Superconducting Fluctuations in One-Dimensional Quasi-periodic Metallic Chains

- The Little Model of RTS Embodied -

Does the

DAVINCI CODE

Hold the Key to Room Temperature Superconductivity?

Room 209, Argyros Forum, 9 May 2017, 9:45 AM – 10:30 AM

Paul Michael Grant

Aging IBM Pensioner

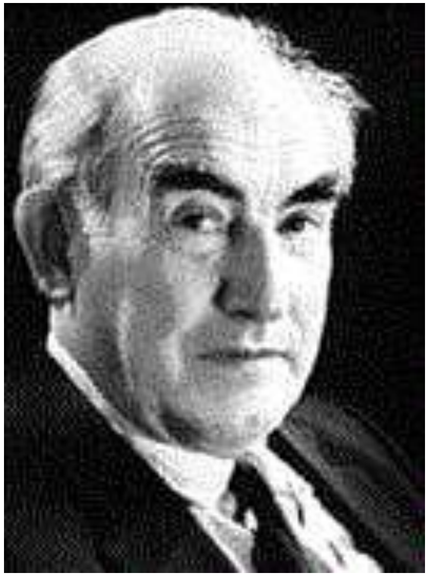
(research supported under the IBM retirement fund)

CHAPMAN UNIVERSITY

8 – 9 May 2017

My Three Career Heroes

“Men for All Seasons”



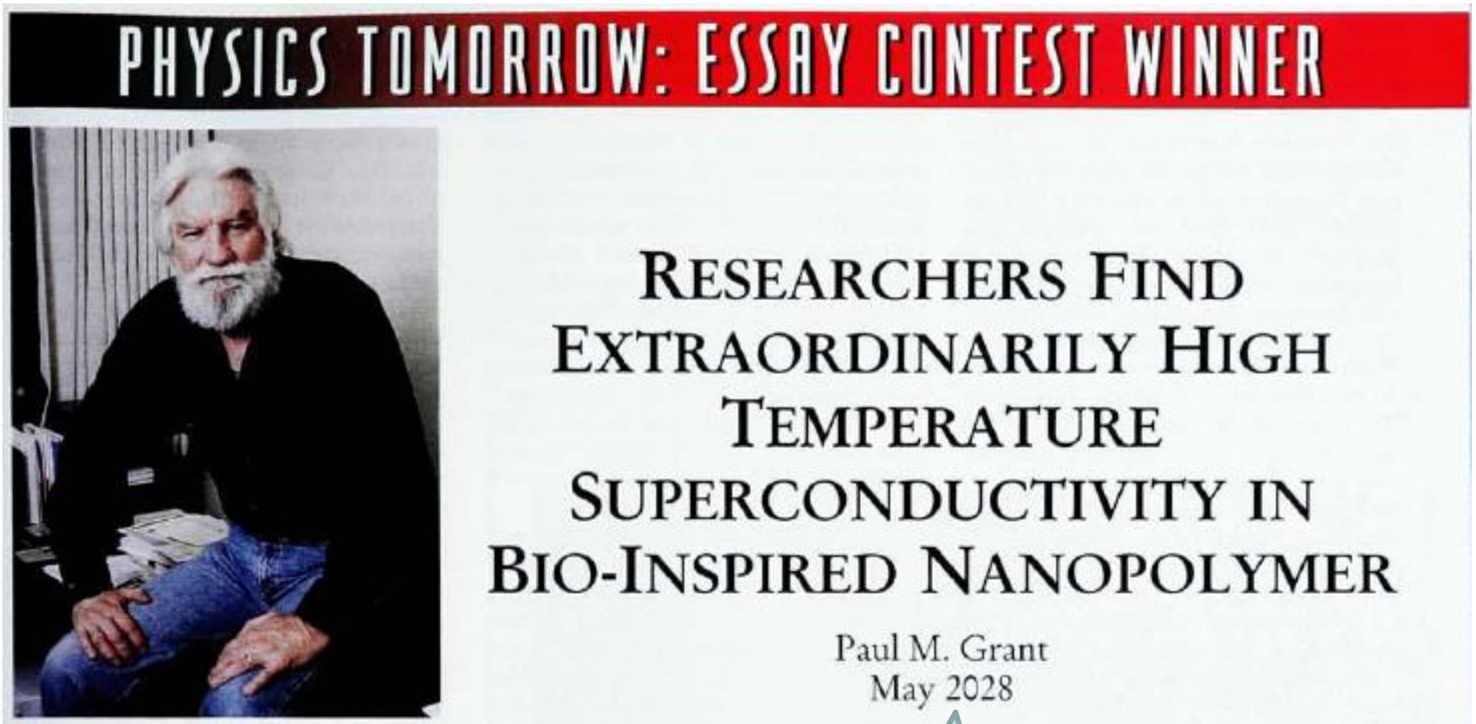
“VL”

“Bill”

“Ted”

50th Anniversary of Physics Today, May 1998

http://www.w2agz.com/Publications/Popular%20Science/Bio-Inspired%20Superconductivity,%20Physics%20Today%2051,%2017%20%281998%29.pdf



May, 2028
(still have some time!)

"Bardeen-Cooper-Schrieffer"

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

$$\lambda k\Theta << E_F$$

Where

Θ = Debye Temperature (~ 275 K)

λ = Electron-Phonon Coupling (~ 0.28)

μ^* = Electron-Electron Repulsion (~ 0.1)

a = "Gap Parameter, ~ 1-3"

Tc = Critical Temperature (9.5 K "Nb")

Electron-Phonon Coupling a la Migdal-Eliashberg-McMillan

(plus Allen & Dynes)

$$H_{el-ph} = \sum_{\mathbf{k}\mathbf{q}\nu} g^{\mathbf{q}\nu,mn}_{\mathbf{k}+\mathbf{q},\mathbf{k}}\; c^{\dagger m}_{\mathbf{k}+\mathbf{q}} c^{n}_{\mathbf{k}}\; (b^{\dagger}_{-\mathbf{q}\nu} + b_{\mathbf{q}\nu}) \qquad (1)$$

