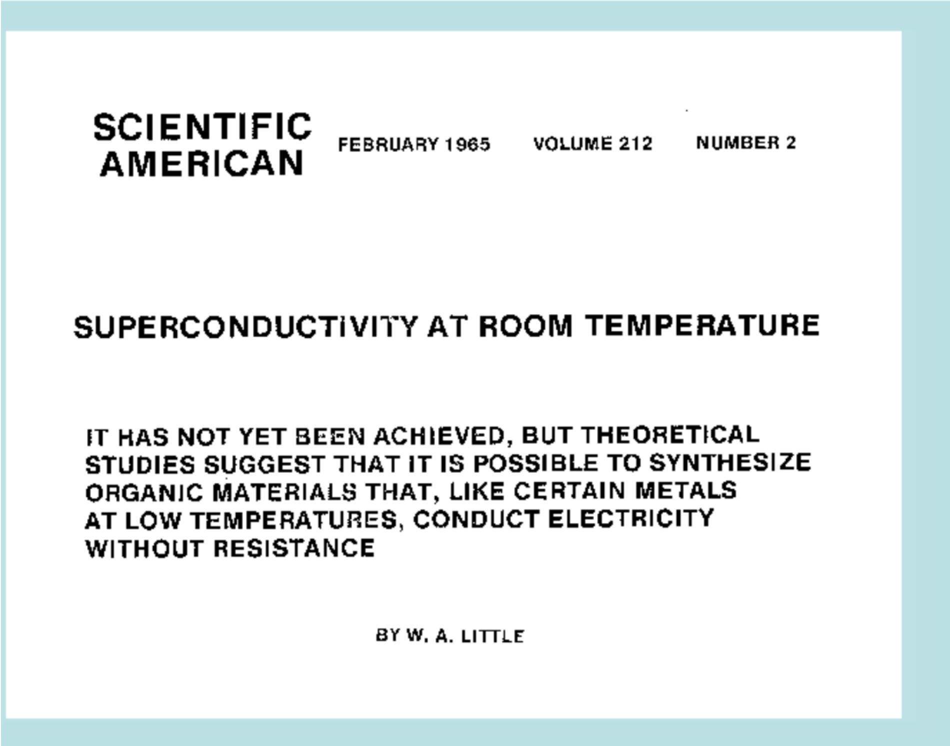
« In the beginning was the Word, …
and without him was not anything made that was made »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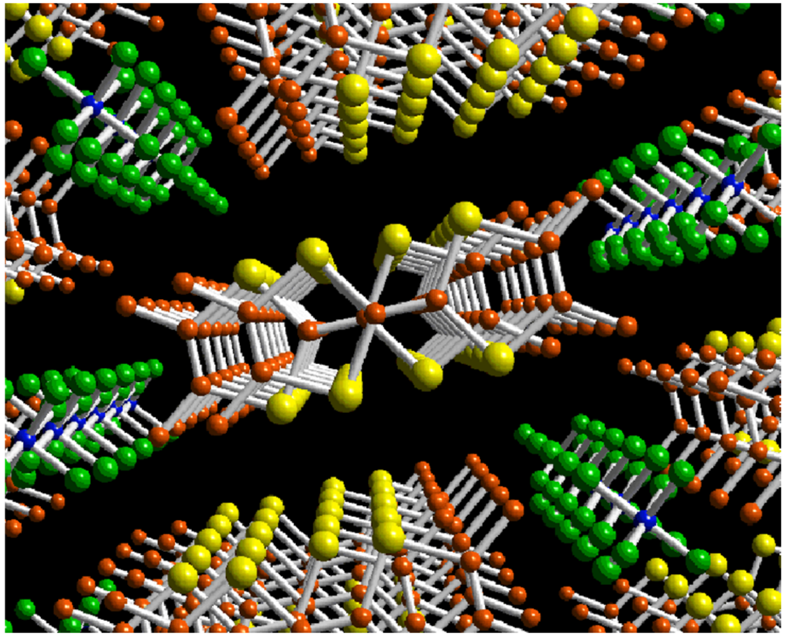
SUPERCONDUCTIVITY AT ROOM TEMPERATURE

IT HAS NOT YET BEEN ACHIEVED, BUT THEORETICAL STUDIES SUGGEST THAT IT IS POSSIBLE TO SYNTHESIZE ORGANIC MATERIALS THAT, LIKE CERTAIN METALS AT LOW TEMPERATURES, CONDUCT ELECTRICITY WITHOUT RESISTANCE

BY W. A. LITTLE



Excursion #4.

