Superconducting Fluctuations in One-Dimensional Quasi-periodic Metallic Chains

Does the

DAVINCI CODE

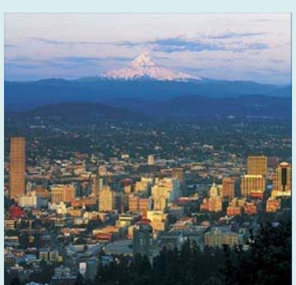
Hold the Key to Room Temperature Superconductivity?

Session T41: T41.00008, Room F152, Wednesday, 4:42 PM

Paul Michael Grant

Aging IBM Pensioner

(research supported under the IBM retirement fund)



Bulletin of the American Physical Society

APS March Meeting 2010
Volume 55, Number 2
Monday–Friday, March 15–19, 2010; Portland, Oregon

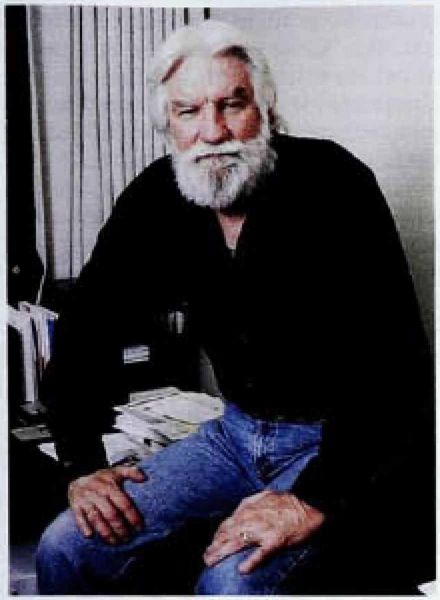
St. Patrick's Day - 2010

Bridget Ann Mullen-Whalen

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

PHYSICS TOMORROW: ESSAY CONTEST WINNER



RESEARCHERS FIND EXTRAORDINARILY HIGH TEMPERATURE SUPERCONDUCTIVITY IN BIO-INSPIRED NANOPOLYMER

Paul M. Grant
May 2028

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)

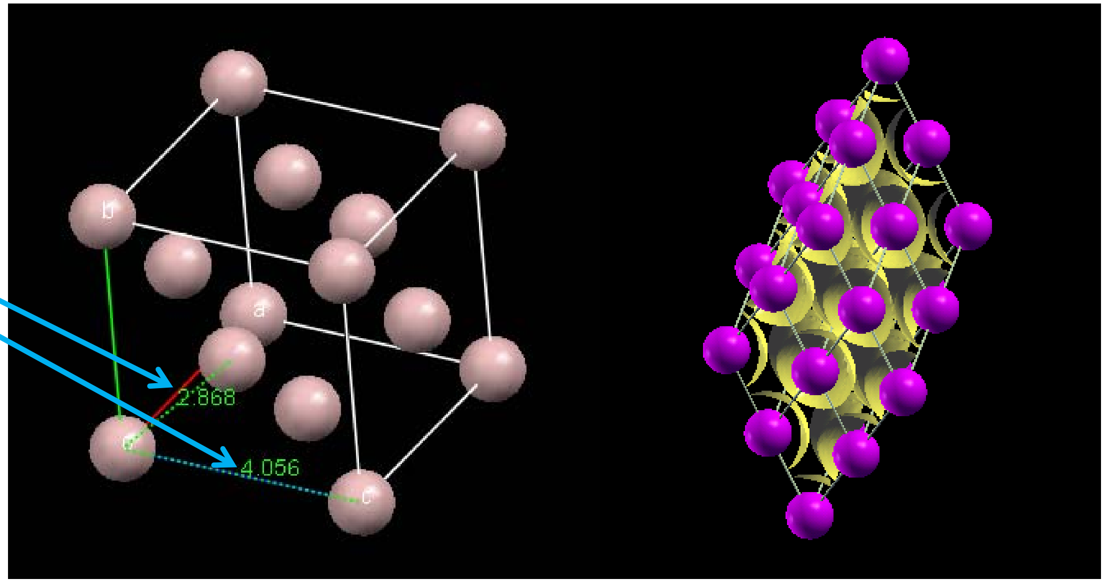
μ^* = Electron-Electron Repulsion (~ 0.1)

