

Road to Room Temperature Superconductivity

17-23 June 2007, Hotel Alexandra, Loen, Norway

AFOSR, Twente, Trondheim, HKUST

<http://www.sruodesigns.com/road2rts/>

<http://www.w2agz.com/rtsc07.htm>

Chu	Varma	Cohen	Bosovic	Kivelson
Kresin	Mannhart	Scalapino	Beasley	Antipov
Akimitsu	Gurevich	Fischer	Pavuna	Hasuo
Ashcroft	Rice	Shimizu	Geballe	Uchida
Sudbo	Klemm	Zakhidov	Raveau	Grant

Theory of Everything

Bob Laughlin's "Theory of Everything" (that matters)

$$\mathcal{H} = - \sum_j \frac{\hbar^2}{2m} \nabla_j^2 - \sum_a \frac{\hbar^2}{2M_a} \nabla_a^2 - \sum_{j,a} \frac{Z_a e^2}{|r_j - R_a|} + \sum_{j,k} \frac{e^2}{|r_j - r_k|} + \sum_{a,b} \frac{Z_a Z_b e^2}{|R_a - R_b|}$$



- | | | |
|--------------------|-----------------|------------------|
| • Hydrogen atom | • Proteins | • Flowers |
| • Methane molecule | • DNA | • Trees |
| • Water | • Viruses | • Cars |
| • Air | • Bacteria | • Cheese |
| • Rocks | • Yeast | • Sauce Bernaise |
| • Concrete | • Slime mold | • Computers |
| • Steel | • Butterflies | • Television |
| • Glass | • Sharks | • Cars |
| • Plastic | • Rats | • Jets |
| • Buildings | • Lawyers | • Lawnmowers |
| • Cities | • Ebola virus | • Sewage |
| • Continents | • Legislatures | • Spotted Oats |
| | • Civilizations | ... |

The crunch comes when \sum_i with $i \geq 3 \rightarrow$ "thermodynamic limit."

"Size Matters !"

“Naked BCS”

$$T_C = a\Theta e^{-\frac{1}{\lambda - \mu^*}}$$

Where

$$\lambda k\Theta \ll E_F$$

T_C = Critical Temperature

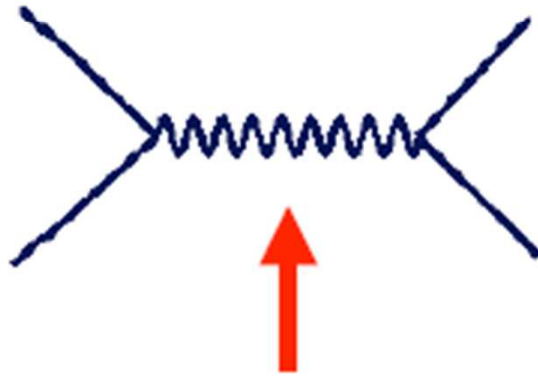
Θ = Boson Characteristic Temperature

λ = Fermion-Boson Coupling Constant

μ^* = Fermion-Fermion Repulsion

a = “Gap Parameter, $\sim 1-3$ ”

When “electron-electron” interactions are involved,
the phrase “pairing glue” can be a dirty word!



Insert your favorite “on” here

(phonon, magnon, exciton, plasmon, anyon, moron ...)

“Put-on !”



Electron-Phonon Coupling a la Migdal-Eliashberg-McMillan

(plus Allen & Dynes)

$$H_{el-ph} = \sum_{\mathbf{k}q\nu} g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{q\nu,mn} c_{\mathbf{k}+\mathbf{q}}^{\dagger m} c_{\mathbf{k}}^n (b_{-\mathbf{q}\nu}^{\dagger} + b_{\mathbf{q}\nu}) \quad (1)$$

First compute
this via DFT...

$$\alpha^2 F(\omega) = \frac{1}{N(\varepsilon_F)} \sum_{mn} \sum_{q\nu} \delta(\omega - \omega_{q\nu}) \sum_{\mathbf{k}} |g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{q\nu,mn}|^2 \times \delta(\varepsilon_{\mathbf{k}+\mathbf{q},m} - \varepsilon_F) \delta(\varepsilon_{\mathbf{k},n} - \varepsilon_F), \quad (2)$$

$$\lambda = 2 \int \frac{\alpha^2 F(\omega)}{\omega} d\omega = \sum_{q\nu} \lambda_{q\nu}, \quad (3)$$

$$\lambda_{q\nu} = \frac{2}{N(\varepsilon_F)\omega_{q\nu}} \sum_{mn} \sum_{\mathbf{k}} |g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{q\nu,mn}|^2 \times \delta(\varepsilon_{\mathbf{k}+\mathbf{q},m} - \varepsilon_F) \delta(\varepsilon_{\mathbf{k},n} - \varepsilon_F). \quad (4)$$

Then this...