Glorious time of early 1980s, superconductivity in organic crystals, after a decade of a crazy and ambitious run over the world , the breakthrough at the LPS in Orsay, Denis Jerome and colleagues.
In a crystal stack of a new molecule synthesized by Klaus Bechgaard.

Those days the 1D models were studies to understand the phase diagram of quasi-1D systems – *the source for this excursion*.

The intrigue against common beliefs: the 1D T=0 phase diagram
based upon diverging power-law susceptibilities,
does not want at all to reproduce itself
when electrons are allowed for the interchain hopping.

The system falls to the Fermi-liquid regime unless real or curious
"imaginary" gaps appear from external symmetry lowering
due to the crystal field or the magnetic field.

S. Brazovskii & V. Yakovenko,
"On the theory of phase transitions in organic superconductors"
J. de Physique Lett. & JETP (1985), JETP Letters (1986);
V. Yakovenko JETP Lett (1992) and cond-mat (2000 – review and rfs.)
"Coherence of tunneling between one-dimensional Luttinger liquids"

Typical types and order parameters of electronic symmetry breaking

$$O_{\mathrm{CDW}}(z)=\sum_{\sigma}\psi^{+}_{\sigma,+}(z)\,\psi_{\sigma,-}(z),$$

$$O^{(j)}_{\mathrm{SDW}}(z)=\sum_{\sigma,\sigma'}\psi^{+}_{\sigma,+}(z)\,\sigma^{(j)}_{\sigma,\sigma'}\psi_{\sigma',-}(z).$$

σ – Pauli matrices

$$O_{\mathrm{SS}}(z)=\sum_{\sigma}\sigma\psi_{-\sigma,+}(z)\,\psi_{\sigma,-}(z),$$

$$O^{(j)}_{\mathrm{TS}}(z)=\sum_{\sigma,\sigma'}\sigma\psi_{-\sigma,+}(z)\,\sigma^{(j)}_{\sigma,\sigma'}\psi_{\sigma',-}(z)$$

Corresponding susceptibilities: $\chi_i(T)=\sum_{\mathbf{m}}\int d^2z\langle O_i^{+}(z,\mathbf{m})O_i(0,\mathbf{n})\rangle$

Phase diagram (PD) of a 3d system of weakly interacting chains is usually supposed to correspond to the conventional 1d PD being defined by divergences of corresponding susceptibilities at **T→0**.

$$\chi^{(i)}_{1\mathrm{d}} \sim T^{-\beta_i} + \mathrm{const.}, \qquad \beta_i = 2 - \eta_i, \qquad i = \mathrm{CDW, SDW, SS, TS}$$

Conditions β_i**>0** with choosing the maximal one were giving rise to the PD in coordinates of many coupling constants of the 1D Hamiltonian which influence β_i

Typical picture of true phase transitions in quasi 1D systems:
on top of T=0 divergences in 1D - interchain coupling of order parameter

$$S_\perp = \sum_{i,\mathbf{m},\mathbf{n}} \int d^2 z \lambda_{\mathbf{m},\mathbf{n}}^{(i)} O_i^+(z,\mathbf{m}) O_i(z,\mathbf{n}), \quad \lambda_i = \sum_{\mathbf{m}} \lambda_{\mathbf{m},\mathbf{n}}^{(i)}$$