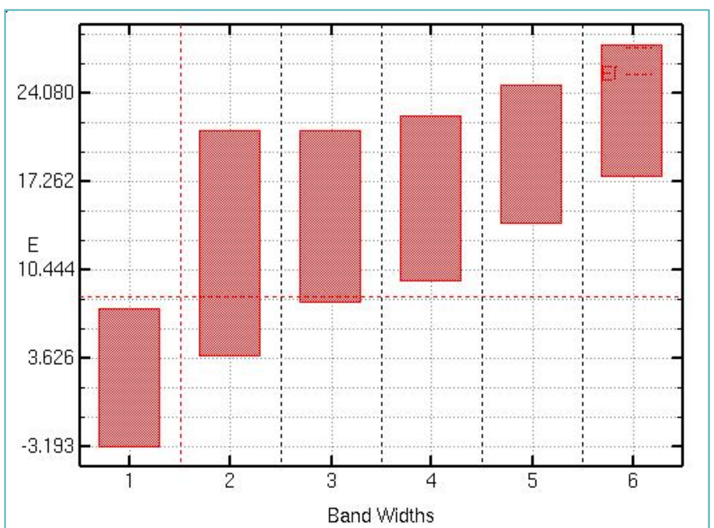
a = "Gap Parameter, ~ 1-3"

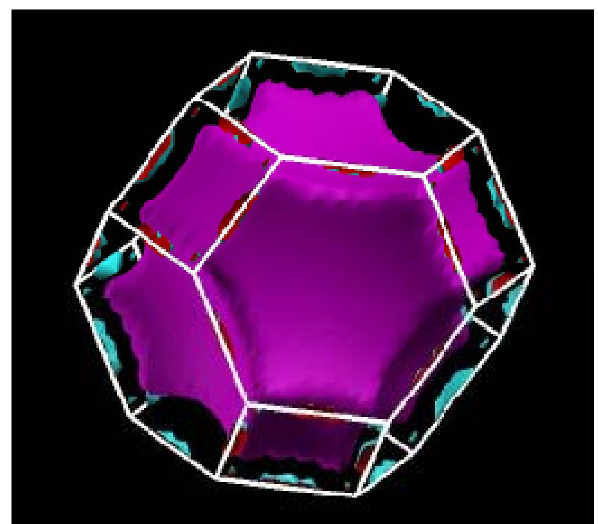
Tc = Critical Temperature (9.5 K "Nb")

“3-D”Aluminum, $T_C = 1.15$ K

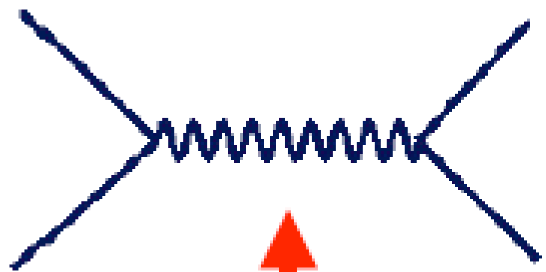
“Irrational”