Quantum-Espresso (Democritos-ISSA-CNR)

<http://www.pwscf.org> Grazie!

Davis – Gutfreund – Little (1975)

PHYSICAL REVIEW B

VOLUME 13, NUMBER 11

1 JUNE 1976

Proposed model of a high-temperature excitonic superconductor*

D. Davis,[†] H. Gutfreund,[‡] and W. A. Little

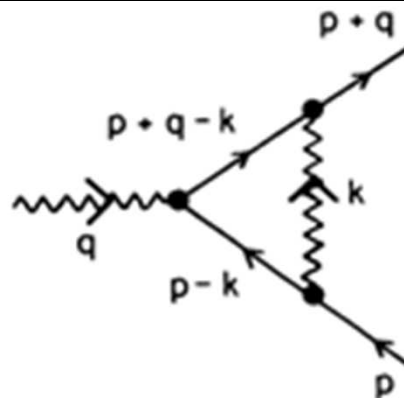
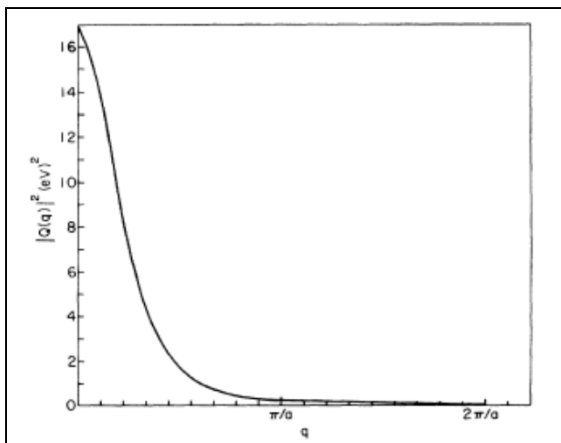
Physics Department, Stanford University, Stanford, California 94305

(Received 16 October 1975)

$g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{qv, mn} \rightarrow$ Kirzhnits, Maximov, Zhomskii

$$\phi^*(r_1 - R_j) \phi(r_1 - R_h) e^{i[kR_h - (k-q)R_j]} V(r_1 r_2) \sum_{m,l,\nu} [u_{\alpha l}^{\nu}(q) + i v_{\alpha l}^{\nu}(q)] e^{-iqR_l} \Psi_{\nu}^*(R_{m l}) \Psi_{00}$$

$$Q_{\alpha}(q) = \frac{1}{N^{3/2}} \int \sum_{j,k} \phi^*(r_1 - R_j) \phi(r_1 - R_h) e^{i[kR_h - (k-q)R_j]} V(r_1 r_2) \sum_{m,l,\nu} [u_{\alpha l}^{\nu}(q) + i v_{\alpha l}^{\nu}(q)] e^{-iqR_l} \Psi_{\nu}^*(R_{m l}) \Psi_{00} d^3 r_1 d^3 r_2$$