First compute this via DFT…

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

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

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

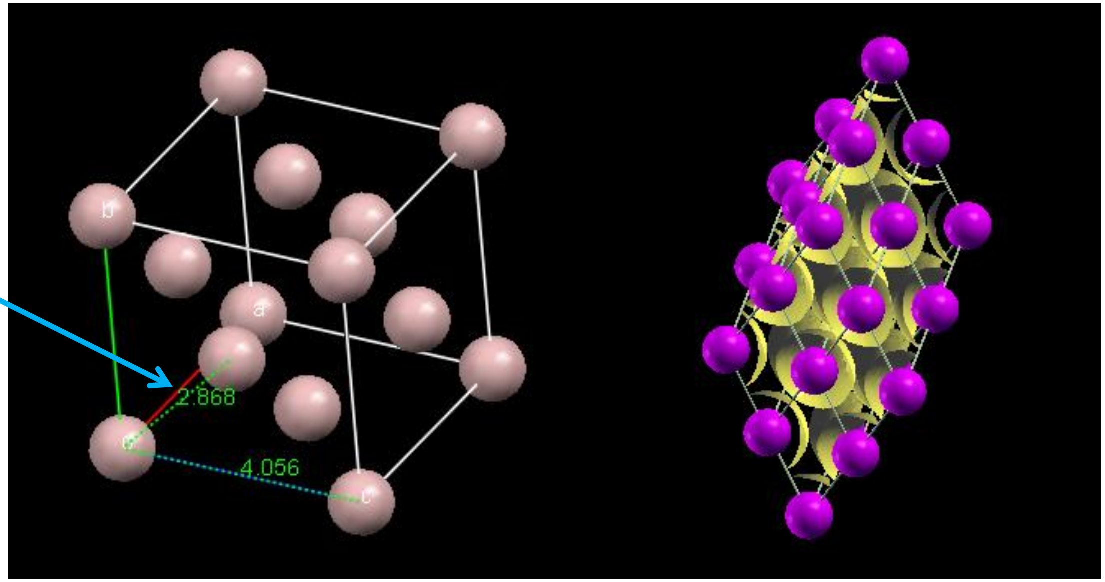
Then this…

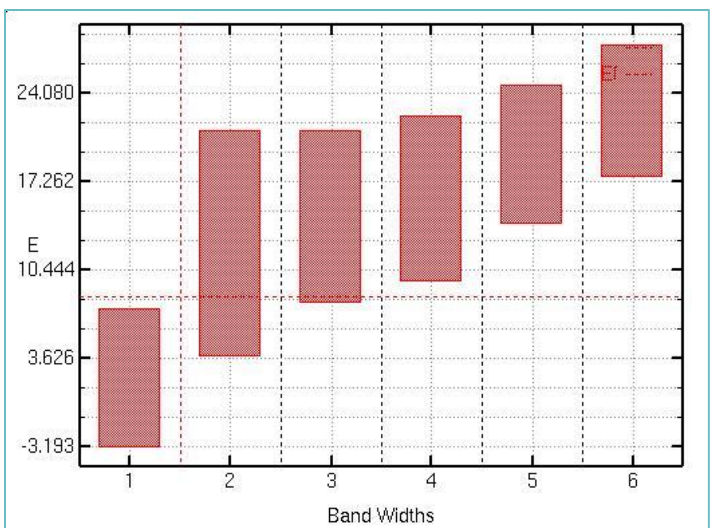
Quantum-Espresso (Democritos-ISSA-CNR)

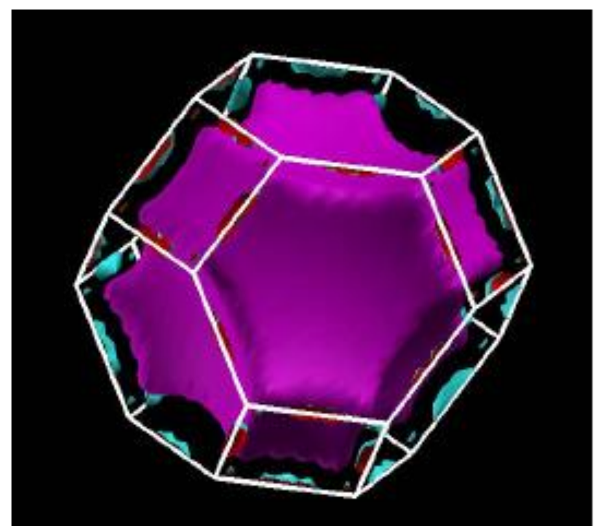
http://www.pwscf.org Grazie!

“3-D”Aluminum, T_C = 1.15 K

“Irrational”

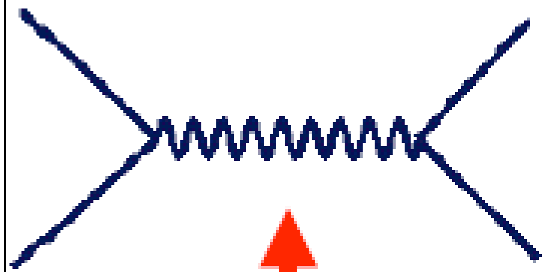






Fermion-Boson Interactions

Phonons:
Θ(Al) ~ 430K ~ 0.04eV
Excitons:
Θ(GaAs) ~ 1eV ~ 12,000K
WOW!



Insert your favorite "on" here

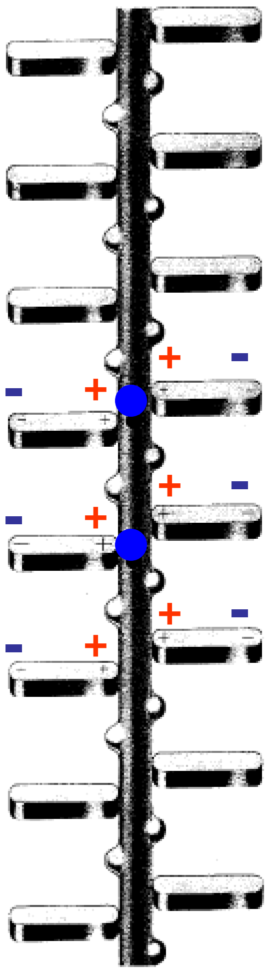
(phonon, magnon, exciton, plasmon, anyon, moron …)