Fermion-Boson Interactions

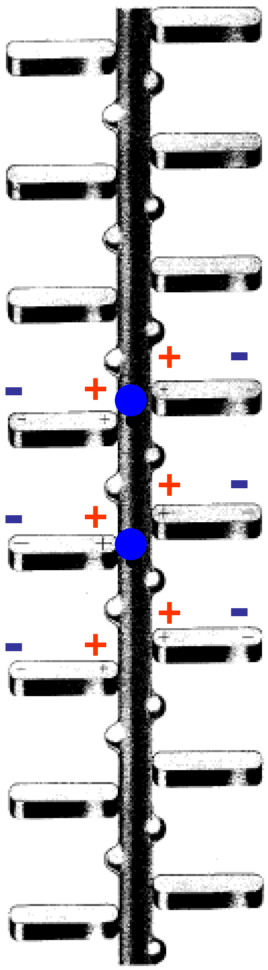


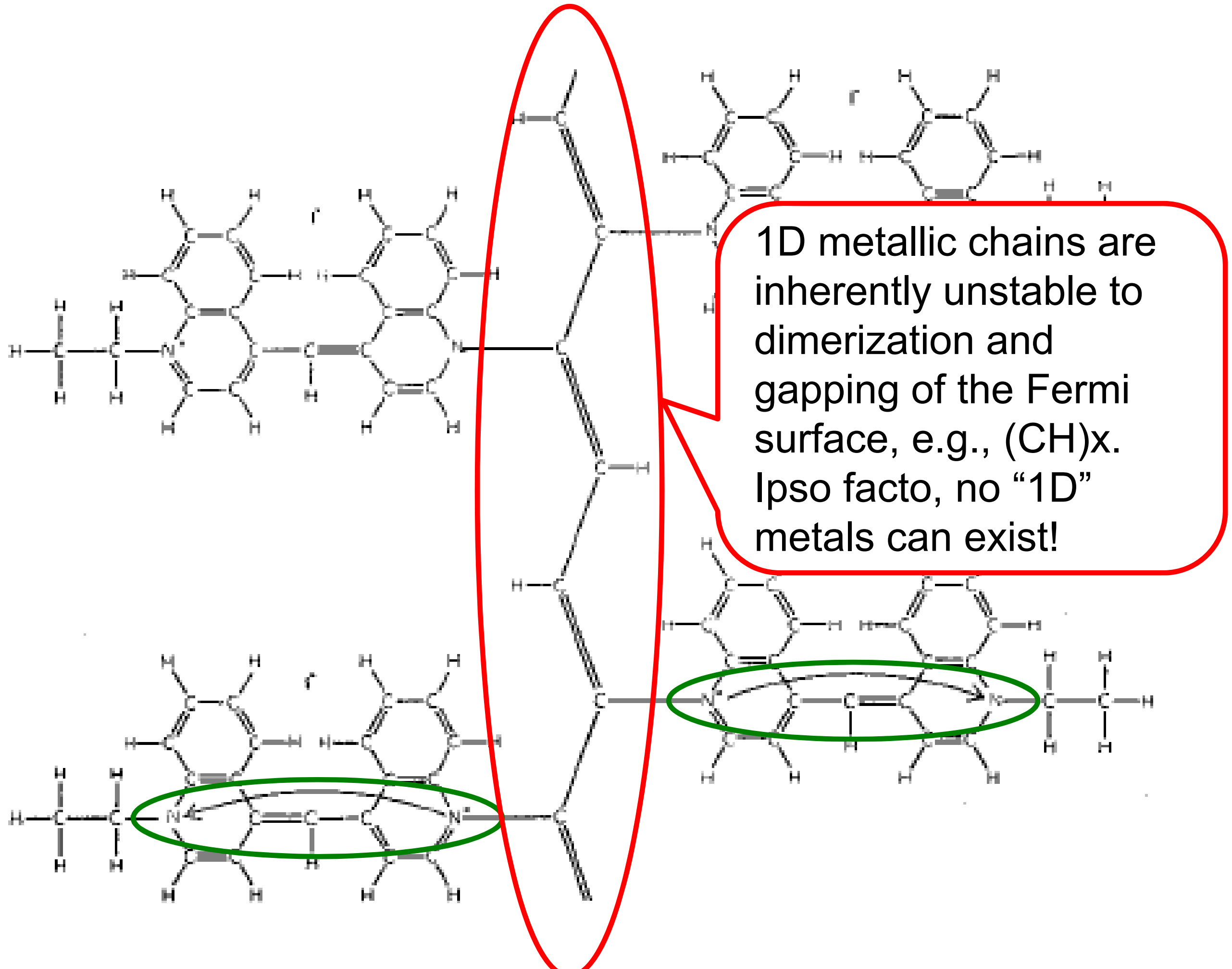
Insert your favorite “on” here

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

“Put-on !”