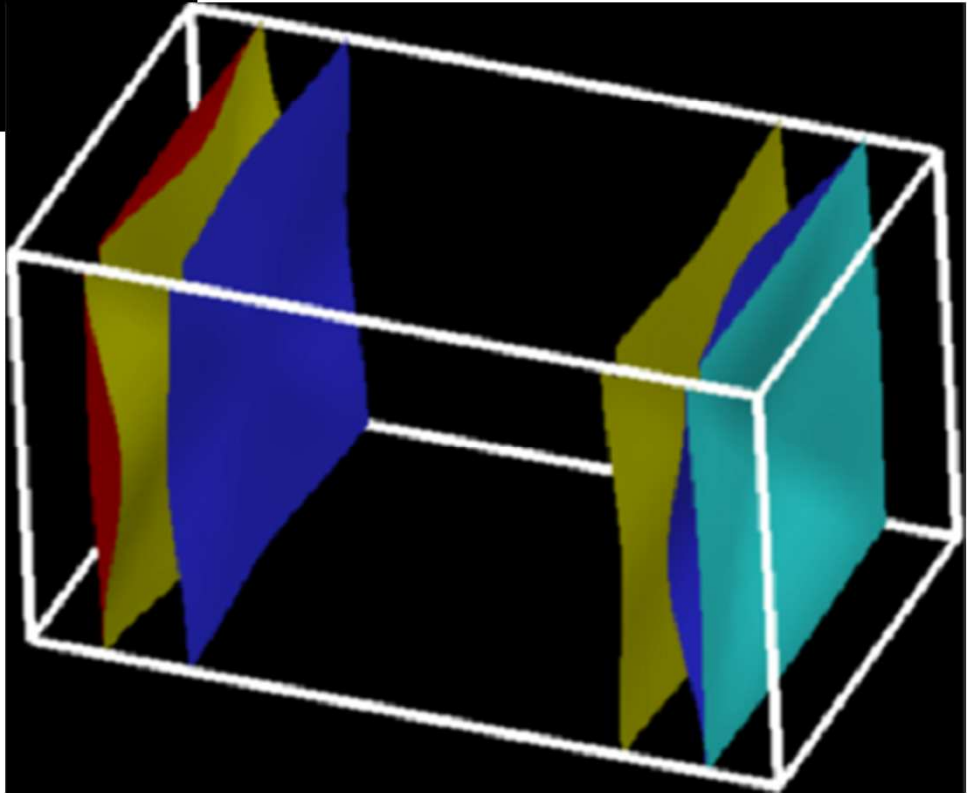
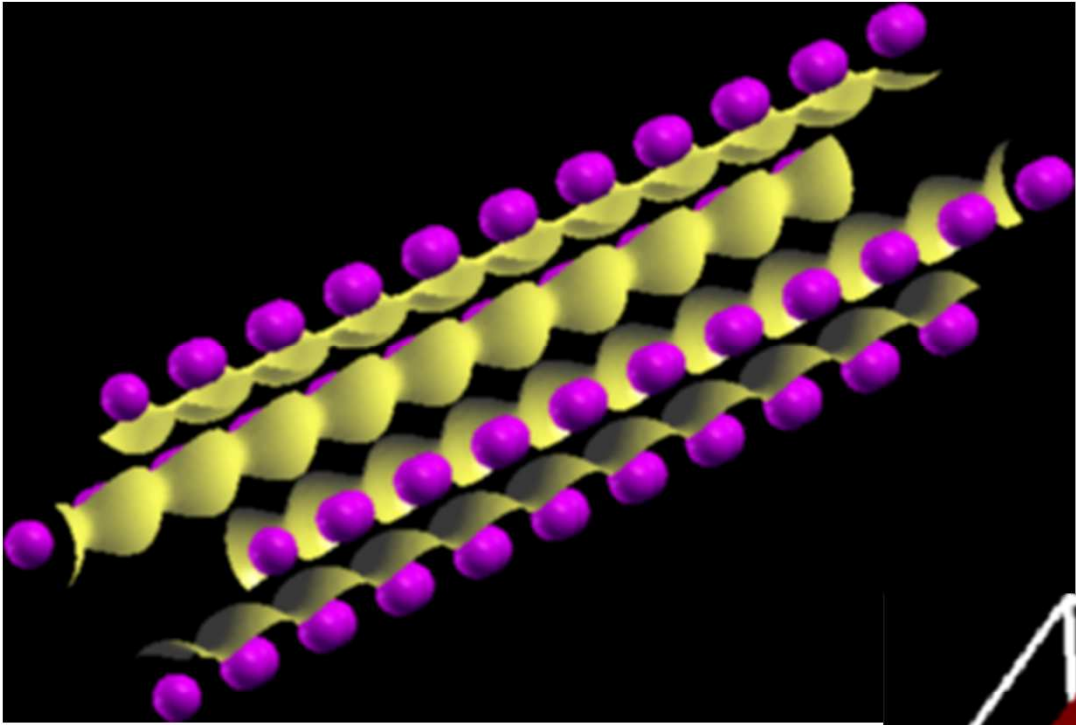


Migdal Issues:

- Only small exciton q 's, $v_q \gg v_f$, couple to the electrons.
- Thus vertex corrections are of order λ^2/θ and we're OK.
- DGL claim this is NOT the case for ABB.
- IMHO, this is an item amenable to numerical analysis.

