Quantum Studies: Mathematics and Foundations

Superconducting fluctuations in one-dimensional quasi-periodic "metallic" chains: The Little Model of room temperature superconductivity embodied.

--Manuscript Draft--

Manuscript Number:	
Full Title:	Superconducting fluctuations in one-dimensional quasi-periodic "metallic" chains: The Little Model of room temperature superconductivity embodied.
Article Type:	Original Paper
Funding Information:	
Abstract:	It is well known that a purely periodic chain of odd-electron atoms, nominally expected to exhibit metallic behavior, is unstable to charge/spin spatial displacement which lowers its ground state energy by gapping its highly-degenerate Jahn-Teller Fermi surface, in this case consisting of nesting parallel Brillouin zone sheets. It is largely for these reasons that superconductivity has not been observed in highly one-dimensional metals -- it is simply energetically more favorable for CDW/SDW gaps to form, via chain dimerization, rather than a BCS state, at the very least one mediated by electron-phonon coupling. In this paper, we explore the hypothetical electronic properties of a nominally "metallic" quasi-periodic chain using both an analytical approach and computationally via density functional theory, searching for configurations which could possibly yield "gap-lets" sufficiently small to permit the formation of BCS pairs as the new energetically favored ground state. The particular embodiment we examine is a proxy structure consisting of a string of odd-electron atoms with interatomic spacing following a Fibonacci sequence, positioned above the surface of an appropriate highly polarizable material substrate. We propose a path to its computational modelling followed by a route to synthesis of such a structure for experimental examination, and thus perhaps leading to an entire new class of near room temperature superconductors. Keywords: -Room temperature superconductors -Quasi-periodic metallic chain structures -Realizable Little models
Corresponding Author:	Paul Michael Grant, Ph.D W2AGZ Technologies UNITED STATES
Corresponding Author Secondary Information:	
Corresponding Author's Institution:	W2AGZ Technologies
Corresponding Author's Secondary Institution:	
First Author:	Paul Michael Grant, Ph.D
First Author Secondary Information:	
Order of Authors:	Paul Michael Grant, Ph.D
Order of Authors Secondary Information:	
Author Comments:	
Suggested Reviewers:	Ted Geballe GEBALLE@STANFORD.EDU Superconductivity Expert

Paul M. Grant

Superconducting fluctuations in one-dimensional quasi-periodic “metallic” chains: The Little Model of room temperature superconductivity embodied.

W2AGZ Technologies
San Jose, CA 95120 USA
1-408-482-8929

Abstract:

It is well known that a purely periodic chain of odd-electron atoms, nominally expected to exhibit metallic behavior, is unstable to charge/spin spatial displacement which lowers its ground state energy by gapping its highly-degenerate Jahn-Teller Fermi surface, in this case consisting of nesting parallel Brillouin zone sheets. It is largely for these reasons that superconductivity has not been observed in highly one-dimensional metals -- it is simply energetically more favorable for CDW/SDW gaps to form, via chain dimerization, rather than a BCS state, at the very least one mediated by electron-phonon coupling. In this paper, we explore the hypothetical electronic properties of a nominally “metallic” quasi-periodic chain using both an analytical approach and computationally via density functional theory, searching for configurations which could possibly yield “gap-lets” sufficiently small to permit the formation of BCS pairs as the new energetically favored ground state. The particular embodiment we examine is a proxy structure consisting of a string of odd-electron atoms with interatomic spacing following a Fibonacci sequence, positioned above the surface of an appropriate highly polarizable material substrate. We propose a path to its computational modelling followed by a route to synthesis of such a structure for experimental examination, and thus perhaps leading to an entire new class of near room temperature superconductors.