Little, 1963





Diethyl-cyanine iodide

NanoConcept

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

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,

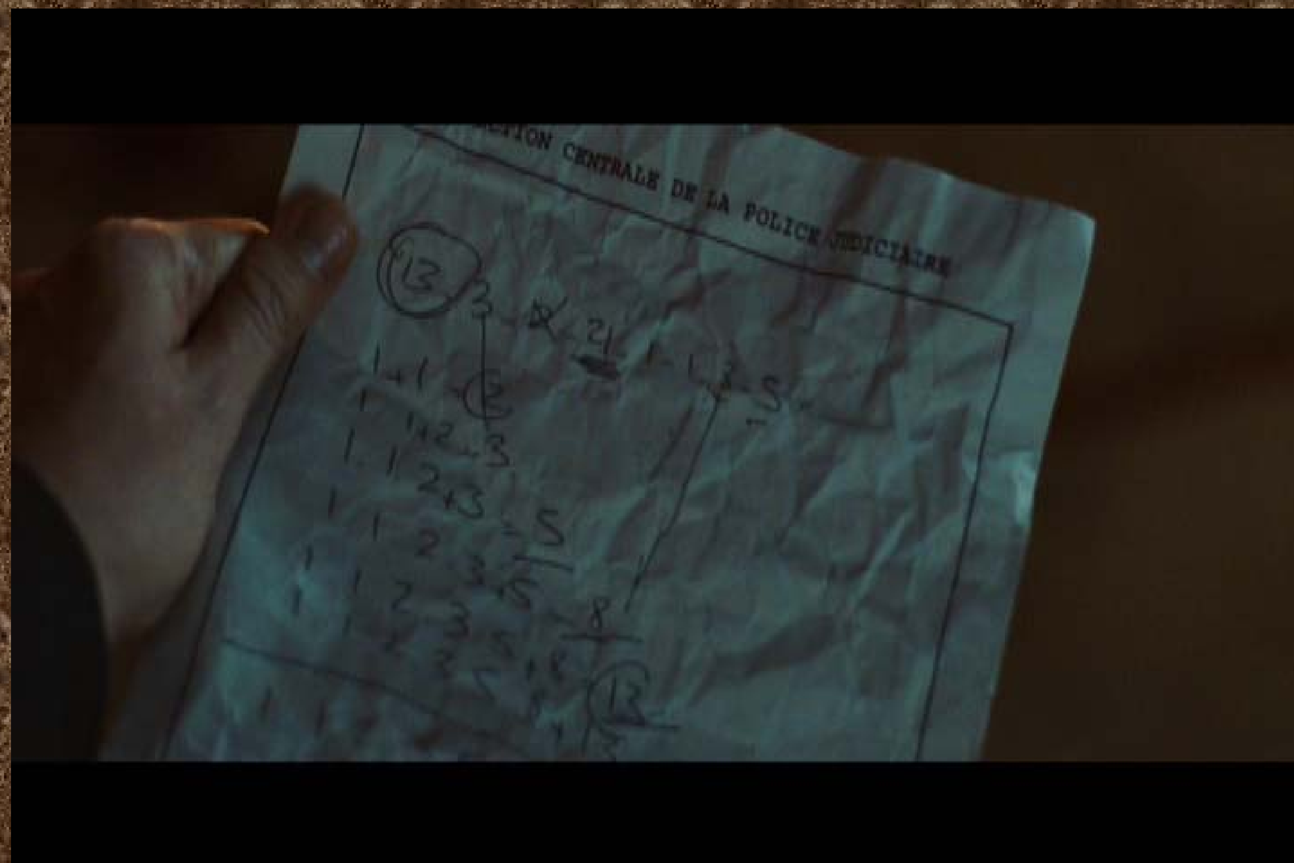