Norwegian Dreams

- Geballe (“Negative U”)
- Kresin (“Magic Clusters”)
- Mannhart-Bosovic (“Interfaces”)
- Gurevich-Beasley (“Large Lambda”)
- Fischer (“Dig out $2\Delta = (8?)kT_c$ ”)
- Ashcroft (“Keep it light”)
- Grant (“da Vinci Code”)



Guidance from Our Elders

- *“Don’t listen to theoreticians”* (B. Matthias, ca. 1970s).
- *“To make a long story short, searches for high-temperature superconductors, especially with the existing obscurities in the area of theory, may lead to unexpected results and discoveries”* (V. L. Ginzburg, 1984).
- *“At the extreme forefront of research in superconductivity is the empirical search for new materials”* (M. R. Beasley (1983), as communicated by K. A. Mueller and J. G. Bednorz, (1986)).
- *“If you find an old metal laying around in the literature, try cooling it down,”* (P. M. Grant, 1976).

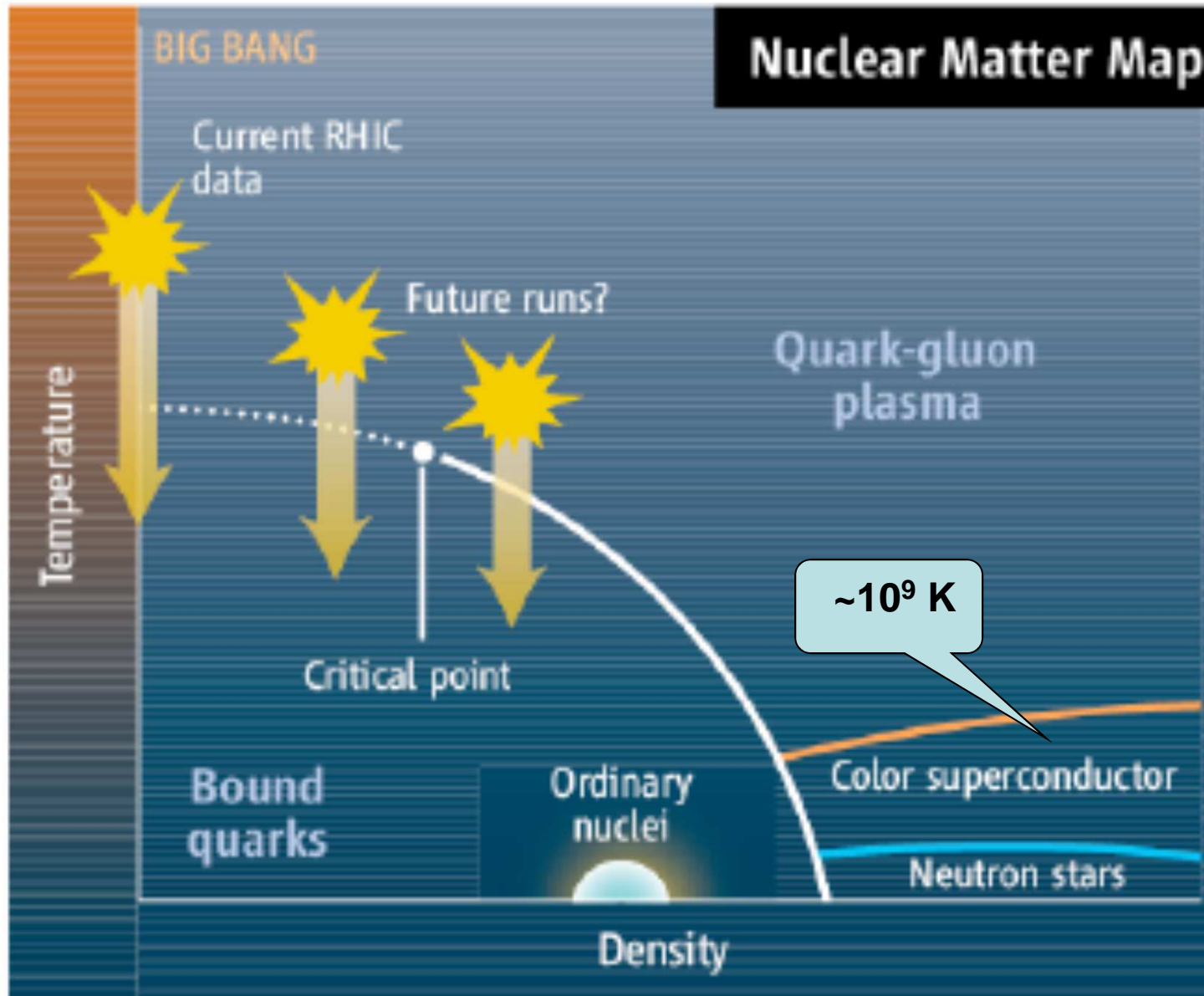
“You can’t always get what you want...”