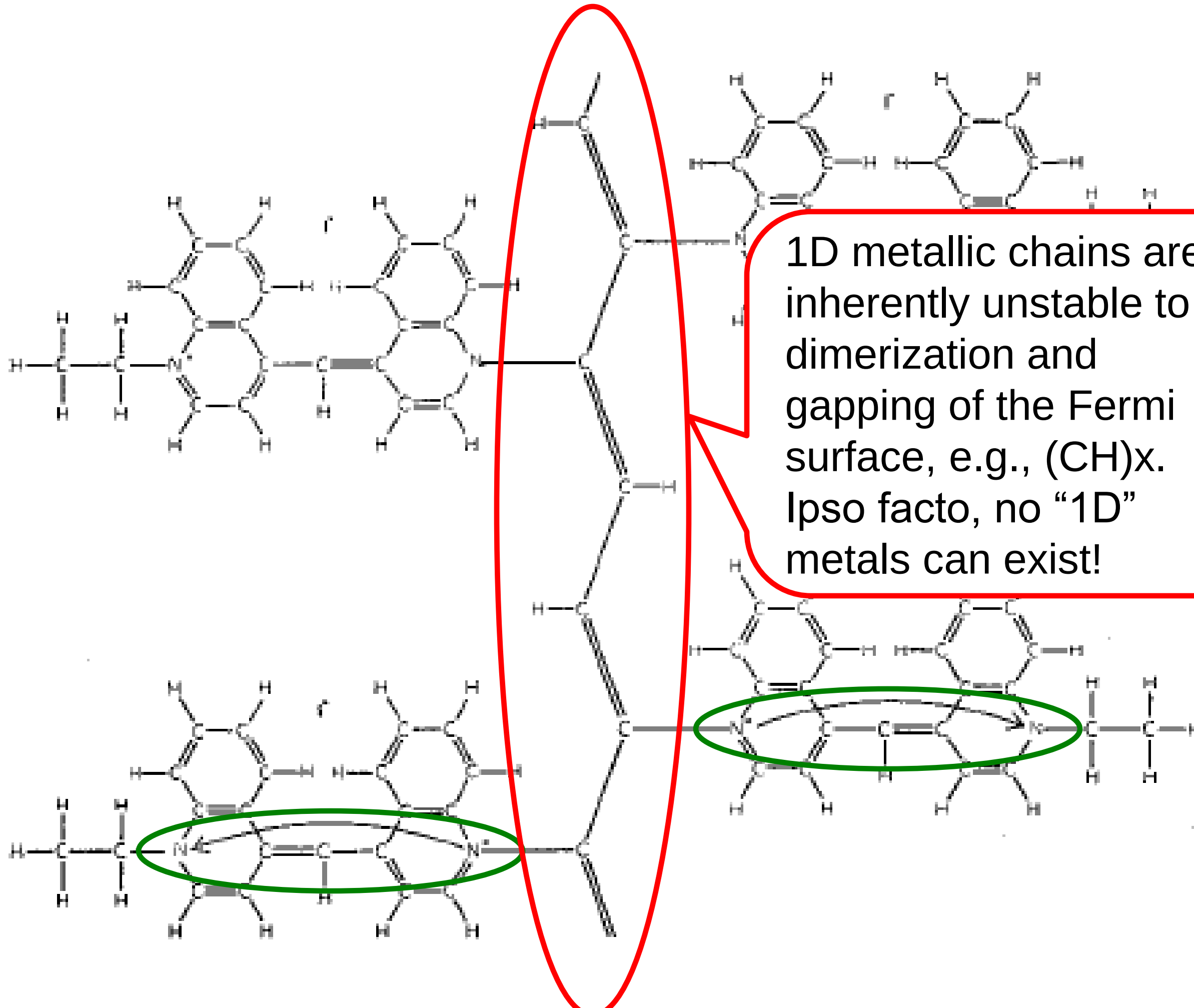
"Put-on !"

NanoConcept

What novel atomic/molecular arrangement might give rise to higher temperature superconductivity >> 165 K?

Little, 1963





1D metallic chains are inherently unstable to dimerization and gapping of the Fermi surface, e.g., (CH)x. Ipso facto, no "1D" metals can exist!

Diethyl-cyanine iodide

NanoBlueprint

- Model its expected physical properties using Density Functional Theory.

$$E_{\mathrm{LDA+U}}\left[n(\mathbf{r})\right] = E_{\mathrm{LDA}}\left[n(\mathbf{r})\right] + E_{\mathrm{HUB}}\left[\left\{n_m^{l\sigma}\right\}\right] - E_{\mathrm{DC}}\left[\left\{n^{l\sigma}\right\}\right]$$

  – DFT is a widely used tool in the pharmaceutical, semiconductor, metallurgical and chemical industries.
  – Gives very reliable results for ground state properties for a wide variety of materials, including strongly correlated, and the low lying quasiparticle spectrum for many as well.
- This approach opens a new method for the prediction and discovery of novel materials through numerical analysis of "proxy structures."

Fibonacci Chains

"Monte-Carlo Simulation of Fermions on Quasiperiodic Chains,"

P. M. Grant, **BAPS March Meeting** (1992, Indianapolis)

$$G_n \equiv G_{n-1} \mid G_{n-2}, \quad n = 3, 4, 5, \ldots, \infty$$

Where $G_1 = a,\ G_2 = ab$

And $\lim_{n \to \infty} N_a(G_n) / N_b(G_n) \equiv \boxed{\tau = (1+\sqrt{5})/2 \approx 1.618\ldots}$

Example: $G_6 = abaababaab\ (N = 13)$

Let $a = c\tau b,$ subject to $\langle a, b \rangle$ invariant,

And take a and b

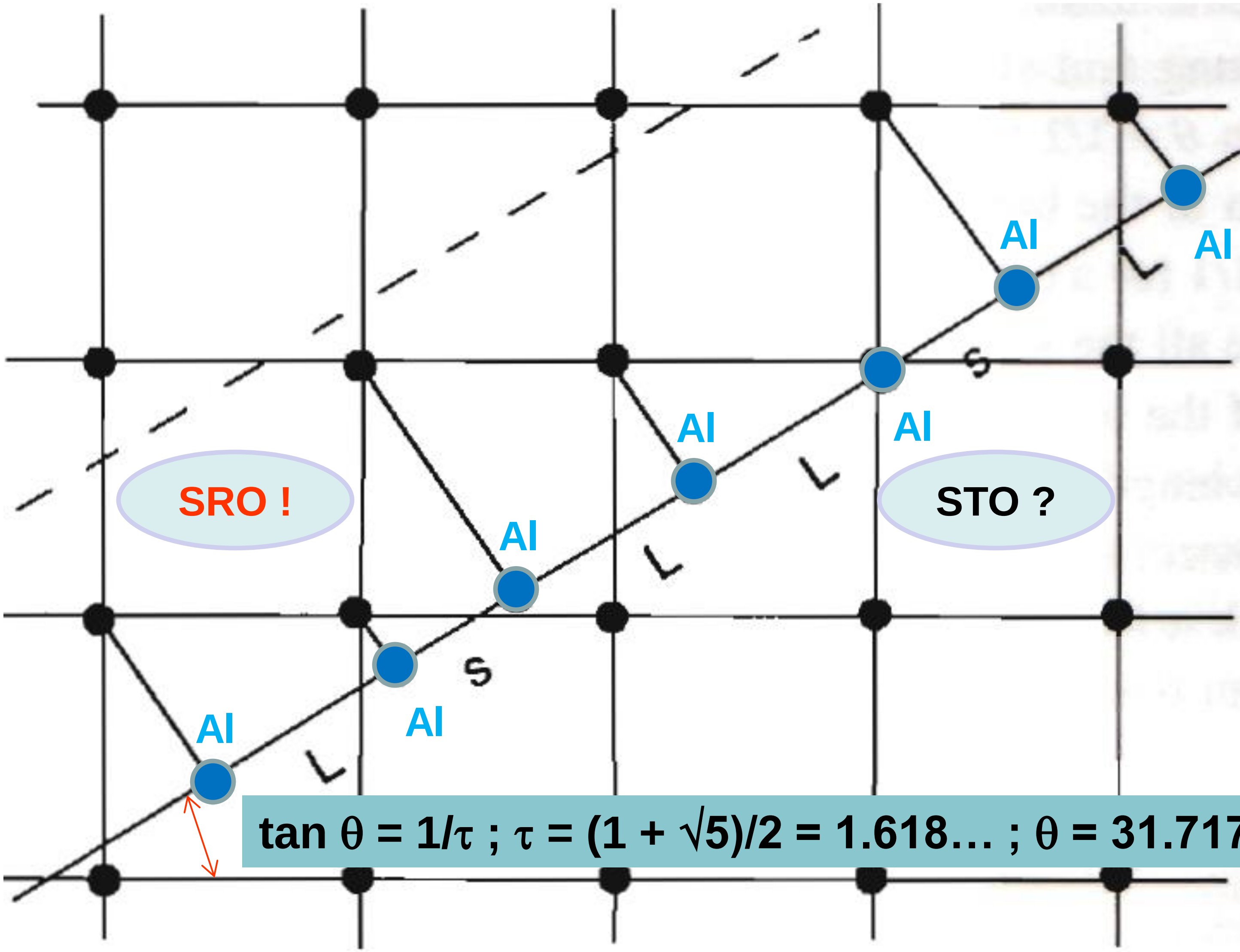
to be "inter-atomic n-n distances,"

Then $b = \tau \langle a, b \rangle / [(1+c)\tau - 1]$.