Given an inter-chain coupling λ_i the total susceptibility yields

$$\chi^{(i)} = \chi_{1d}^{(i)} + \lambda_i (\chi_{1d}^{(i)})^2 + \cdots \approx [(\chi_{1d}^{(i)})^{-1} - \lambda_i]^{-1}$$

$$\chi_{1d}^{i} \sim T^{-\beta_i} \quad \chi^{(i)}(T_c) = \infty, \quad \chi_{1d}^{(i)}(T_c) \sim \lambda_i^{-1}, \quad \beta_i > 0$$

The unattended problem: 3d couplings λ_i do not appear explicitly (except for i = CDW) due to the loss of electronic coherence in the course of an interchain tunneling. λ may or rather cannot be generated from the interchain hopping Hamiltonian

$$S_t = \sum_{\sigma,\mathbf{m},\mathbf{n},\alpha} \int d^2 z [t_{\mathbf{m}-\mathbf{n}} \psi_{\sigma,\alpha}^{+}(z,\mathbf{n}) \psi_{\sigma,\alpha}(z,\mathbf{m}) + \text{H.c.}] \qquad z = x + it$$

Conventional systems: **λ∝t²/Δ** for SC or CDW, **λ∝t²/U** for AFM,SDW - gaps **Δ** or **U** are required to generate either Josephson or spin-exchange couplings

Gapless Tomonaga-Luttinger regime

$$G = \langle \psi_{n\alpha}(0)\psi^{+}_{na}(z)\rangle \sim |z|^{-\eta_F}\ ,\ z = x + it,\ \ \eta_F = 2 - \beta_F$$

$$K^{\sigma\sigma'}_{n_1 n_2 n_3 n_4}(z_1, z_2, z_3, z_4) = \left\langle \psi_{\sigma^+}(z_1, n_1)\psi^{+}_{\sigma'^+}(z_3, n_3)\psi_{\sigma'^-}(z_2, n_2)\psi^{+}_{\sigma'^-}(z_2, n_2)\right\rangle$$

Up to Log scaling:

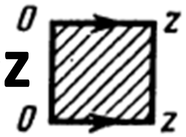
$$K(z_1..z_4) \propto (|z_1 - z_3|\,|z_2 - z_4|)^{\eta}\left(\frac{|z_1 - z_4||z_2 - z_3|}{|z_1 - z_2|\,|z_4 - z_3|}\right)^{\nu}$$

$$\gamma = \gamma_\rho = K_\rho \quad \eta_i = 1 + \gamma\ (\mathrm{SC}) \quad \eta_i = 1 + 1/\gamma (DW)$$

$$\eta = \eta_F = (2 + \gamma + 1/\gamma)/4 \quad \nu = (\gamma - 1/\gamma)/4$$

No interactions: $\eta_F = 1$ $\nu = 0$, Attraction: $\gamma > 1$, Repulsion: $\gamma < 1$, Mott instability: $\gamma < 1/2$

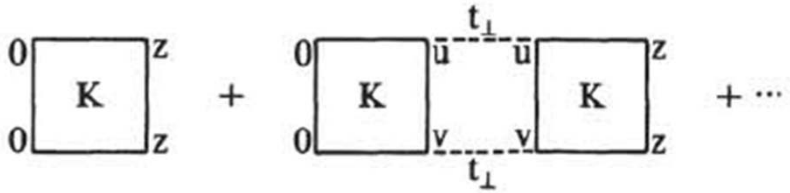
Expressions for χ_{1d} follow from K if we bind the ends z_j by pairs,

e.g. for SC $z_1 = z_2$, $z_3 = z_4$, and integrate over them. $\int d^2z$  $= \chi$