And take a and b

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

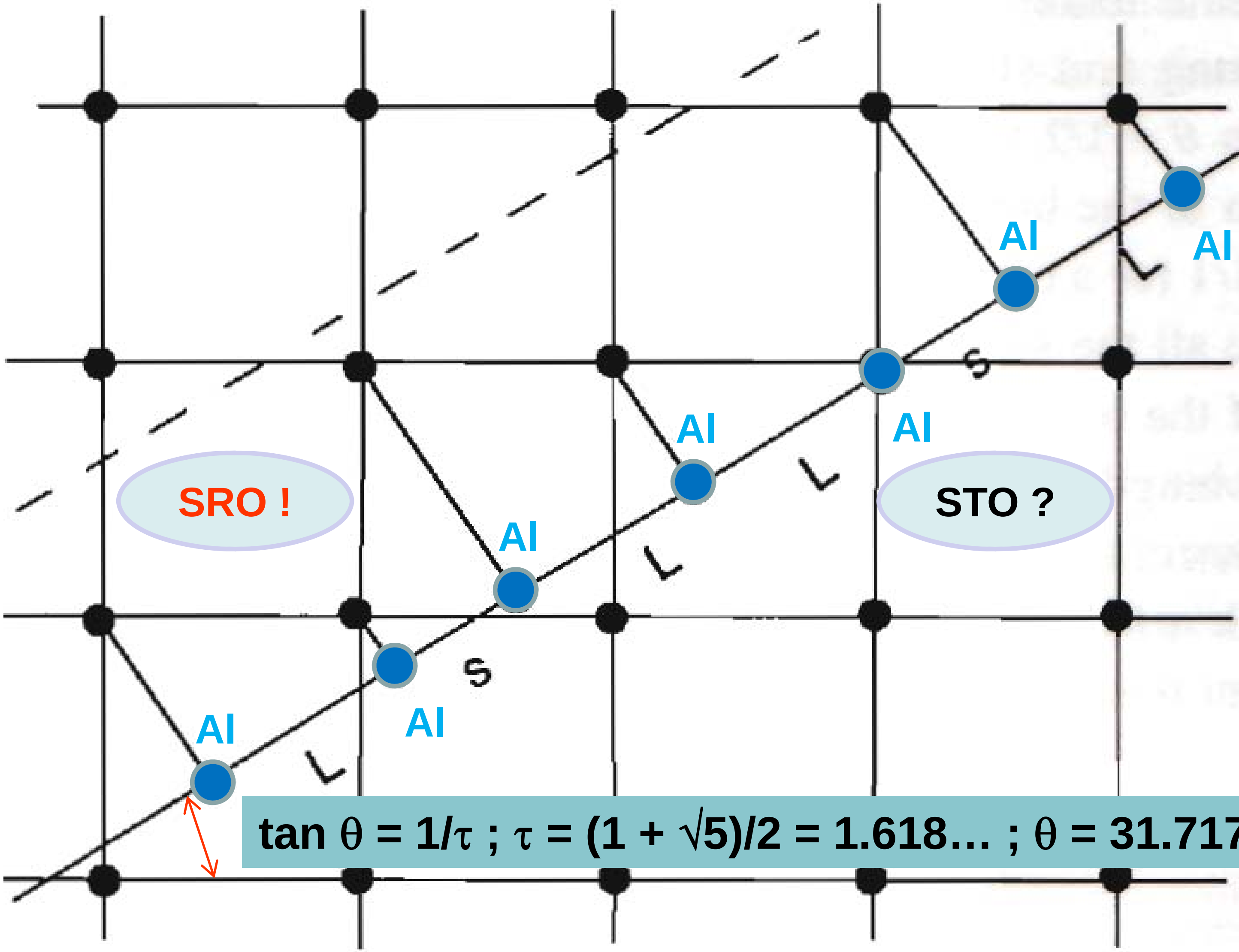
Then $b = \tau \langle a,b \rangle / [(1+c)\tau - 1]$.

Where c is a "scaling" parameter.