Where c is a "scaling" parameter.

A Fibonacci fcc "Dislocation Line"

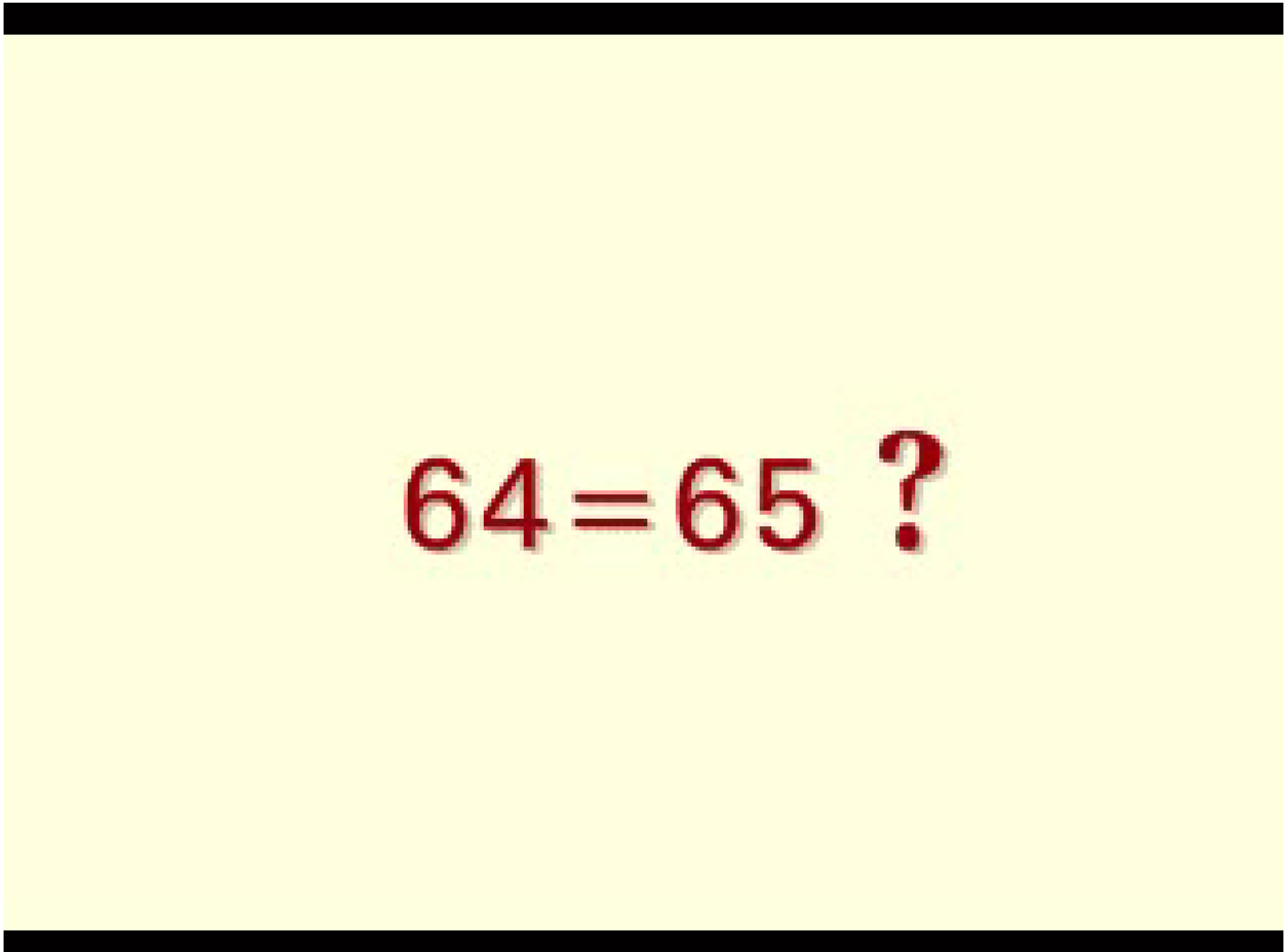
...or maybe Na on Si?...in other words..."a proxy Little model!"



tan θ = 1/τ ; τ = (1 + √5)/2 = 1.618… ; θ = 31.717…°

L = 4.058 Å (fcc edge) **s = 2.869 Å (fcc diag)**

64 = 65



“Not So Famous Danish Kid Brother”

Harald Bohr

Silver Medal, Danish Football Team, 1908 Olympic Games

Almost Periodic Functions

"Electronic Structure of Disordered Solids and Almost Periodic Functions,"

P. M. Grant, **BAPS 18**, 333 (1973, San Diego)

Definition I: Set of all summable trigonometric series:

$$f(x) = \sum_n A_n e^{i\lambda_n x}$$

where $\{\lambda_n\}$ are denumerable.

Type (1) Purely Periodic: $\lambda_n = cn$, n = 0, ± 1, ± 2, ...

Type (2) Limit Periodic: $\lambda_n = cr_n$, $r_n \in$ {rationals}

Type (3) General Case: One or more λ_n irrational

==

Definition II: Existence of an infinite set of "translation numbers," $\{\tau_\varepsilon\}$, such that:

$$| f(x+\tau_\varepsilon) - f(x) | \le \varepsilon; \ -\infty < x < \infty$$

where $\varepsilon \ge 0$.

==

Parseval's Theorem:

$$\sum_n | A_n |^2 = \lim_{L\to\infty} \frac{1}{2L} \int_{-L}^{L} | f(x) |^2 \, dx$$

Mean Value Theorem:

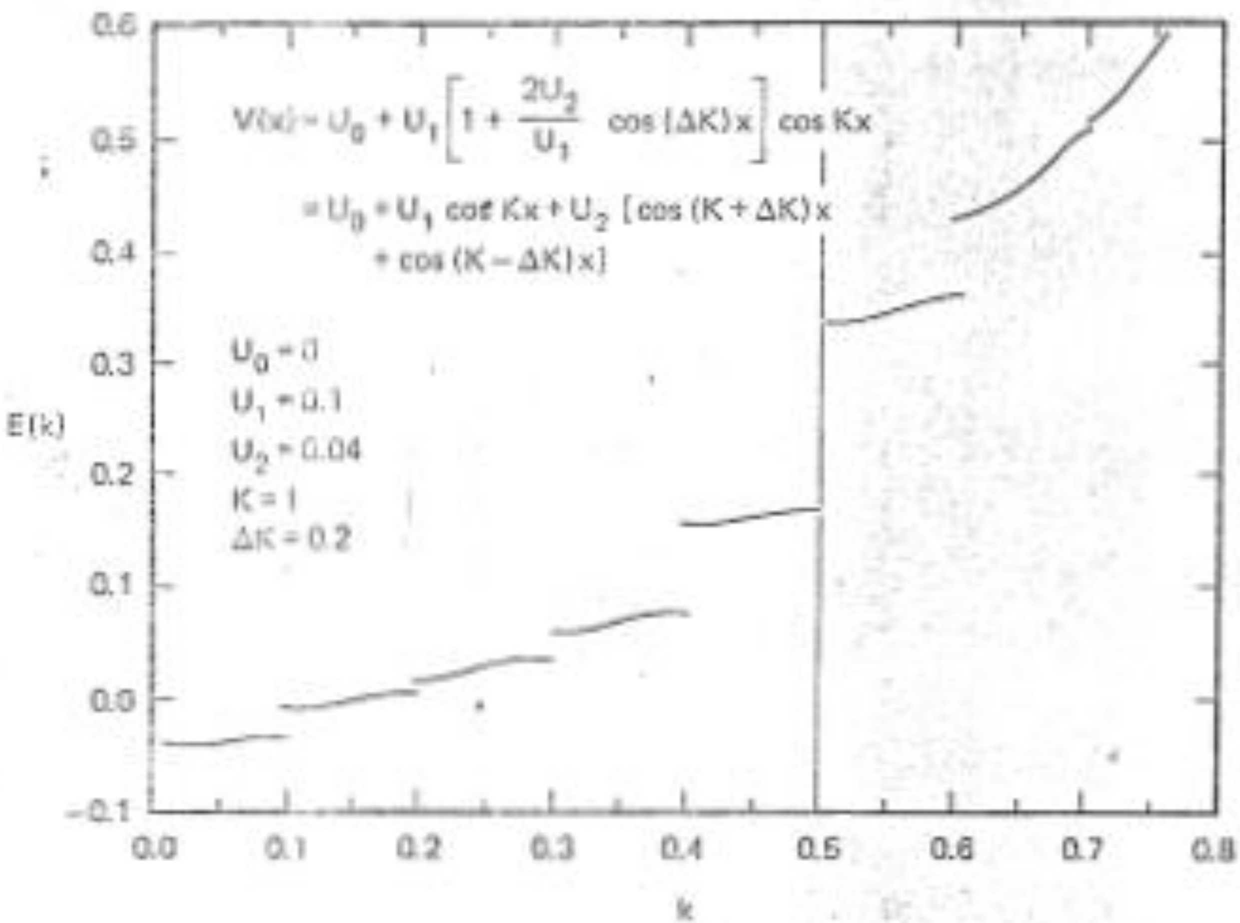
$$\int_{-\infty}^{\infty} f(x) e^{i\lambda x} dx = A_n \delta(\lambda - \lambda_n)$$

$$\text{Example}: f(x) = \cos x + \cos\sqrt{2}x$$

APF "Band Structure"

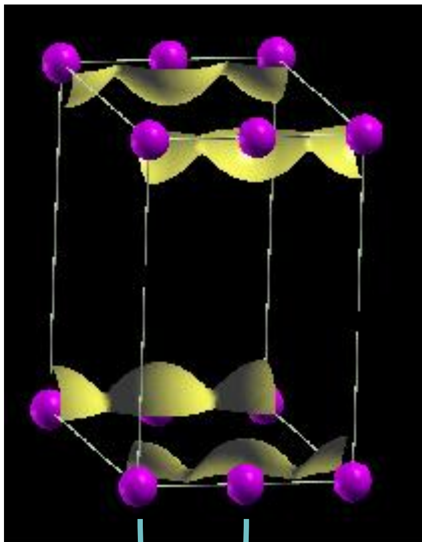
"Electronic Structure of Disordered Solids and Almost Periodic Functions,"

P. M. Grant, **BAPS 18**, 333 (1973, San Diego)

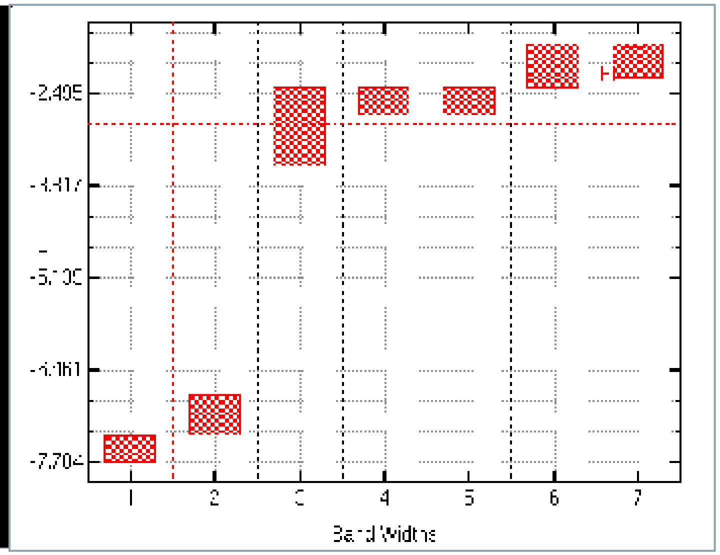


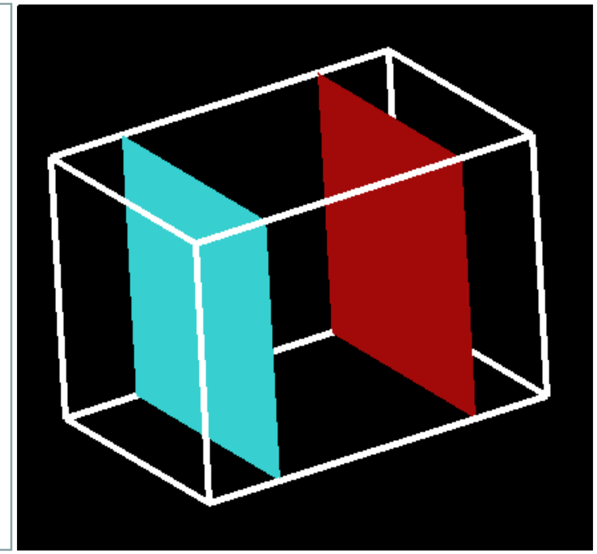
Doubly Periodic Al Chain

(a = 4.058 Å [fcc edge],   b = c = 3×a)



