Unconventional density waves in quasi-one dimensional systems

Balázs Dóra, Attila Virosztek, Kazumi Maki

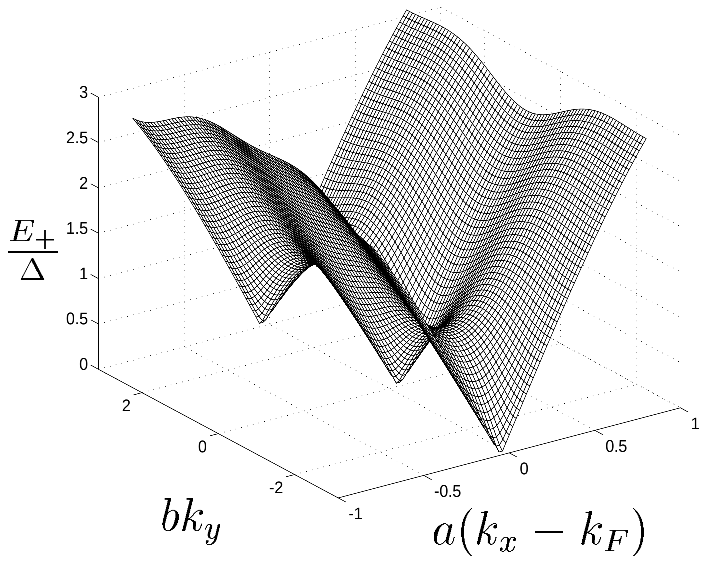
Outline:
- The model
- Order parameter
- Possible materials
- Optical conductivity
- Effect of magnetic field
- Threshold electric field

The Hamiltonian of the system of quasi-one dimensional interacting electrons is given by:

$$H = \sum_{\mathbf{k},\sigma} \varepsilon(\mathbf{k}) a^+_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{1}{2V} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} \tilde{V}(\mathbf{k},\mathbf{k}',\mathbf{q}) a^+_{\mathbf{k}+\mathbf{q},\sigma} a_{\mathbf{k},\sigma} a^+_{\mathbf{k}'-\mathbf{q},\sigma'} a_{\mathbf{k}',\sigma'},$$

Interaction between at most nearest neighbour electrons is taken into account: on site and direct Coulomb, exchange, pair-hopping and bond-charge terms. Diagonalizing H, the energy spectrum is given by:

$$E_\pm(\mathbf{k},\sigma) = \frac{\varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k}-\mathbf{Q})}{2} \pm \sqrt{\left(\frac{\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}-\mathbf{Q})}{2}\right)^2 + |\Delta(\mathbf{k},\sigma)|^2}$$



The gap equation: $\Delta(\mathbf{l}) = \sum_{\mathbf{k}}' \frac{1}{V} \overline{P(\mathbf{k},\mathbf{l})} \frac{\Delta(\mathbf{k}) \tanh\left(\frac{\beta}{2} E(\mathbf{k})\right)}{2E(\mathbf{k})}$, where the kernel is the linear combination of the different matrix elements of the interaction.

From this the gap reads as:

$$\Delta(\mathbf{l}) = \Delta_0 + \Delta_1 \cos(l_y b) + \Delta_2 \sin(l_y b) + \Delta_3 \cos(l_z c) + \Delta_4 \sin(l_z c)$$

From these we take one component. If it is wavevector dependent (unconventional): $\langle m(\mathbf{Q})\rangle = 0$, $\langle n(\mathbf{Q})\rangle = 0$, "hidden-order".
$\Delta(\sigma) = \Delta(-\sigma)$: UCDW, $\Delta(\sigma) = -\Delta(-\sigma)$: USDW
The order parameters of the different phases:

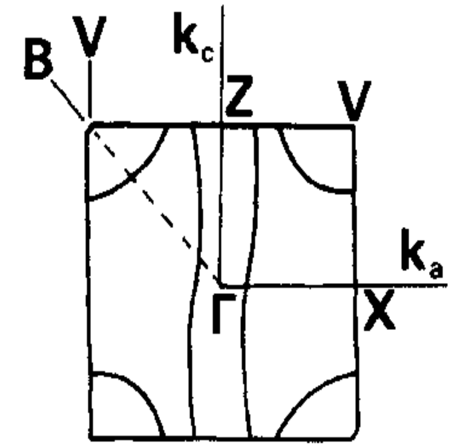
phase	gap	order parameter: the **Q**-th Fourier component of
UCDW	$\Delta\cos(bk_y)$	electric current density
UCDW	$\Delta\sin(bk_y)$	kinetic energy density
USDW	$\Delta\cos(bk_y)$	spin current density
USDW	$\Delta\sin(bk_y)$	spin kinetic energy density