DA VINCI CODE



A Fibonacci "Dislocation Line"



$\tan\theta = 1/\tau$; $\tau = (1 + \sqrt{5})/2 = 1.618\ldots$; $\theta = 31.717\ldots°$

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

64 = 65

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:

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

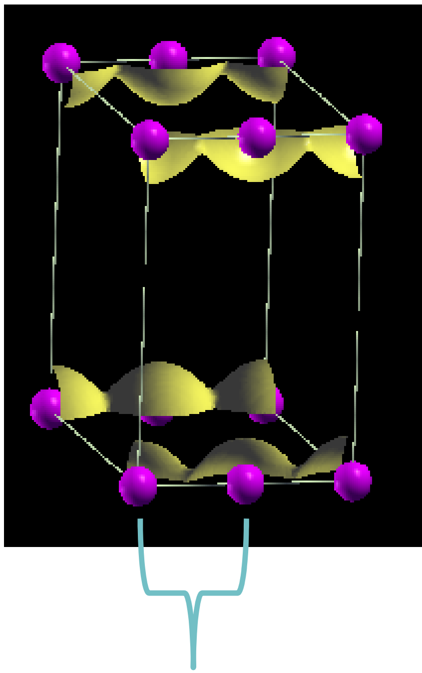
Mean Value Theorem:

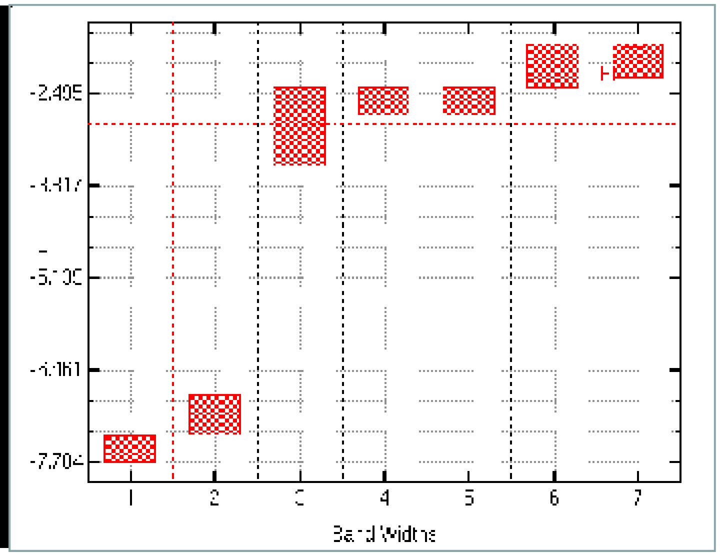
$$\int_{-\infty}^{\infty} f(x) e^{i\lambda x} dx = A_n \delta(\lambda - \lambda_n)$$

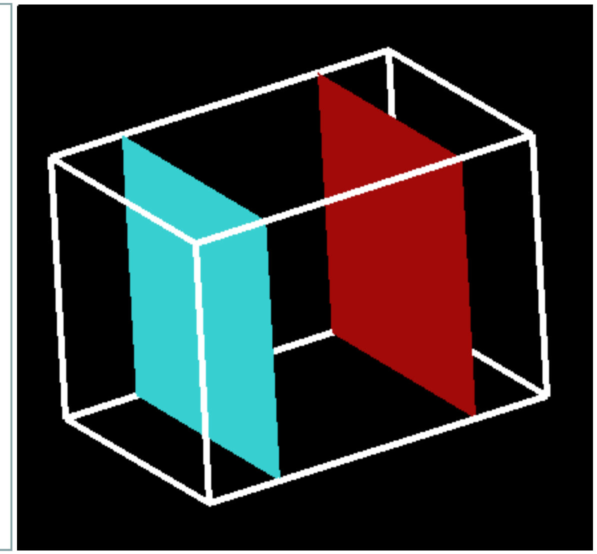
$$\text{Example}: f(x) = \cos x + \cos \sqrt{2} x$$

Doubly Periodic Al Chain

(a = 4.058 Å [fcc edge], b = c = 3×a)