“...you get what you need!”



Really High-Tc



Exactly What is a “Superconductor?”

- Does it have to be a “perfect conductor?”
 - i.e., zero TAFF
- Does it have to exclude flux (Meissner)?
- Or does it only need to be a “real good conductor (“ultraconductor”)?”
 - $200\times \sigma_{\text{Cu}} @ 300 \text{ K} @ 1000 \text{ Hz}$
 - Ballistic CNTs
 - Sliding P-F CDWs
 - Charged Solitons
 - ???

“From Rags to Riches”

The Road to Room-Temperature Superconductivity

For Fame:

- $T_c = 300 \text{ K}$
- no layered cuprate

Thanks, Jochen !

For Fortune:

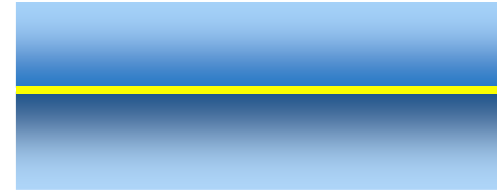
- $T_c > 500 \text{ K}$
- $J_e (350 \text{ K}) > 10^4 \text{ A/cm}^2$ in 5 T
- ductile, robust, good thermal properties
- good Josephson junctions
- environmentally friendly compound
- available in large quantities
- $< 20 \text{ € kA/m}$

Design and Fabrication of New Superconducting Materials

II) Boosting T_c by Optimizing the Mesoscopic Structure

1) Kresin Effect: nanoclusters with number of electrons close to magic

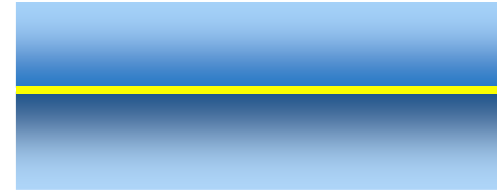
Using Interfaces to Enhance T_c



Interfaces to:

- 1) stabilize superconducting phase / suppress phase transitions
- 2) optimize doping
 - spatially separate doping layer from layer with pair interaction (see HTS)
- 3) create novel electronic phases:
 - correlation parameters at interfaces different from those of bulk —
- 4) use interface chemistry / induce defects
- 5) create E and B – fields, break inversion symmetry
- 6) spatially separate pairing interaction from flow of carriers

