

\[ T_P^{MF} \]

• Coupled chains
Interchain coupling restores a Peierls 3D LRO at finite \( T_p \)

\[ T_P \sim T_P^{MF}/3 \]
X-ray diffuse scattering

$T_F \sim T_{MF}$

$T > T_P$

1D regime

Short Range Order

$T < T_P$

3D regime

3D Long Range Order

Direct space

Reciprocal space

pre-transitional fluctuations $\rightarrow$ diffuse scattering

(2$k_F)^{-1}$

$2k_F$

$\xi_{//}$

$\xi_{//}^{-1}$

$\xi_{\perp}$

$\xi_{\perp}^{-1}$

* start of 1D fluctuations

satellite reflections

$T > T_P$

$X$-ray diffuse scattering

$T_F * \sim T_{MF}$

$T > T_P$

1D regime

Short Range Order

$T < T_P$

3D regime

3D Long Range Order

$T_P$

$T_F * \sim T_{MF}$

$T > T_P$

1D regime

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Short Range Order

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3D Long Range Order

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1D regime

Short Range Order

$T < T_P$

3D regime

3D Long Range Order

$T_P$

$T_F * \sim T_{MF}$

$T > T_P$

1D regime

Short Range Order

$T < T_P$

3D regime

3D Long Range Order

$T_P$
Blue bronze: $2k_F$ CDW superlattice spots

$q_{\text{CDW}} = (1, 2k_F, 1/2)$

$I_{\text{CDW}} \sim 10^{-2} I_{\text{Bragg}}$

$I_{\text{CDW}}(Q) \sim |Q u_{\text{CDW}}|^2; \quad u_{\text{CDW}} \sim 0.05\text{Å}$

$2k_F \sim 3/4 b^*$

shifts in $T$

$T_p = 180\text{K}$

J. P. Pouget & al J. Physique 46, 1731 (1985)
S. Girault & al PRB 39, 4430 (1989)
Peierls transition in a non interacting electron gas opens the same gap in conductivity (charge degrees of freedom) and in magnetism (spin degrees of freedom).

\[ \Delta_0^{\text{spin}} \sim 50 \text{meV} \]

\[ \Delta_0^{\text{charge}} \sim 40 \text{meV} \] (75 meV in optics)

(D.C. Johnston PRL 52, 2049 (1984))
1D fluctuation regime:
\[ \xi_\perp < d_\perp \]

\[ \pm 2k_F \] diffuse sheets in reciprocal space
X-ray diffuse scattering

\[ T_F \approx T_{MF} \]

**direct space**

\[ T > T_P \]

**1D regime**

Short Range Order

pre-transitional fluctuations \( \rightarrow \) diffuse scattering

\( (2k_F)^{-1} \)

\[ 2k_F \]

**3D regime**

\[ T_P \]

\[ T < T_P \]

3D Long Range Order

**reciprocal space**

\[ \xi_{//}^{-1} \]

\[ \xi_{//} \]

\[ \xi_{\perp}^{-1} \]

\[ \xi_{\perp} \]

* start of 1D fluctuations

\( T > T_P \)

3D Long Range Order

\[ 2k_F \]

\[ \xi_{//}^{-1} \]

\[ \xi_{//} \]

\[ \xi_{\perp}^{-1} \]

\[ \xi_{\perp} \]

satellite reflections
TSF-TCNQ: 2kF CDW instability

Charge transfer
\( \rho = 0.63 \)

2kF CDW on the TSF stack
Thermodynamics of 1D classical systems

Exact treatment of 1D fluctuations

\[ F[u] = \int dz \left[ a |u(z)|^2 + b |u(z)|^4 + c |\frac{\partial u}{\partial z}|^2 \right] \]

\[ a = a'(T - T_p^{MF})/T_p^{MF} \]

\[ <u(z)u(0)> \propto \exp(\pm i2k_Fz) \exp(-z/\xi) \]

Inverse correlation length \( \xi(T)^{-1} \)

Complex order parameter

\[ u(z) = u_0 \exp(i\phi) \exp(\pm i2k_Fz) \]

(Scalapino et al, PRB 6, 3409 (1972); H. J. Schulz)

fluctuations of the phase \( \phi \)
fluctuations of the amplitude \( u_0 \)

Fluctuations controlled by the Ginzburg critical region: \( \Delta t_{1D} = (b T_p^{MF})^{2/3}/\varepsilon \)