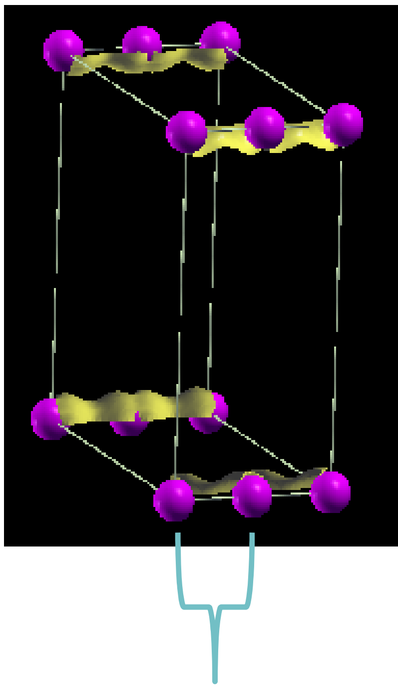


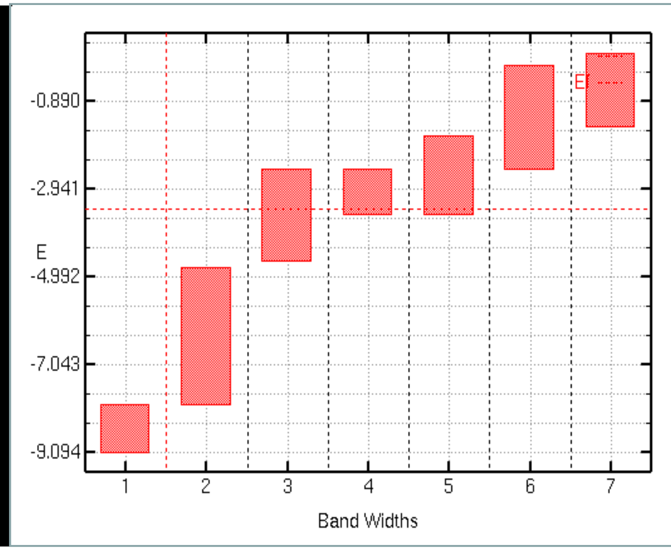


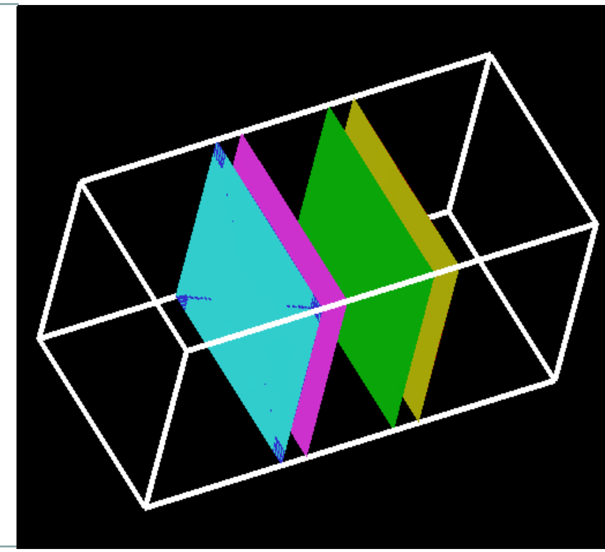


Doubly Periodic Al Chain

(a = 2.869 Å [fcc diag], b = c = 6×a)