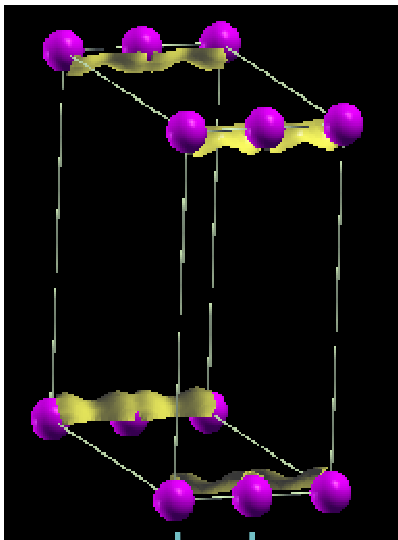
a

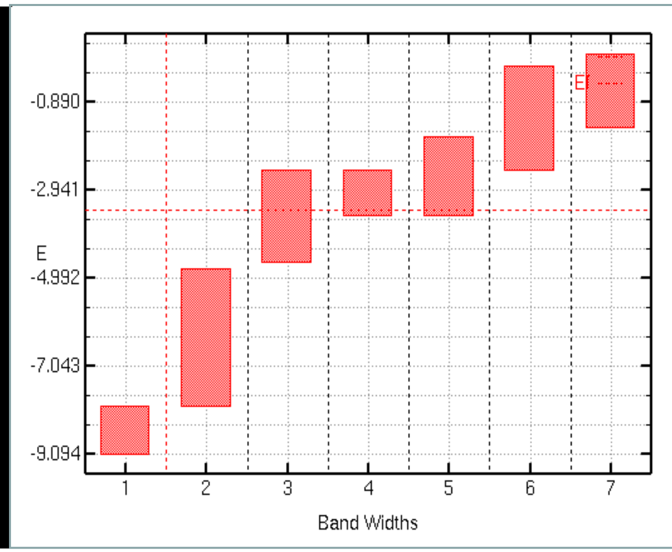


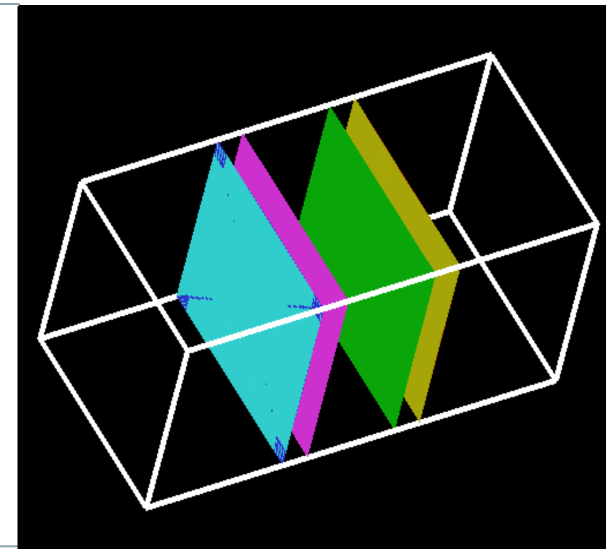


Doubly Periodic Al Chain

(a = 2.869 Å [fcc diag], b = c = 6×a)





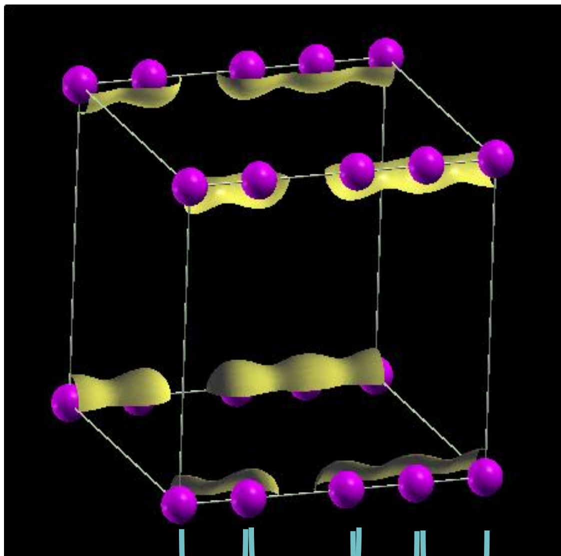


a

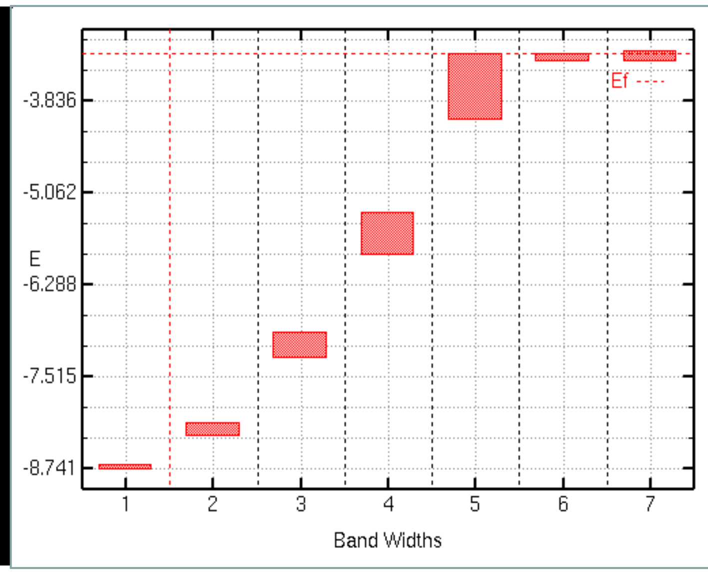
Quasi-Periodic Al Chain

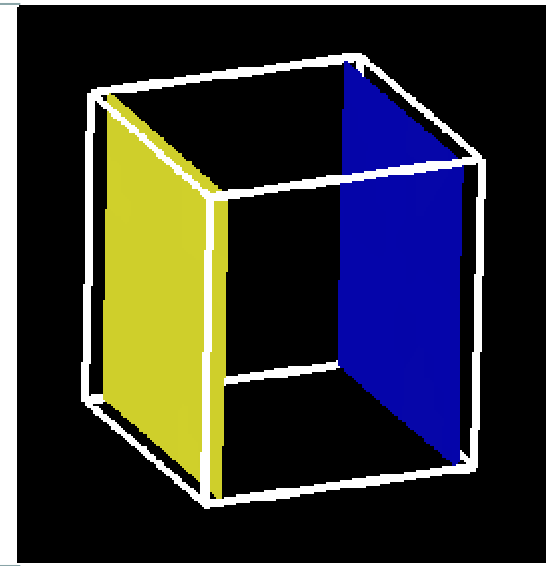
Fibo G = 6: s = 2.868 Å, L = 4.058 Å

(a = s+L+s+s = 12.66 Å, b = c ≈ 3×a)



s L s s





Preliminary Conclusions

- 1D Quasi-periodicity can defend a linear metallic state against CDW/SDW instabilities (or at least yield an semiconductor with extremely small gaps)
- Decoration of appropriate surface bi-crystal grain boundaries or dislocation lines with appropriate odd-electron elements could provide such an embodiment.

What’s Next (1)
- Do a Better Job Computationally -

- We now have computational tools (DFT and its derivatives) to calculate to high precision the ground and low level exited states of very complex “proxy” structures.
- In addition, great progress has been made over the past two decades on the formalism of “response functions,” e.g., generalized dielectric “constant” models.
- It should now be possible to “marry” these two developments to predict material conditions necessary to produce “room temperature superconductivity.

A possible PhD thesis project?