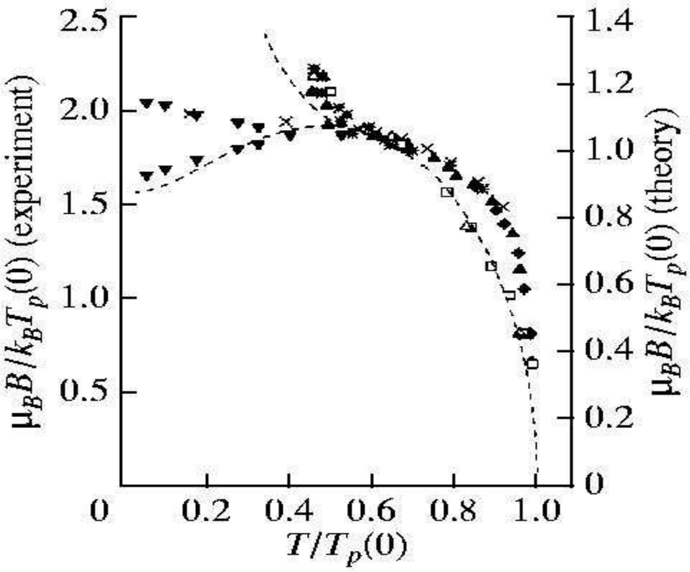
These phases are already known in two dimensional systems as orbital antiferromagnet, bond-order wave, spin nematic state and spin bond-order wave.

The thermodynamics is identical to those of a d-wave superconductor in spite of the dissimilar Fermi surfaces: the gap vainshes on lines at the Fermi surface.
Possible materials with UDW ground state:

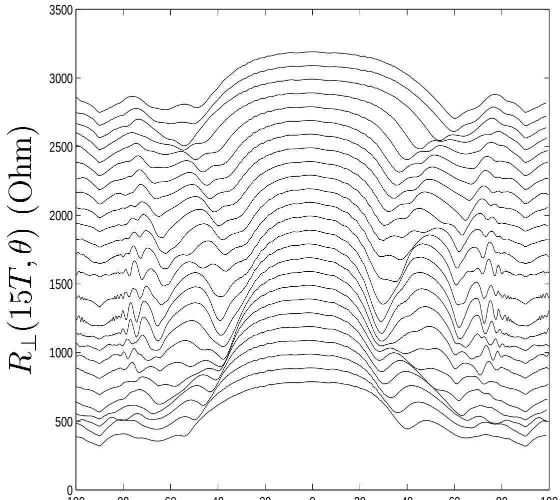
- URu_2Si_2
- $\alpha-(BEDT\text{-}TTF)_2KHg(SCN)_4$
- 2H-$TaSe_2$
- pseudogap: $(TaSe_4)_2I$, HTSC, transition metal oxides ($SrRuO_3$, $BaRuO_3$)

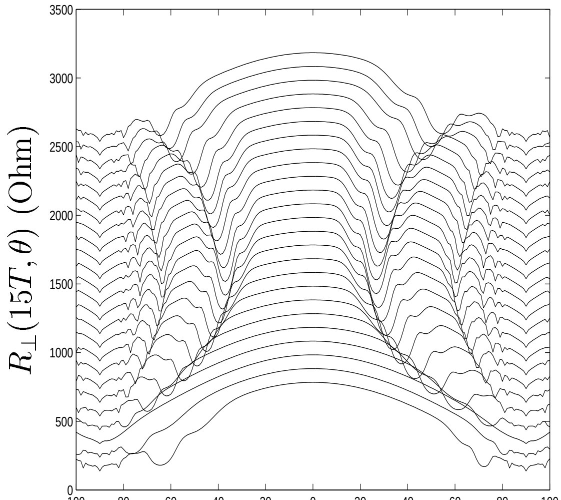
$\alpha-(\mathrm{BEDT\text{-}TTF})_2\mathrm{KHg(SCN)}_4$ salt