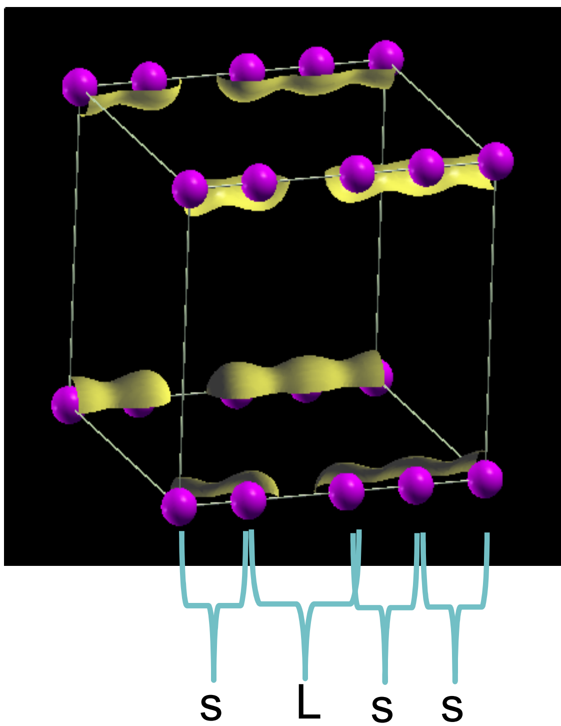


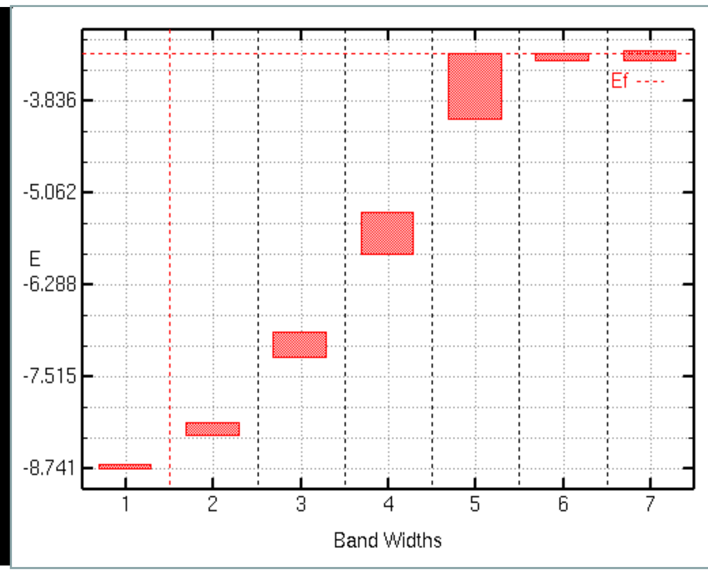


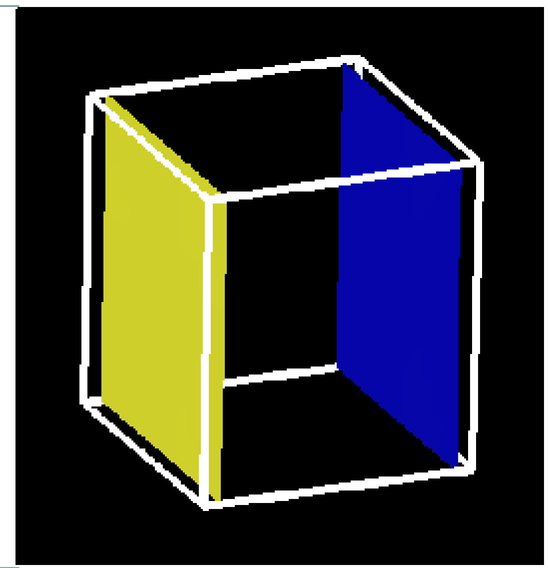
Quasi-Periodic Al Chain

Fibo G = 6: s = 2.868 Å, L = 4.058 Å

(a = s+L+s+s = 12.66 Å, b = c ≈ 3×a)







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.

Homework

- Computational physics and chemistry has attained the potential to assess the physical possibility of other-than-phonon mediated superconductivity via examination of “proxy structures” such as the example proposed in this talk.
- However, better and more comprehensive “post-processing” software tools are required to supplant and substitute for Eliashberg-McMillan based algorithms.
- The formalism already exists within the framework of the momentum-dependent dielectric function, $\varepsilon(q, \omega+i\gamma)$, e.g., the generalized Lindhard expression and/or the work of Kirzhnitz, Maksimov and Khomski……., but no code implementation is currently available (as far as I know…possibly soon from Yambo)!

Éireann go Brách