It was just the artificial confining of the ends

that usually brought the over-optimistic result of reproducibility of χ_{1d}

Series of $\mathbf{t}_\perp$=$\mathbf{t}$ for any $\boldsymbol{\chi}$:



$$\chi^{(i)}(T) = \frac{1}{T^{2-\eta_i}} + t_\perp^2 \int \frac{\mathrm{d}^2 z\, \mathrm{d}^2 u\, \mathrm{d}^2 v\, f_i(u, v)}{|u - v|^{2\eta_F - \eta_i}\, [|u|\,|v|\,|z - u|\,|z - v|]^{\eta_i/2}} + \cdots$$

i=SS, TS: $\eta_i = 2(\eta_F - \nu)$ $\quad$ i=CDW, SDW: $\eta_i = 2(\eta_F + \nu)$

$$\eta_F = (2 + \gamma + 1/\gamma)/4 \quad , \; 2\eta_F - \eta_i = \pm 2\nu = \pm(\gamma - 1/\gamma)/2$$

f= f(u, v) *may come* from additional symmetry lowering, otherwise ***f*** = ***const***.

Regime 1: $\int d^2 w$, $w=u-v$, is convergent, two particles tunnel together, series of χ^i_{1d} is reproduced accumulating to divergent χ^i_{3d}.

Regime 2: divergence towards upper limit ~***1/T***; series of χ^i_{1d} is not reproduced: independently on the channel (i), the series goes in powers with the non-specific index η_F of the one-particle Green function, apparently working out the quasi-1d band picture.

If the integral over **(u - v)** converges at some length ξ.
The intermediate ends **u, v** (tunnelling space-time points) become confined at the scale ξ. Then, the subseries of powers $(\lambda_i \chi_i)^n$
with the effective coupling constant λ_i :

$$\lambda_i \sim \frac{t_\perp^2}{\xi^{\beta_i - 2\beta_F}} \qquad\qquad T_{3d} \sim \xi^{-1}\left(t_\perp \xi^{\beta_F}\right)^{2/\beta_i}$$

Symmetry lowering to the Mott state - the gap **Δ** in the charge channel.
Or a singlet superconductivity or CDW - the gap **Δ** in the spin channel.
The convergence length **ξ~1/Δ** is worked out

$$\lambda_i = t^2 \int \frac{d^2 w}{w^{2\eta_F - \eta_i}} \exp\left(-\frac{|w|}{\xi}\right) \propto \frac{t^2}{\Delta^{2 - 2\eta_F + \eta_i}}$$

Particles tunneling is confined –
generalization of Josephson or exchange coulplings

But if no gaps, Δ=0 ?
Common believe of 1980’s-90’s : the temperature **T** takes the duty.
WRONG

Brutal-force power law convergence of the sub-integral over **w=u-v**

$$\int \frac{d^2 w}{w^{\pm\nu}} = \int \frac{d^2 w}{w^{2\eta_F - \eta_i}}$$

In a common TL case with no gaps and symmetry lowering effects the convergence requires for $\boldsymbol{2\eta_F-\eta_i>2}$.
Not excluded for extremely strong long range repulsions,
but still so far: for free fermions $\boldsymbol{2\eta_F-\eta_i=0}$ since $\boldsymbol{\gamma=1}$*!*
Even for **U** $\boldsymbol{\to\infty}$ Hubbard model: $\boldsymbol{\gamma=1/2}$, $\boldsymbol{\eta_F=9/4}$, $\boldsymbol{2\eta_F-\eta_i=1/2<2}$
Here we need truly strong interaction, well beyond stability criteria,
e.g. $\boldsymbol{\gamma<1/2}$ for repulsion (Mott state = $4K_F$ anomaly):

$$\boldsymbol{2\eta_F-\eta_i=\pm 2\nu>2}\ , \qquad \boldsymbol{\gamma>\sqrt{5}+2\approx 4.24}\ \text{(SC)}$$
$$\text{or}\quad \boldsymbol{\gamma<\sqrt{5}-2\approx 0.24}\ \text{(DWs)}$$

This consideration touches hot topics from all 1990's of
one- and two-particle inter-chain coherence of coupled TL chains
Bourbonnais&Caron; Clark,Strong&Anderson; Fabrizio et al; Finkelstaein&Larkin; Kusmartsev,Luther&Nersesyan; Mila&Poilblanc; H.Schultz; Tsvelik; Yakovenko