Keywords:
- Room temperature superconductors
- Quasi-periodic metallic chain structures
- Realizable Little models

I. Introduction

It is now slightly more than a century…and exactly 60 years…since the discovery of superconductivity in mercury metal by Gilles Holst in 1914 [1], to its explanation by Bardeen, Cooper and Schrieffer (aka "BCS") in 1957 [2]. Throughout all the years following, many refinements, both experimental and theoretical, to this remarkable phenomenon have taken place [3-7]. What has remained common and constant is that superconductivity, from millikelvin organic compounds to terakelvin neutron stars, results from a generalization of fermion pairing inevitably arising in a given boson field, as formulated within the BCS framework. In its simplest formulation, superconductivity can be described by,

$$T_C \sim \Theta \exp(-1/\lambda) , \qquad [1]$$

where Θ is the characteristic energy of the boson field (usually proportional to the Debye temperature for a lattice of phonons), and λ the dimensionless coupling constant between the respective boson/fermion fields (e.g., the scattering of electrons in a simple metal brought on by "lattice shakings"). Typical computational values for basic metals, like Al , (as obtained employing the Quantum Espresso package [19]), are T_C,s ranging from 0.9 to 2.0 K, λ's ~ 0.4 with Debye temperatures averaging 411 K. Not bad, given experimental values for Θ ranging from 390-433 K, and T_C's ~ 1.2 K!

Around 1964-65, W. A. ("Bill") Little at Stanford University recognized that should the boson field be comprised of excitons ($\Theta \approx$ 1-2 eV, or $\geq$ 12,000 K), the mediation of an even relatively weak electron-exciton coupling $\lambda \sim 0.5$, could result in a T_C well above room temperature (300 K) [8-12]. Little's conjecture encouraged other speculations as well, particularly by Allender, Bray and Bardeen [13], a conjecture that remains controversial to the present day. One must remain aware, however, that the basis of the speculations surrounding references [8-13] were anticipated by Ginzburg [1] (search all references within, many of which were "unreachable" during the Cold War).

Little's basic idea is summarized in Fig. 1. Major features are a dimerized polyacetylene ($(CH)_x$) chain (red encircled) surrounded by polarizable excitonic groups of diethyl-cyanine-iodide (polarizable component green enclosed). It is important to note that trans-polyacetylene has a band gap roughly 1-2 eV, requiring an exciton energy of at least that magnitude to effect pairing. Although fascinating, his model is structurally complex, and thus difficult to assess, even given present materials synthesis and computational tools.

In this paper, we undertake a description of a possible novel path involving computational DFT plus "response function" studies of feasible "proxy" structures perhaps achievable by emerging nano-fabrication technologies. We do this in the spirit of promoting a doctoral or post-doctoral effort at an appropriate institution. Pero, con quidado! Andale pues! Rough Mexican-American translation: "But watch out! Hurry up!" There is a preprint available

from Physics Today published in 1998 [16] announcing its discovery in 2028 by the North American Physical Society!

II. A Proxy Structure Embodiment of Little's Vision

Thus, let's address a rather simple "proxy model" engendered mathematically by the Fibonacci "arithmetic" summarized in Fig. 2, and embodied by the Al atomic chain structure outlined in Fig. 3, where we imagine such a chain deposited along a lattice dislocation line, either "cracked" or "scratched" on the (001) face of a cubic perovskite crystalline substrate. Exactly how such a "proxy" could be realized remains in the imagination of the reader, but instinctively given the plethora of presently emerging epitaxial growth methods combined with nano-manipulation of atomic surface "decoration," all which are emerging as future tools of materials science, now live in the "inbox." Of course, it is important to keep in mind that it is only physically possible to approximate a truly Fibonacci chain, just as one can only approximate a transcendental number by a ratio of integers (recall being taught in the 4^{th} grade that π is 22/7!), thus any practical realization of such a chain will certainly be periodic at some finite length.

This fact is made quite clear in Fig. 4 where we attempt a crude "band structure" calculation of a "quasiperiodic" Al string by imposing a three-fold periodicity s+L+s+s along the a-direction of a proxy cubic unit cell. Please see its caption for more details. The principal "take home" message is that increasing the length of the a lattice parameter following a Fibonacci sequence will not fundamentally result in a non-metallic state, but which would likely be eventually gapped by a small lattice distortion, but with a gap far smaller than that produced by dimerization as was the case of the trans-polyacetylene backbone chain of the classic Little model outlined in Fig. 1, and a gap easily bridged by excitons formed in a polarizable substrate (STO, SRO or Si), rather than at the more remote distance as would be the case for the cyanide side groups shown. As such, our model is perhaps more in line with the "Ginzburger" [5] or the metal-semiconductor interface proposed by Allender, Bray and Bardeen [13].