Davis – Gutfreund – Little (1975)

PHYSICAL REVIEW B VOLUME 13, NUMBER 11 1 JUNE 1976

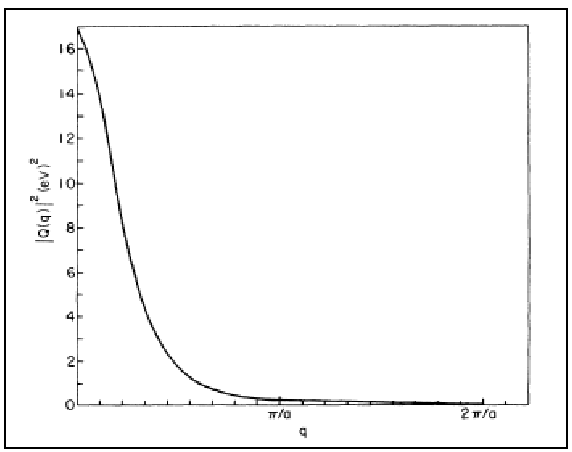
Proposed model of a high-temperature excitonic superconductor*

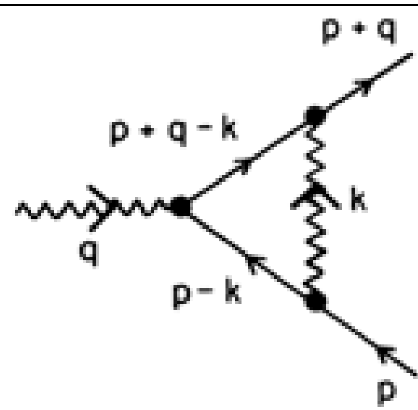
D. Davis,† H. Gutfreund,‡ and W. A. Little
Physics Department, Stanford University, Stanford, California 94305
(Received 16 October 1975)

$$g^{q\nu,mn}_{k+q,k} \longrightarrow$$

$$\phi^*(r_1-R_j)\,\phi(r_1-R_h)e^{i[kR_h-(k-q)R_j]}V(r_1r_2)\sum_{m,l,\nu}\left[u^{\nu}_{\alpha l}(q)+i\,v^{\nu}_{\alpha l}(q)\right]e^{-iqR_l}\,\Psi^*_\nu(R_{ml})\Psi_{00}$$

$$Q_\alpha(q)=\frac{1}{N^{3/2}}\int\sum_{j,k}\phi^*(r_1-R_j)\,\phi(r_1-R_h)e^{i[kR_h-(k-q)R_j]}V(r_1r_2)\sum_{m,l,\nu}\left[u^{\nu}_{\alpha l}(q)+i\,v^{\nu}_{\alpha l}(q)\right]e^{-iqR_l}\,\Psi^*_\nu(R_{ml})\Psi_{00}\,d^3r_1\,d^3\tau$$





Migdal Issues:

- Only small exciton q's, $v_q > v_F$, 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.

Journal of Low Temperature Physics, Vol. 10, Nos. 1/2, 1973

The Description of Superconductivity in Terms of Dielectric Response Function

D. A. Kirzhnits, E. G. Maksimov, and D. I. Khomskii

P. N. Lebedev Physical Institute, Moscow, USSR

(Received May 30, 1972)

A critical temperature T_c of a superconducting transition is calculated for a rather general form of the electron–electron interaction. It is shown that even if both the energy and momentum dependence of the interaction is included, the equation determining T_c coincides formally with the corresponding equation of the BCS theory. The kernel of this equation is a smooth real function of its variables; it is expressed through $\rho(\mathbf{k}, E)$, the spectral density of the inverse dielectric function of the system. The expression for T_c is written in terms of $\rho(\mathbf{k}, E)$; this enables us to analyze the dependence of the critical temperature on the properties of the metal in a normal state. Some simple models illustrating the results are considered, and a discussion of the limits on T_c is given.

Filamentary-Chaotic Conductance and Possible Routes to Room Temperature Superconductivity

Hans Hermann Otto

Materialwissenschaftliche Kristallographie, Clausthal University of Technology, Clausthal-Zellerfeld, Lower Saxony, Germany

World Journal of Condensed Matter Physics, 2016, 6, 244-260
Published Online August 2016 in SciRes. http://www.scirp.org/journal/wjcmp
http://dx.doi.org/10.4236/wjcmp.2016.63023

Scientific Research Publishing

Keywords

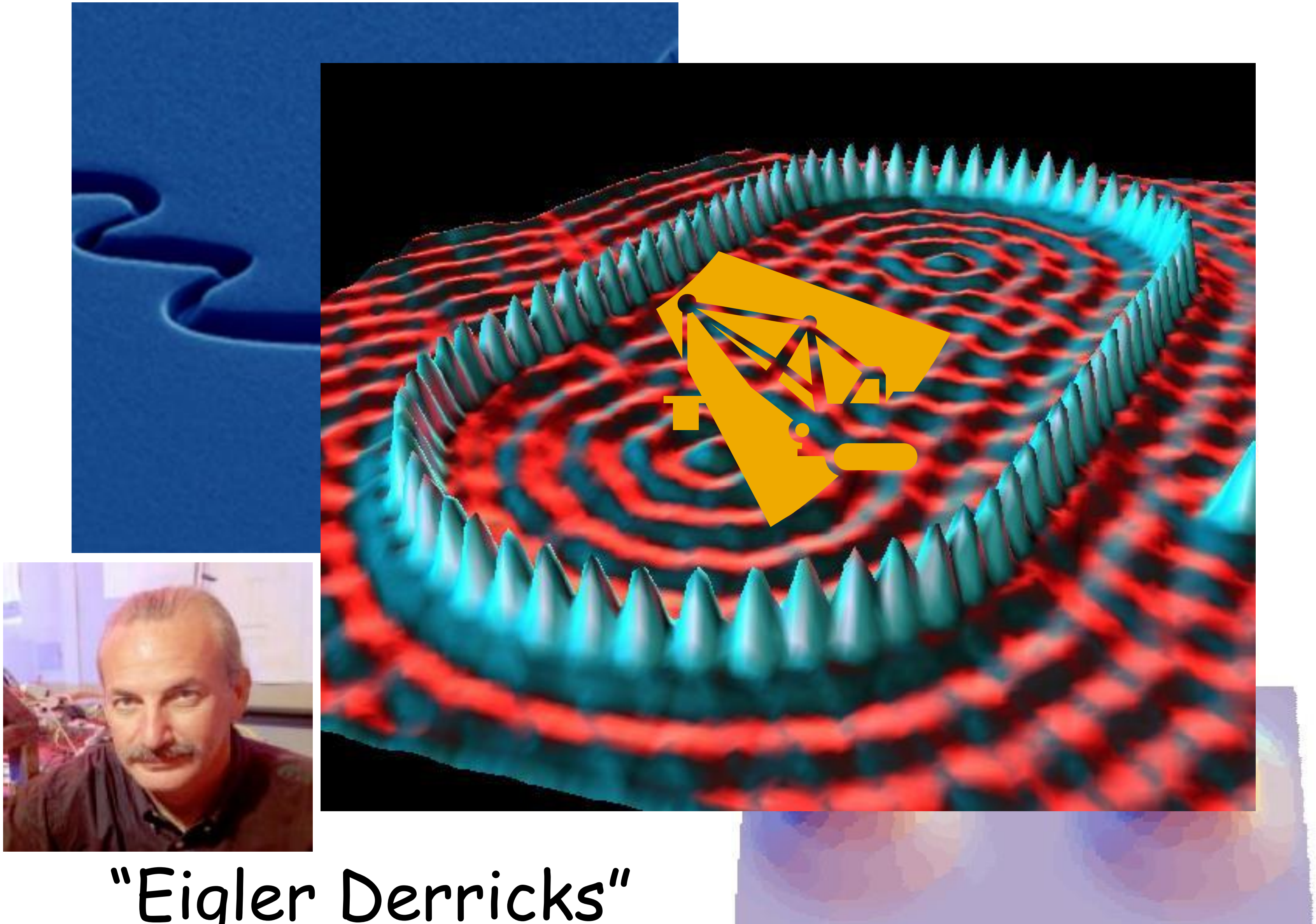
Superconductivity, Fractals, Chaos, Feigenbaum Numbers, Fibonacci Numbers, Golden Mean,