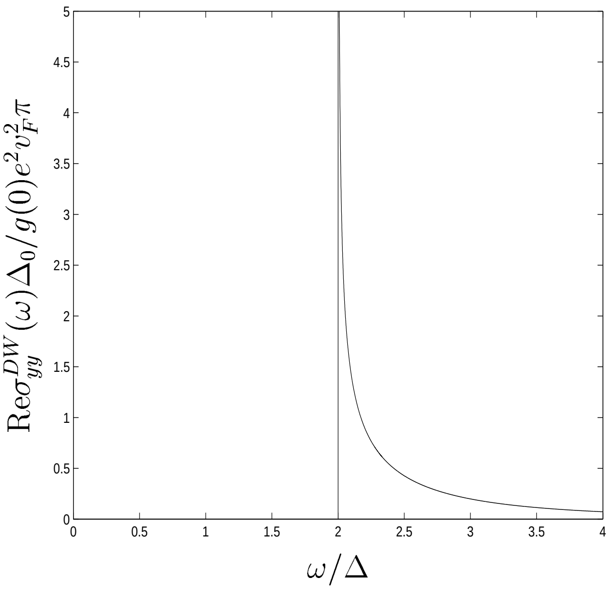
Fermi surface B-T phase diagram⇒ a kind of CDW



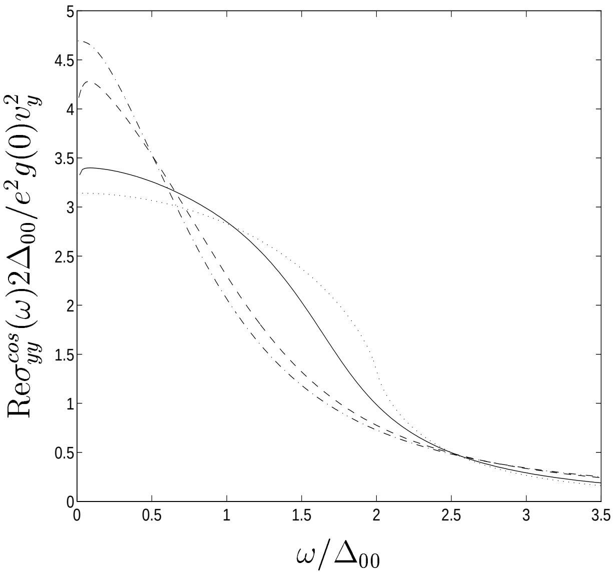


Angular dependent magnetoresistance (Landau quantization of the quasiparticle spectrum)

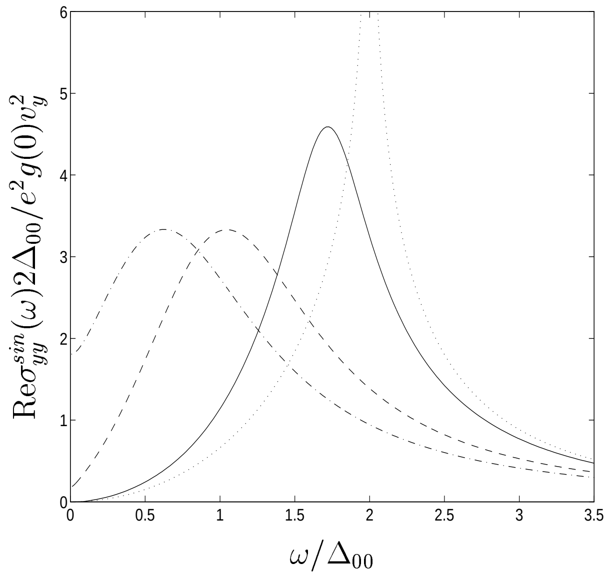
Optical conductivity in the presence of impurities