For the non-interacting Peierls chain: \( \Delta t_{1D} = 0.8 \)
2kF Fluctuations in charge transferred salts

Reduced Ginzburg critical region of the Peierls chain $\Delta t_{1D} = 0.8$

2kF CDW fluctuations

Thermal length scale: \( \xi_0 = \frac{\hbar v^*}{\pi k_B T_p^{MF}} \)

<table>
<thead>
<tr>
<th>SALT</th>
<th>( T_F ) (K)</th>
<th>( \xi_0 ) (nm)</th>
<th>( \hbar v^*) (eVÅ)</th>
<th>( \hbar v_F ) (eVÅ)</th>
<th>( v^*/v_F )</th>
</tr>
</thead>
<tbody>
<tr>
<td>TSF-TCNQ</td>
<td>230</td>
<td>1.5</td>
<td>0.92</td>
<td>1</td>
<td>0.9</td>
</tr>
<tr>
<td>HMTSF-TCNQ</td>
<td>~300</td>
<td>2.2</td>
<td>1.80</td>
<td>2.3</td>
<td>0.8</td>
</tr>
<tr>
<td>NMP-TCNQ</td>
<td>~300</td>
<td>1.9</td>
<td>1.54</td>
<td>~1.35</td>
<td>1.15</td>
</tr>
<tr>
<td>HMTSF-TNAP</td>
<td>~300</td>
<td>0.9</td>
<td>0.74</td>
<td>0.6</td>
<td>1.2</td>
</tr>
</tbody>
</table>

Start of 2kF fluctuations: \( T_F \sim T_p^{MF} \)

From plasma edge measurements

In 1D: \( \hbar v_F = 2t_{//} d_{//} \sin \left( \pi \rho /2 \right) \)
interacting electron gas coupled to the lattice

Organic conductors
Density waves
Charge ordering
Spin-Peierls instability
ORGANIC CHARGE TRANSFER SALTS

1D

2 bands crossing at $E_F$

$2k_F(A) = 2k_F(D)$

Only a single $2k_F$

critical wave vector!

TTF-TCNQ and TSF-TCNQ are isostructural
TSF-TCNQ: 2kF CDW instability

Charge transfer
\( \rho = 0.63 \)

2kF CDW on the TSF stack
TTF-TCNQ: 2kF and 4kF CDW!

2kF CDW on the TCNQ stack

4kF CDW on the TTF stack

2$k_F$ Peierls transition for non interacting Fermions
(exists whatever the strength of the electron-phonon coupling)

4$k_F$ Peierls transition for spinless Fermions (no double occupancy $U >> t$)
(exists only if the electron-phonon coupling is strong enough)

$\rho = 4k_F$ Average distance between charges: $1/\rho = (4k_F)^{-1}$

The 4$k_F$ CDW can correspond at the first Fourier component of a 1D Wigner lattice of localized charges
$4k_F$ phase diagram for spinless fermions with long range coulomb interactions

\[ H = -t \hat{T} + V \hat{W} = \sum_k \epsilon_k c_k^+ c_k + \frac{1}{2L} \sum_q V(q) \rho_q \rho_{-q}, \]
\[ \epsilon_k = -2t \cos k, \quad V(q) = -V \ln[2(1-\cos q)] \]
\[ \rho_q = \sum_k c_k^+ c_{k+q} c_k \]

$4k_F = n (d_{\parallel}^*)$

FIG. 3. Average occupation of site $l$ for different values of the interaction strength at $n = 1/8$: $V = 0.5t$ (triangles), $V = 20t$ (circles), $V = 500t$ (squares). Lines are guides to the eye.

FIG. 5. Phase diagram for the spinless model (9). A charge-ordered state persists for all commensurate fillings with three characteristic regimes, from top to bottom: (I) generalized Wigner lattice, (II) Wigner crystal and (III) small-amplitude charge-density wave.