A low mean cationic charge allows the development of a frustrated nano-sized fractal structure of possibly ferroelastic nature delivering nano-channels for very fast charge transport, in common for both high-T_c superconductor and organic-inorganic halide perovskite solar materials. With this backing superconductivity above room temperature can be conceived for synthetic sandwich structures of $\langle q \rangle_c$ less than 2+. For instance, composites of tenorite and cuprite respectively tenorite and CuI (CuBr, CuCl) onto AuCu alloys are proposed. This specification is suggested by previously described filamentary superconductivity of "bulk" CuO_{1-x} samples. In addition, cesium substitution in the Tl-1223 compound is an option.

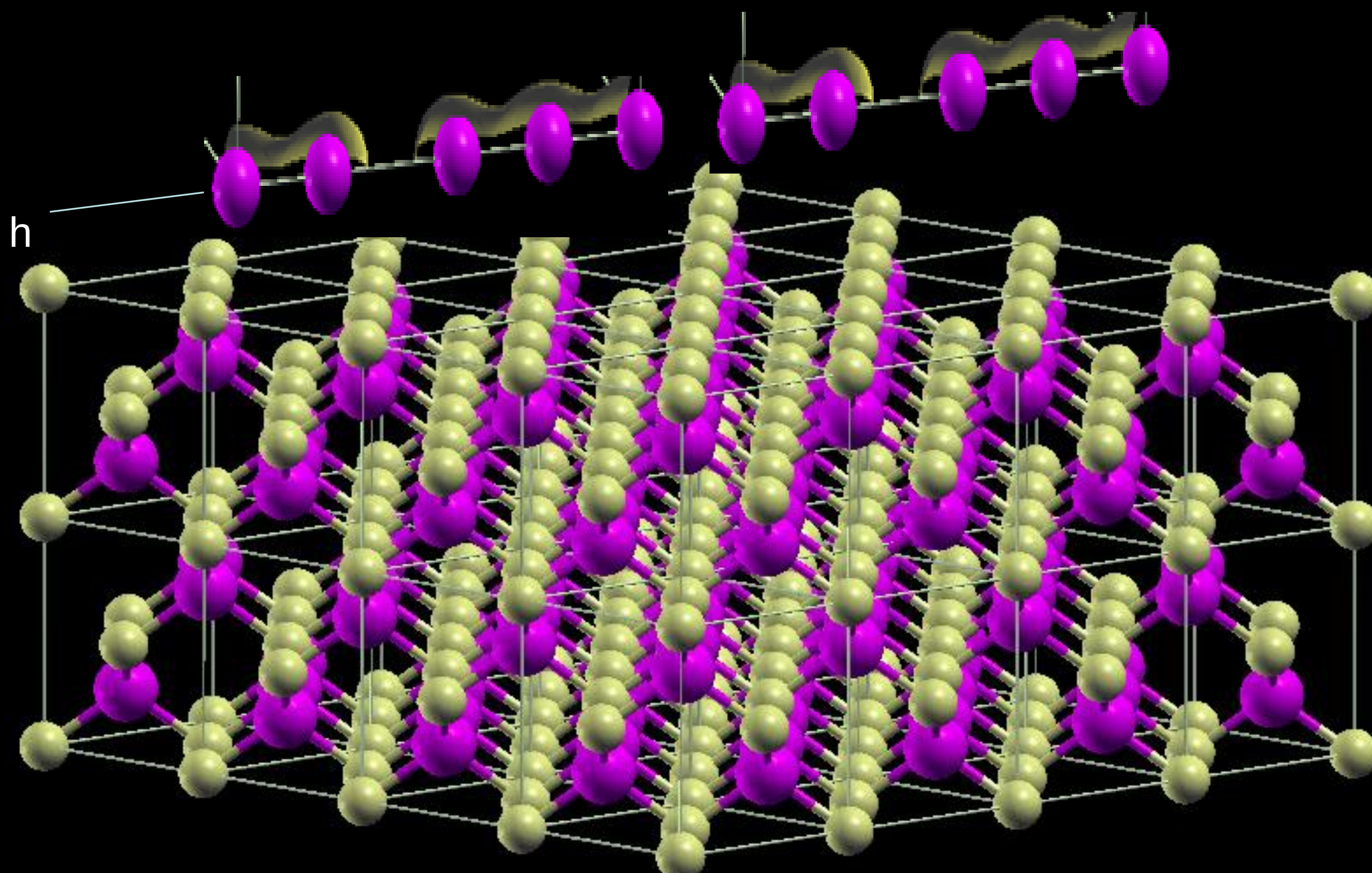
What’s Next (2)
- Build It! -

- Today we have lots of tools...MBE (whatever), “printing,” bio-growth...
- So, let’s do it!

NanoConstruction



"Eigler Derricks"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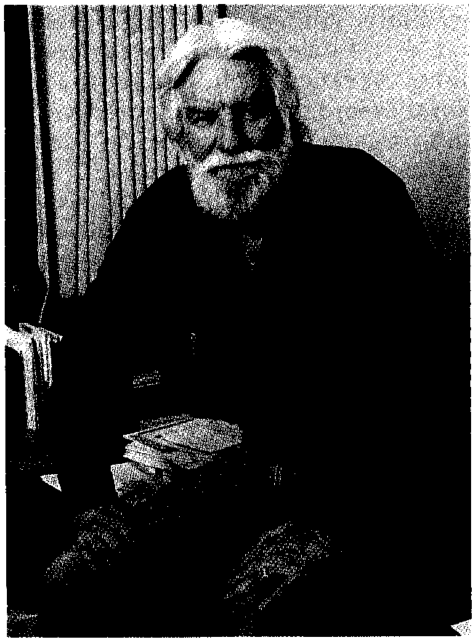
Fast Forward: 2028

PHYSICS TOMORROW: ESSAY CONTEST WINNER



RESEARCHERS FIND EXTRAORDINARILY HIGH TEMPERATURE SUPERCONDUCTIVITY IN BIO-INSPIRED NANOPOLYMER

Paul M. Grant
May 2028

“You can’t always get what you want…”

“…you get what you need!”