"Imaginary correlation lengths" or virtual attractions from inequivalence of chains

A. Fortunate present from tiny structures of the Q-1D organic superconductors: alternating mean densities at neighboring chains (n)

$$k_f^{(a)} = k_F + (-1)^n \kappa \rightarrow f_i(u,v) = \cos\left[2\kappa(x_u - x_v)\right] \quad \textbf{\textit{i=SS, TS}}$$

B. Spin density waves under magnetic field **H** transverse to the inter-chain ***b*** direction - progressive increments of Fermi wave numbers among neighboring chains:

$$\psi_{\sigma,\alpha}(\mathrm{z},\mathrm{n}) \rightarrow \psi_{\sigma,\alpha}(\mathrm{z},\mathrm{n})\exp\left(iqnx\right), \quad q = (e/c)bH$$

$$f_i(u,v) = \exp\left[-iq(x_u - x_v)\right] \qquad \textbf{\textit{i=CDW, SDW}}$$

These external fields provide oscillating factors, which greatly improve the convergence of tunneling points

$$I_{SC} = \int d^2z \frac{\cos(2\kappa x)}{|z|^{2\nu}} \quad \nu = (\gamma - 1/\gamma)/4$$

$$I_{DW} = \int d^2z \frac{\cos(2qx)}{|z|^{2\nu}} \quad \nu = -(\gamma - 1/\gamma)/4$$

with $\nu>0$ being the sufficient condition
rather than **ν>1** for super-strong interactions.
ν≠0 at any **γ≠1** – already for small interactions.

The confinement within the tunneling pair is maintained, effective interchain coupling constant is worked out

$$\lambda \sim \frac{t_\perp^2}{\kappa^{2-2\nu}}$$

WHERE WE ARE?

$H \sim = (\hbar/4\pi\gamma)\,[v_\rho(\partial_x\varphi)^2 + (\partial_t\varphi)^2/v_\rho]$

$- U\cos(2\varphi+2kx) - W\cos(4\varphi+4kx) + \{aU^2/2 + bW^2/2 + ck^2/2\}$

U- dimerization, build-in or spontaneous

W- effect of ¼ filling, octamerization

k – deviation from the commensurability

$\gamma = K_\rho$ controls renormalization of U and W, *without interactions* $\gamma=1$

$\gamma<1$: renormalized **$U\neq0$** - gap originated by build-in dimerization.

$\gamma<1/2$: spontaneous **U** is formed (**$4K_F$** condensed = charge ordering,
- electronic energy gain **$\delta F_e \sim -U^\zeta$ ($\zeta=1/(1-\gamma)<2$**
overcomes the energy lost **$\sim U^2$** to pay spontaneous deformations.

$\gamma<1/4 = 0.25$ renormalized **$W\neq0$** - gap originated by generic ¼ filling (*recall ThG*)

$\gamma<\sqrt{5}-2=0.24$ ultimate 3D SDW instability – today's lesson.

$\gamma<3-\sqrt{2}=0.17$ last features (ARPES) of electrons disappear.

$\gamma=1/8=0.125$ spontaneous W is formed – gratest Coulomb enhancement of repalsive interactions; close to estimate from optical tails (*ThG, LD*)

Only atomic gases in the vacuum can pass $\gamma=1/2$ in 1D and $\gamma=0.24$ for an array of 1D.

Outcome:

Interchain mismatches **κ,q** of wave numbers work as imaginary gaps,

1/κ,1/q work as imaginary correlation lengths of e-e or e-h pairs.

Having found, after tunnelings, themselves together away from the Fermi points, the particles get confined, keep coherence, and transmit on-chain divergences of pair-wise correlation functions.

Methodological hint for these observations:
A lesson from the diagram technique epoch
– always check for cumbersome higher order terms,
above the happily found seemingly significant ones.
An advice hardly realizable in earlier time of decoupling techniques
and the later RG epoch.