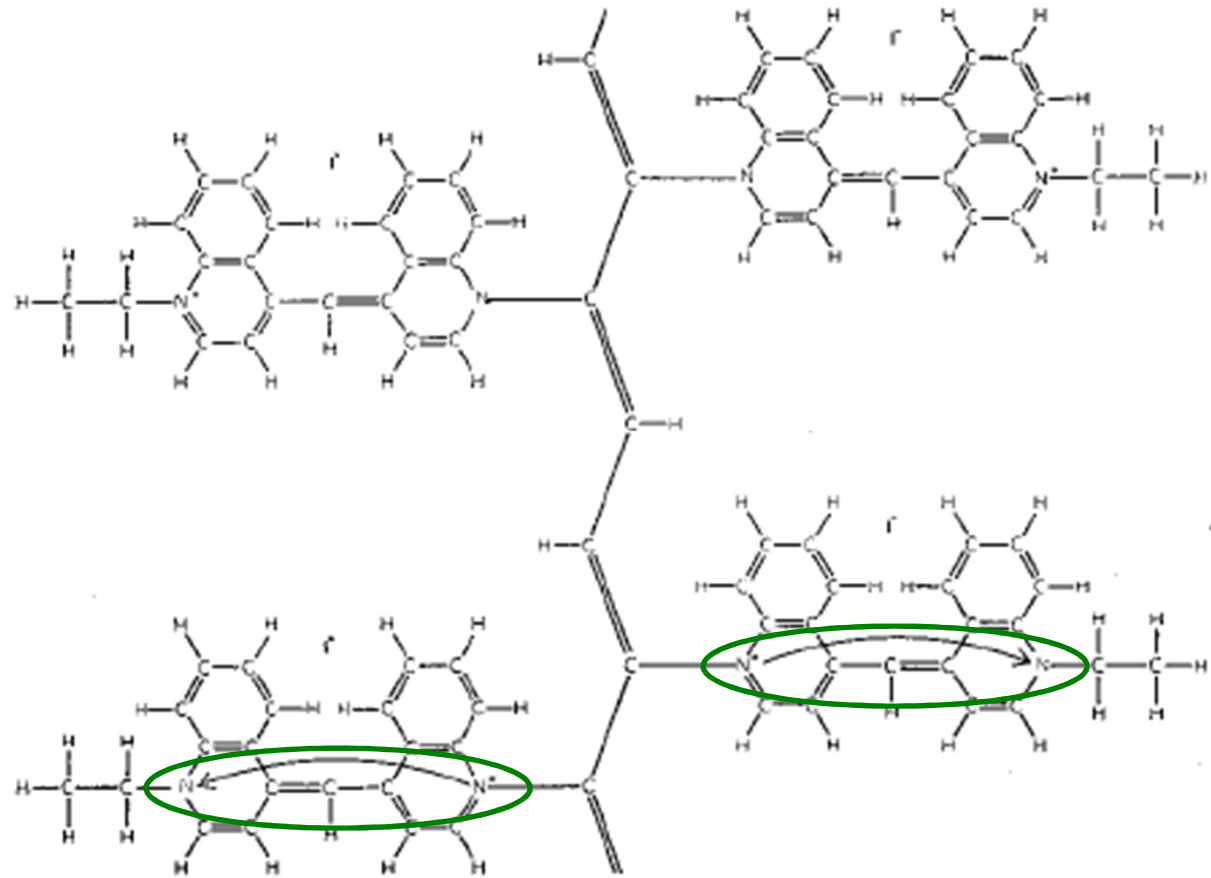
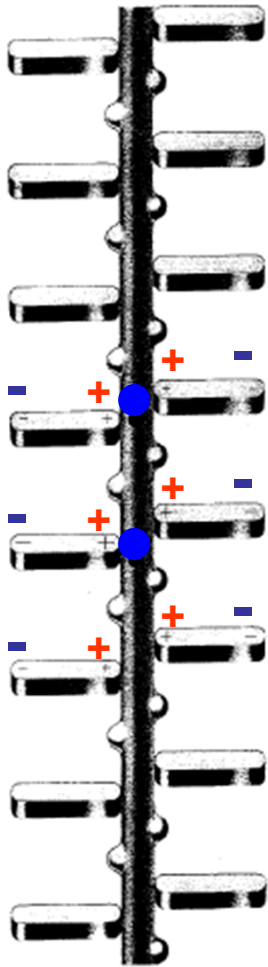
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Little, 1963



Diethyl-cyanine iodide

Theory of Everything

Bob Laughlin's "Theory of Everything" (that matters)

$$\mathcal{H} = - \sum_j \frac{\hbar^2}{2m} \nabla_j^2 - \sum_\alpha \frac{\hbar^2}{2M_\alpha} \nabla_\alpha^2 - \sum_{j,\alpha} \frac{Z_\alpha e^2}{|r_j - R_\alpha|} + \sum_{j,k} \frac{e^2}{|r_j - r_k|} + \sum_{\alpha,\beta} \frac{Z_\alpha Z_\beta e^2}{|R_\alpha - R_\beta|}$$

Where's spin, Pauli and Darwin? Ya screwed up, Bob...should'a used the many boy Dirac equation! Oh yeah, and maybe Maxwell, Boltzman and Gibbs, too...and Newton's Apple.

- | | | |
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| | • Civilizations | ... |

The crunch comes when \sum_i with $i \geq 3 \rightarrow$ "thermodynamic limit."

"Size Matters !"

"Superconduct-ress"