Besides requiring a sound ground state calculation, we also, and perhaps even more critically, must possess an inclusive response function from which to compute relevant superconducting properties, particularly T_C!

Such can be abstracted from Ref. [11], which follows on pioneer work by Kirschnitz, et al. [6], perhaps the premier study focused on formulating a generalized dielectric function derived from an arbitrary basis set…just simply follow Eq. (24) in [11]. Much more algebraic manipulation is required for generalization to our quasiperiodic model string structure, but today the analytic path forward is straightforward, nevertheless tedious. See Fig. 5 and its caption.

Let's consider explicitly the structural model shown in Fig. 6, and as detailed in its caption, and then apply DFT followed by the calculation of Kirschnitz's dielectric constant, all as a function of the distance "h" from the Si (001) surface to the midline of the Na quasiperiodic chain, in the spirit of Fig. 3c. At what value of "h" is it necessary stay within in order to realize Little's vision as applied to this embodiment? Should our results show promise, how do we next fabricate a Fig. 6 reality? With today's rapidly expanding nano-fabrication toolbox, such structures might be possible employing AFM "nano-derricks!"

III. Conclusions

As stated earlier in the Introduction, the purpose of the present paper is to propose a "proxy" approach to the realization of room temperature superconductivity, via a simple computationally tractable structural model, as suggested in Figs. 3-4 and Fig. 6, yet practically realizable via emerging nano-fabrication technology. The availability of a wide variety of DFT tools enables not only very accurate examination of the ground state eigenfunctions of a given model, but also a variety of nearby excited states outside the reach of first and second order perturbation theory. The path to a general and appropriate "boson-fermion coupling" response function, an extension of the Kirschnitz, et al., dielectric model [6], would next computationally be applied. Finally, should the model of Fig. 6, or similar structural proxies, prove promising, their nano-fabrication should be actively considered. As suggested in the Introduction, a possible doctoral or post-doctoral undertaking indeed!

Figure Captions

Fig. 1. Graphical summary of the original Little model (outlined in Refs. 8-11). Central features are a dimerized polyacetylene ($(CH)_x$) chain (red encircled) surrounded by polarizable excitonic groups of diethyl-cyanine-iodide (polarizable component green enclosed). It is important to note that trans-polyacetylene has a band gap roughly 1-2 eV, requiring an exciton energy of at least that magnitude to effect pairing.

Fig. 2. Mathematical outline of a quasiperiodic sequence of Fibonacci numbers. Note that the $n = \infty$ limit of the ratio of the number of two possible seqential interatomic distances, a and b, is defined as a transcendental number, thus assuring quasiperiodicy.

Fig. 3. One possible embodiment of a quasiperiodic sequence would be metallic Al atoms, deposited along a dislocation line, or "scratch," on the [001] surface of strontium ruthenate (SRO) or strontium titanate (STO) "decorated" by Al atoms. The efficacy of this embodiment needs to undergo study by appropriate DFT modelling prior to attempting fabrication.

Fig. 4. Elementary DFT study of a "bare" Al chain as envisioned in Fig. 3 [19]. (a): The 3-D crystal structure of such a chain, with lattice parameters b= c = 3a sufficiently separate to approximate its 1D nature. Note the nearest neighbor distances s and L are taken from the Fibonacci sequence postulated in Fig. 3, but the lattice constant for a = s+L+s+s imposes an arbitrary periodicity required to perform a DFT calculation. The "yellow surfaces" depict an arbitrarily selected charge density resulting from the calculation. (b): Selected "mid-band energies" plotted as a function of band number, with the red bars reflecting total individual band widths. Note that the Fermi energy, E_f, passes through a very narrow band (7), thus imposing a small "metallicity." (c): The Fermi surfaces resulting from this weak metallic state are shown. In principle, this degeneracy would be removed by nesting as the a parameter increases by including more s and L units and approaches ideal quasiperiodicity. See body of text for further discussion.