J. Hubbard; B. Valenzuela et al PRB 68, 045112 (2003)
**ORGANIC CONDUCTORS**

Extended Hubbard Model:

\[
H = H_0 + U \sum_i n_i \uparrow n_i \downarrow + \sum_{i,m > 0} V_{m} n_i n_{i+m}
\]

1D correlated fermion gas: no quasiparticle

only CDW, SDW and supraconductivity fluctuations

The most diverging fluctuation at low T depends upon:

- The strength and range of Coulomb interactions: \( K_\rho (>1) \)
  
  \( K_\rho < 1 \) density waves \( / \) \( K_\rho > 1 \) superconductivity

- The sign of the 2kF Fourier transform of the Coulomb interaction:
  
  \( g_1 (= U + 2V_1 \cos \pi \rho) \)
  
  If repulsion (\( g_1 > 0 \)): Luttinger Liquid
  
  If attraction (\( g_1 < 0 \)): Luther Emery Liquid
Ground states with $K_ρ<1$: illustration in the commensurate case of $ρ=1$

**U<0: Luther Emery liquid**

2$k_F$ « site » CDW - no magnetism

**U>0: Luttinger liquid**

AF

2$k_F$ SDW

SP

S = 0

2$k_F$ « bond » CDW (BOW)
PHASE DIAGRAM OF THE 1D INTERACTING ELECTRON GAS

Charge sector ($K \sigma = 1$)

Coexistence of $2k_F$ and $4k_F$ CDW!

($H.~Schultz$)

2$k_F$ incommensurate
no unklapp scattering
Divergence of the CDW electron-hole response function (U, V \geq 0 case)

T → 0: χ(2k_F) diverges

V \sim U/2

T → 0: both χ(2k_F) and χ(4k_F) diverge

CDW instability on the donor stack

Increase of the polarizability of the molecule

- HMTSF
- TSF
- HMTTF
- TTF

- 2kF CDW
- 2kF + 4kF CDW
- 4kF CDW

two more cycles
4\(k_F\) charge localization

- In 1D for strong enough coulomb repulsion \((U,V)\) 4\(k_F\) charge localization (4\(k_F\) CDW)
- For **commensurate band filling** the electrons can be localized either on the sites or on the bonds (ground states of different symmetry/ energy)

  **case of quarter filled band \((\rho=1/2)\):** the 4\(k_F\) instability corresponds to a lattice dimerization of:
  - either the bonds: 4\(k_F\) BOW (Mott dimer)
    
    ![Diagram of Mott dimer]
    
    \(I\): inversion center on the bonds
  - or the sites: 4\(k_F\) CDW (Wigner charge order)
    
    ![Diagram of Wigner charge order]
    
    \(I\): inversion center on the sites

  (If BOW+CDW mixture no inversion symmetry: polar chain)
(TMTCF)$_2X$: BECHGAARD and FABRE SALTS

zig-zag chain of TMTCF

X centrosymmetrical: AsF$_6$, PF$_6$, SbF$_6$, TaF$_6$, Br

X non centro: BF$_4$, ClO$_4$, ReO$_4$, NO$_3$
Phase diagram of (TMTCF)$_2$X

4$K_F$BOW
4$K_F$ CDW

Temperature (K)

Pressure

10 kbar
Charge ordering transition ($4k_F$ CDW)

- Charge disproportion at $T_{CO}$
  
  2 different molecules: NMR line splitting

Chow et al PRL 85, 1698 (2000)

- Charge disproportion + incipient dimerization ($4k_F$ BOW)
  
  Ferroelectricity at $T_{CO}$

Monceau et al PRL 86, 4080 (2001)
Charge ordering transition

Enhancement of the charge localization gap at $T_{CO}$

(4$K_F$BOW)$^{-1}$
Structural dimerization

$PF_6(H_{12})$: $T_{CO}=69K$
$PF_6(D_{12})$: $T_{CO}=90K$
$AsF_6(H_{12})$: $T_{CO}=100K$
Spin susceptibility measurements: \((TMTTF)_2X\)

No anomaly at \(T_{CO}\): spin charge decoupling
Non magnetic ground state develops below \(T_{SP}\)
Ground states of the 1D Heisenberg chain

CO state: charge degrees of freedom frozen
Spin degrees of freedom remain

Spin-Peierls

\[ \rho = \frac{1}{2} \text{ (1 electron per dimer)} \]

Case of (TMTTF)\(_2\)X

2\( k_F \) SDW

2\( k_F \) bond « CDW » (BOW)
Phase diagram of the (TMTCF)$_2$X
Spin-Peierls ground state: Singlet-Triplet splitting gap

\[ \chi_T \sim \exp\left(-\frac{\Delta}{T}\right) \quad \text{(ground state is a singlet } S=0) \]

\begin{align*}
\text{PF}_6\text{(H}_{12}\text{)} & : \Delta = 79K \\
\text{PF}_6\text{(D}_{12}\text{)} & : \Delta = 75K \\
\text{AsF}_6\text{(H}_{12}\text{)} & : \Delta = 70K
\end{align*}