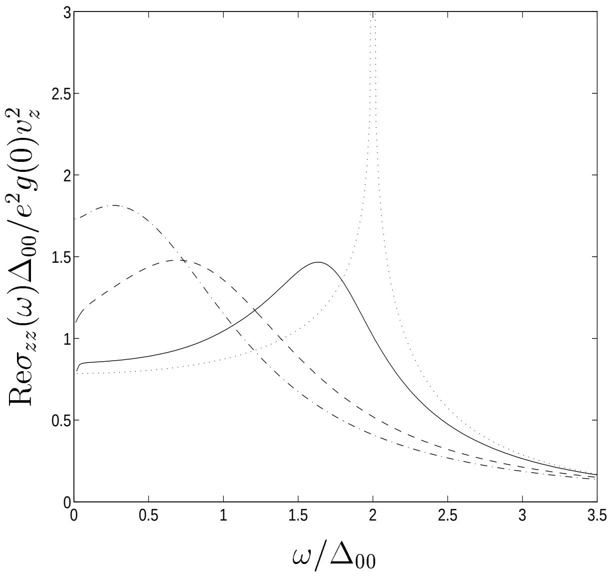
$\Delta(\mathbf{k}) = \Delta_0$



$\Delta(\mathbf{k}) = \Delta\cos(bk_y)$



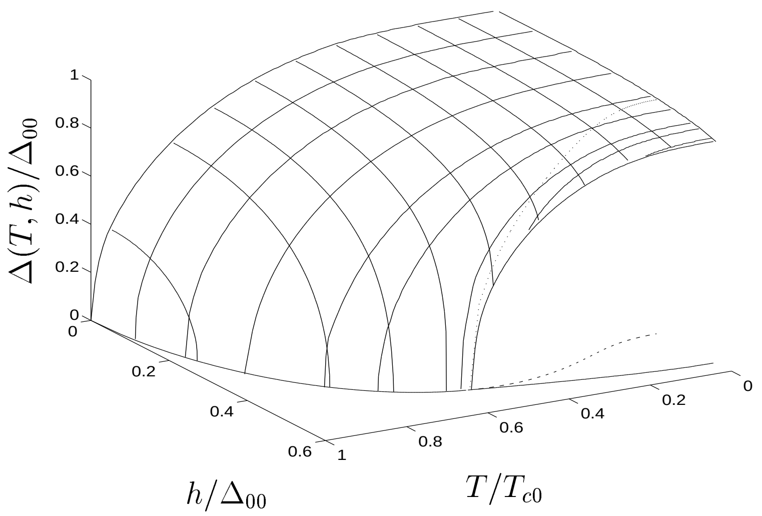
$\Delta(\mathbf{k}) = \Delta\sin(bk_y)$



$\Delta(\mathbf{k}) = \Delta\cos(bk_y)$ or $\Delta\sin(bk_y)$

Magnetic field effects

Magnetic field in the chain directon, Zeeman term. USDW remains unaffected due to spin-flop. The phase diagram of UCDW:



Threshold electric field (E_T): impurities pin the DW, the electric field tries to move the condensate. Strong (small n_i and strong V) and weak (large n_i and weak V) pinning.

- For point-like impurity: $E_T = 0$.
- For finite (nonzero) E_T, extended impurities are needed: $U(\mathbf{Q}+\mathbf{q}) = V_0 + \sum\limits_{i=y,z} V_i \cos(q_i \delta_i)$,

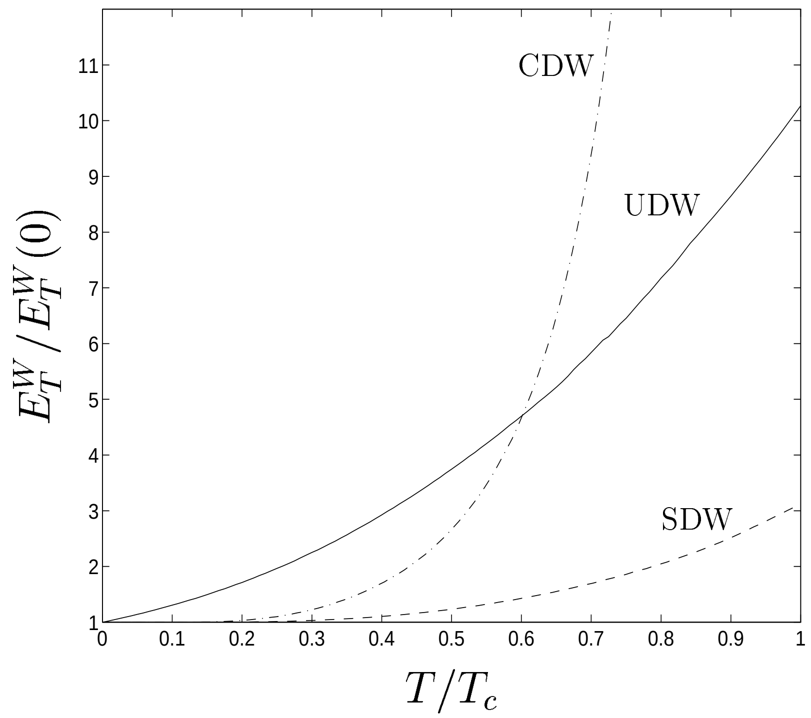
The threshold electric field depends strongly on the magnetic field. At the bicritical point:

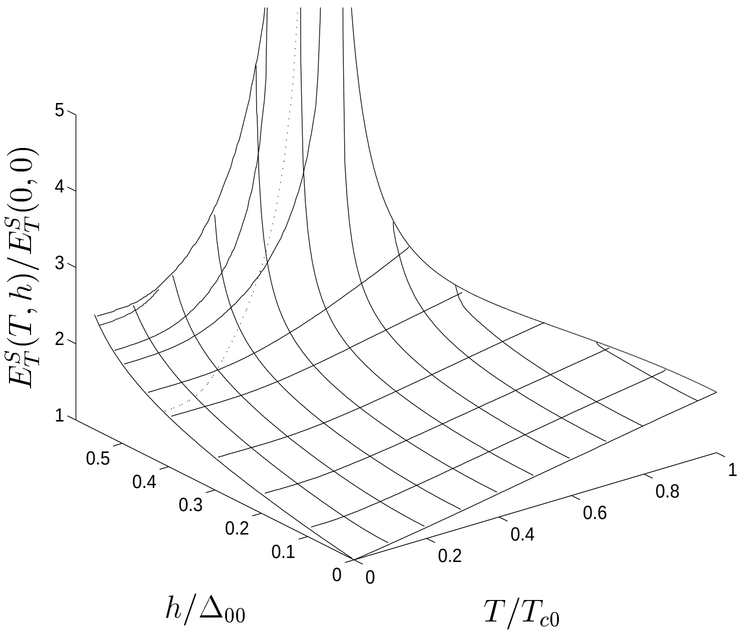
$$\frac{E_T^S(T,h)}{E_T^S(0,0)} = \frac{1.12}{1.91 - h/T}.$$

Threshold electric field

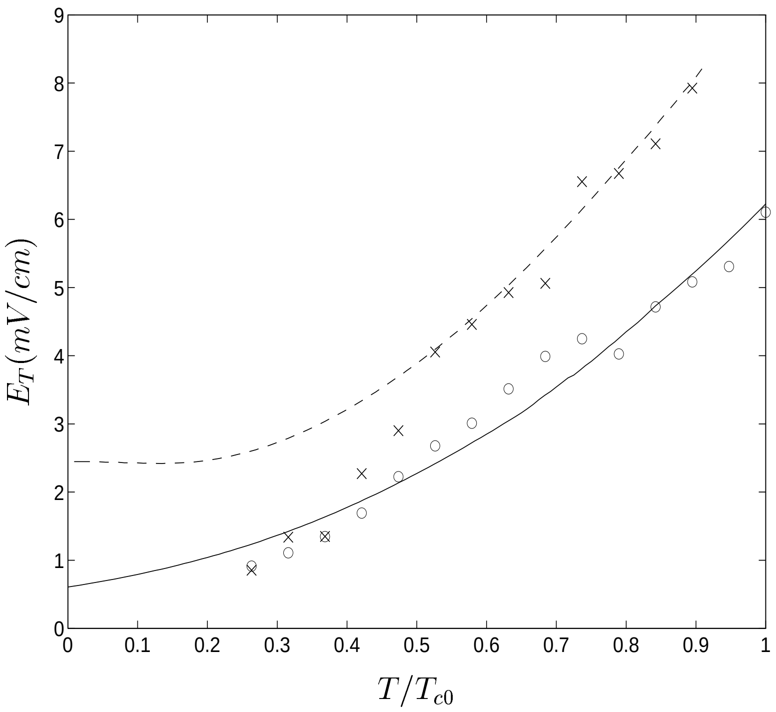
	CDW	SDW	UDW
$\frac{E_T^S(T\to 0)}{E_T^S(0)}$	$1+\sqrt{\frac{2\Delta\pi}{T}}e^{-\frac{\Delta}{T}}$	$1+\sqrt{\frac{2\Delta\pi}{T}}e^{-\frac{\Delta}{T}}$	$1+2\ln(2)\frac{T}{\Delta}$
$\frac{E_T^S(T_c)}{E_T^S(0)}$	∞	1.33	1.793

$$\frac{E_T^W(T)}{E_T^W(0)} = \left(\frac{E_T^S(T)}{E_T^S(0)}\right)^{\frac{4}{4-D}}$$





The threshold electric field of α-(BEDT-TTF)$_2$KHg(SCN)$_4$ at $H = 0$T és $H =$ 1T: comparison of theory and experiment.



Conclusion

- $\mathbf{k}, \mathbf{k}'$ dependent potential for wavevector dependent gap
- Small energy excitations at the zeros of the gap $\Rightarrow$ power-law temperature dependence at $T \to 0$
- No finite magnetic moment, no charge modulation$\Rightarrow$ hidden-order
- In the conductivity, absorption at small frequencies. At certain gap structure, no divergence in the conductivity at 2Δ!
- Strong magnetic field effects on UCDW, good agreement with the experimental data on α-(BEDT-TTF)$_2$KHg(SCN)$_4$!