Fig. 5. All portions clipped and pasted from Ref. [11]. (a): Eq. (23), a tight-binding approximation to the matrix element bonding adjacent "chains." The path forward is to "adjust" all for the present model. (b): Resolution of the Migdal

issues relative to the Little model. (c): Dispersion of the relevant coupling boson strength vs. its quasi-momentum. Note the rather sharp "cutoff" and the connection to the distance "h" in Fig. 6 following.

Fig. 6. A possible structural realization of the concepts presented in Figs. 3-4. Shown is substrate consisting of the (001) surface of an otherwise single crystal of silicon, "decorated" along an appropriate quasiperiodic dislocation line with sodium, the latter positioned a distance "h" above that surface. Such could possibly be synthesized using AFM-derived "nano-derricks."

References

[1] "Superconductivity: The Day Before Yesterday - Yesterday - Today - Tomorrow," V. L. Ginzburg, Physics - Uspekhi 43, 573 (2000).

[2] "Theory of Superconductivity," J. Bardeen, L. N. Cooper and J. R. Schrieffer, Phys. Rev. 108, 1175 (1957).

[3] "Interactions Between Electrons and Lattice Vibrations in a Superconductors," G. M. Eliashberg, Sov. Phys. JETP 11, 1364 (1959).

[4] Transition Temperature of Strong-Coupled Superconductors," W. L. McMillan, Phys. Rev. 167, 331 (1968).

[5] "The Problem of High-Temperature Superconductivity, II," V. L. Ginzburg, Sov. Phys. Uspekhi 13, 335 (1970).

[6] "The Description of Superconductivity in Terms of Dielectric Response Function," D. A. Kirzhnits, E. G. Maksimov, and D. I. Khomskii, J. Low Temp. Phys. 10, 79 (1972).

[7] "Transition Temperature of Strong-Coupled Superconductors Reanalyzed," P. B. Allen and R. C. Dynes, Phys. Rev. B 12, 905 (1975).

[8] "Possibility of Synthesizing an Organic Superconductor," W. A. Little, Phys. Rev. 134, A1416 (1964).

[9] "Superconductivity at Room Temperature," W. A. Little, Scientific American 212, 21 (1965).

[10] "Dynamic Effective Electron-Electron Interaction in the Vicinity of a Polarizable Molecule," W. A. Little and H. Gutfreund, Phys. Rev. B 4, 817 (1971).

[11] "Proposed Model of a High-Temperature Excitonic Superconductor," D. Davis, H. Gutfreund, and W. A. Little, Phys. Rev. B 13, 4766 (1976).

[13] "Model for an Exciton Mechanism of Superconductivity," D. Allender, J. Bray and J. Bardeen, Phys. Rev. B 7, 1020 (1973)

[14] "June 2005 Notre Dame Workshop on the Possibility of RTSC," [Abstract List]