(C. Coulon)
elastic neutron scattering evidence of SP superlattice reflexions in (TMTTF)$_2$PF$_6$ (D$_{12}$)

(2.5,0.5,-0.5) reflexion

h = $\frac{1}{2}$ a* : 2a periodicity chain dimerization (pairing into S=0 singlet)
Thermal dependence of the (TMTTF)$_2$PF$_6$ superlattice peak intensity

\( T_{SP} = 18 \pm 1 \text{K} \)

(P. Foury-Leylekian et al PRB 70, R180405 (2004))
Analogy between the spin-Peierls transition and the Peierls transition

AF chain: $H = \Sigma_j [J_{xy} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + J_z S_j^z S_{j+1}^z]\$

XY term  

Ising term

Wigner Jordan transform spins 1/2 into fermionic operators:

$S_j^+ = (S_j^-)^* = \exp(-i\pi \Sigma_l a^+_l a_l) a_j^+$

$S_j^z = a_j^+ a_j - 1/2$

$S_j^+ S_{j+1}^- = a_j^+ a_{j+1}^-$

Vacuum $|0\rangle = |\downarrow\downarrow\downarrow\downarrow\downarrow\rangle$

One pseudo-fermion added: $a_j^+ |0\rangle = |\-downarrow\downarrow\downarrow\uparrow\downarrow\rangle$ spin up in j

AF chain: half filled band of pseudo-fermions

In k space: Fourier transform $a_j \rightarrow a_k$

$H = \Sigma_k \varepsilon(k) a^+_k a_k + (1/N) \Sigma_{k,k',q} V(q) a^+_k a^+_q a_{k'} a_{k'-q}$

with: $\varepsilon(k) = J_{xy} \cos(ka) - J_z$

$V(q) = J_z \cos(qa)$

Half filled band of spinless fermions:
- free fermions for XY chain ($J_z = 0$)
- interacting fermions for Heisenberg chain ($J_{xy} = J_z = J$)
half filled band of spinless fermions coupled to the lattice

$2k_F \sim \text{Peierls instability leads to a lattice dimerization}$

(because $2k_F = a^*/2 \rightarrow \lambda_{\text{CDW}} = 2a$)

Spin-Peierls transition in the Heisenberg chain equivalent to the Peierls (CDW) transition in a Luther-Emery liquid with:

$V(q=2k_F) = -V(q=0) = -J_z < 0$

« Peierls » transition opens a gap $\Delta$ in the pseudo-fermion dispersion

(gap opened in the spin degrees of freedom: **spin-Peierls transition**
Phase diagram of the (TMTCF)$_2$X

D. Jérome
$(\text{TMTSF})_2\text{PF}_6$: $2k_F$ SDW insulating ground state

- $T_{\text{SDW}} = 12K$
- First order metal-insulator transition
- $m \approx 0.1 \mu_B$
- From NMR: $q_{\text{SDW}} = (2k_F = 0.5; 0.2 \pm 0.05; 0.06)$
- $q_{\text{SDW}}$ nests the quasi-1D FS

Magnetization jump of $\sigma$
Slater metal –insulator transition to a SDW ground state (1951)

Analogous to a Peierls transition with the Hubbard term playing the role of the electron phonon coupling

\[ U_{n_i, n_i} \text{ set a potential } U_{\uparrow}(x) \text{ to the charge density } \rho_{\uparrow}(x) \]

If this potential is modulated at \( 2k_F \): a gap \( \Delta \) is opened in \( E[\rho_{\downarrow}(x)] \) at \( \pm k_F \)

Gain of electronic energy as for the Peierls transition.

Loss of energy by double occupancy of site \( i \).

Loss minimized if:

\( \rho_{\uparrow}(x) \) and \( \rho_{\downarrow}(x) \) are out of phase

this leads to the stabilization of a \( 2k_F \) Spin Density Wave
In fact hybrid $2k_F$ CDW-SDW ground state in $(TMTSF)_2PF_6$!

Very weak $2k_F$ and $4k_F$ CDW satellite reflections $10^{-5}$-$10^{-6}$ Bragg intensity!

$q_{CDW} \sim (1/2, 1/4, 1/4)$

Generalized density waves (Overhauser 1968)

\[ \rho^\uparrow = \rho^\downarrow \exp i\Theta \]

2k_F CDW
- \[ \downarrow \equiv \uparrow \] \( \Theta = 0 \)
- U and V weak
- (4k_F CDW for strong U and V)

2k_F SDW
- \[ \downarrow \] \[ \uparrow \] \( \Theta = \pi \)
- U > V

Hybrid 2k_F SDW/CDW
- \[ \downarrow \] \[ \uparrow \] \( 0 < \Theta < \pi \)
- U ~ V

Case of \((\text{TMTSF})_2\text{PF}_6\)

\[ H = H_0 + U \sum_i n^\uparrow_i n^\downarrow_i + \sum_{i, m > 0} V m n^i n^i_{i+m} \]
Phase diagram of the (TMTCF)$_2$X

D. Jérome
Superconducting State of the Organic Conductor \((\text{TMTSF})_2\text{ClO}_4\)

\(T_c = 1.4\text{K}\)

J. Shinagawa, 1 Y. Kurosaki, 1,2 F. Zhang, 1 C. Parker, 1,3 S. E. Brown, 1 D. Jérôme, 4 J. B. Christensen, 5 and K. Bechgaard 5

Singlet superconductor at low \(H\) at high \(H\) transition to:

- inhomogeneous FFLO state
- triplet paired state
Drastic effect of a non magnetic disorder on the superconductivity of (TMTSF)$_2$ClO$_4$/ReO$_4$

nR: substitionnal disorder ReO$_4$/ClO$_4$

nQ: orientational disorder of ClO$_4$

Depairing of Cooper pairs

Figure 27: Superconducting critical temperature as a function of the residual resistivity for samples with different amounts of disorder either chemical (nR) or orientational (nQ)[145]. The solid line is a least square fit of the digamma pair-breaking function to the data which reaches zero at $\alpha = 0.88$.

\[
\ln \left( \frac{T_{c0}}{T_c} \right) = \Psi \left( \frac{1}{2} + \frac{\alpha T_{c0}}{2 \pi T_c} \right) - \Psi \left( \frac{1}{2} \right)
\]

with $\Psi$ being the digamma function, $\alpha = \hbar / 2 \pi k_B T_{c0}$ the depairing parameter, $\tau$ the elastic scattering time and $T_{c0}$ the limit of $T_c$ in the absence of any scattering.

Elastic collisions on non magnetic punctual defects mix \(-k_F\) to \(+k_F\) states (scattering momentum \(2k_F\)).

Elastic process: not allowed if the gap is always \(>0\) (s superconductor) allowed if elastic scattering link gap regions of opposite sign (unconventional superconductor).

Unconventional gap symmetry averaged out by finite electron lifetime due to elastic scattering.

(rate of decrease of \(T_C\) given by the pair breaking Abrikosov-Gorkov equation)

\[
\Delta_k = \text{cte} \ cos(k_{\perp}b)
\]

\(\Delta_k\) node
Superconducting order parameter in quasi-1D conductors

TABLE I. Superconducting order parameters in a quasi-1D geometry. The names are assigned according to the number of sign changes along the Fermi surface.

<table>
<thead>
<tr>
<th>name</th>
<th>spin pairing</th>
<th>$\Delta_r(k_\perp)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s$</td>
<td>singlet</td>
<td>$\mathbf{1}$</td>
</tr>
<tr>
<td>$p_x$</td>
<td>triplet</td>
<td>$\mathbf{r}$</td>
</tr>
<tr>
<td>$p_y$</td>
<td>singlet</td>
<td>$\sin k_\perp$</td>
</tr>
<tr>
<td>$d_{xy}$</td>
<td>singlet</td>
<td>$\cos k_\perp$</td>
</tr>
<tr>
<td>$d_{x^2-y^2}$</td>
<td>singlet</td>
<td>$r \sin k_\perp$</td>
</tr>
<tr>
<td>$f$</td>
<td>triplet</td>
<td>$r \cos k_\perp$</td>
</tr>
<tr>
<td>$g$</td>
<td>singlet</td>
<td>$\cos 2k_\perp$</td>
</tr>
<tr>
<td>$h$</td>
<td>triplet</td>
<td>$r \sin 2k_\perp$</td>
</tr>
<tr>
<td>$i$</td>
<td>singlet</td>
<td>$\cos 3k_\perp$</td>
</tr>
</tbody>
</table>

Increasing number of nodes

warped FS
wave vector ($r k_F, k_\perp$); $r = \pm$

SS in 1D

TS in 1D

nodes

d, f
Purely **intrachain repulsive interactions** leads to unconventional superconductivity (only interchain hopping $t_{\perp}$ and nesting deviation $t_{\perp2}$).

Interference between SDW instability and Cooper pairing
Attraction takes place between electrons on neighboring chains as a result of their coupling to spin fluctuations

**d-wave superconductivity:** interchain singlet pairing, nodes

Duprat et al EPJB 21, 219 (2001); Fusaya et al JPSJ 74, 1263 (2005)
Extended quasi-1D electron gas
(interchain coulomb interactions $g_{\perp}$)

Stabilization with increasing $g_{\perp}$ of:
CDW and f triplet SC ($r \cos k_{\perp}$)

Interference between density wave and pairing

Boundary between SDW and CDW ground states (hybrid SDW/CDW state?)

Nickel et al PRL 95,247001 (2005)
& PRB 73,165126 (2006)

Impact of electron-phonon interactions
(retardation effects)

For weak coulomb interactions SCd robust

Electron-phonon interactions:
enlarge the $g_{\perp}$ interval for SDW to SCf
increases the SDW gap and CDW correlations

Bakrim and Bourbonnais ISCOM 2007
Main messages

• 1D (quasi-1D) systems allow to test exact calculations of the many body problem
• 1D conductors exhibits unconventional behavior:
  – Large regime of fluctuations
  – Collective behavior
  – Exotic ground states

Thank you for your attention
Documents supplémentaires
N. Joo et al Europhys. Lett. 72, 645 (2005)
• **Charge density wave modulation (CDW)**

\[
\frac{\Delta n_i}{n} = \rho_{4k_F} \cos(2\pi \frac{r_i}{2a}) + \rho_{2k_F} \cos(2\pi \frac{r_i}{4a} + \Phi_{2k_F})
\]

- **4\(k_F\) term**
- **2\(k_F\) term**

site i: \(\Delta n_i = \langle n_i \rangle - n\)

Modulation of the charge on site i

average charge per site: \(n = \frac{1}{2}\)

• **Bond order wave modulation (BOW)**

\[
\delta^B_i = \delta_{4k_F}^B \cos(2\pi \frac{r_i}{2a}) + \delta_{2k_F}^B \cos(2\pi \frac{r_i}{4a} + \Phi_{2k_F}^B)
\]

- **4\(k_F\) term**
- **2\(k_F\) term**

bond i \(a + \delta^B_i\)

Modulation of the bond length i-i+1

\[-n = \frac{1}{2}\]

- **2\(k_F\)**
- **4\(k_F\)**

2\(a\) crystallographic periodicity (1 electron per 2 sites)
1D Hubbard model at quarter-filling \( (\rho = \frac{1}{2}) \) coupled with classical phonon field

\[
H_{1D} = \sum_i \varepsilon(i)n_i + \sum_{i,\sigma} t(i)(c_{i,\sigma}^\dagger c_{i+1,\sigma} + h.c.) + U\sum_i n_{i,\uparrow} n_{i,\downarrow} + V\sum_i n_i n_{i+1} + H_{ph}
\]

Electron–phonon coupling

\( \varepsilon(i) = \varepsilon(1-\alpha \delta_i^S) \Rightarrow H_{Holstein} \)

local deformation of the molecule \( i \) changes the on site energy \( \varepsilon(i) \) at a cost of

\[
H_{elas} = \frac{1}{2} K_S \sum_i (\delta_i^S)^2
\]

\( t(i) = t(1-\beta \delta_i^B) \Rightarrow H_{SSH} \)

change of the inter stack distances modulates the single particle hopping integral \( t(i) \) at a cost of an elastic energy

\[
H_{ph} = H_{elas} = \frac{1}{2} K_B \sum_i (\delta_i^B)^2
\]

\( n_{i,\sigma} = C_{i,\sigma}^\dagger C_{i,\sigma} \)

\( n_i = n_{i,\uparrow} + n_{i,\downarrow} \)

« Internal » phonon mode

Modulation of the charge on site \( i \): CDW

idem for \( U \)

« External » phonon mode

Modulation of the bond length \( i-i+1 \): BOW

idem for \( V \)