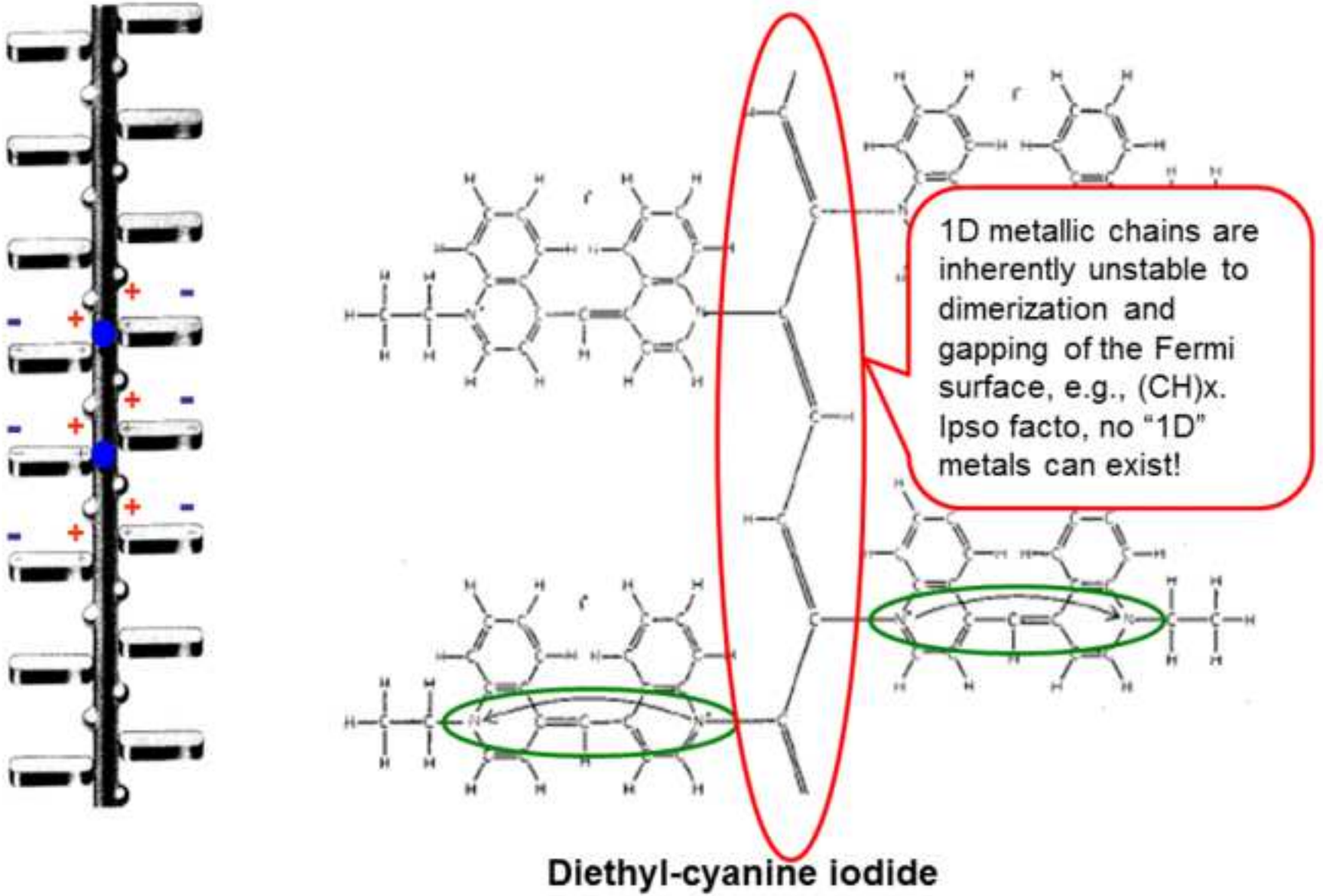
[15] "Design for a Room Temperature Superconductor," W. E. Pickett, BES Workshop on Superconductivity, May 2006.

[16] "Researchers Find Extraordinarily High Temperature Superconductivity in Bio-Inspired Nanopolymer," Paul M. Grant, Physics Today, May 1998.

[17] Quasiperiodic Quasi-1D Metal Chains , P. M. Grant, *February 2009: ICQNM - Quantum, Nano and Micro Technologies, Cancun* (pdf of presentation on mathematical properties of quasiperiodic arrays as a basis for a room temperature superconductor).

[18] Superconducting Fluctuations in One-Dimensional Quasi-periodic Metallic Chains , P. M. Grant, *BAPS APS March 2010, Vol. 55, 2, Portland* (pdf of presentation outlining physical principles underpinning the present work).

[19] All density functional calculations were performed using the open source Quantum Espresso package. Please visit the Quantum Espresso Web Page. For details regarding computations presented in Figs. 3-4, please email w2agz@w2agz.com.



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

Where $G_1 = a,\ G_2 = ab$

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

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

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

And take a and b

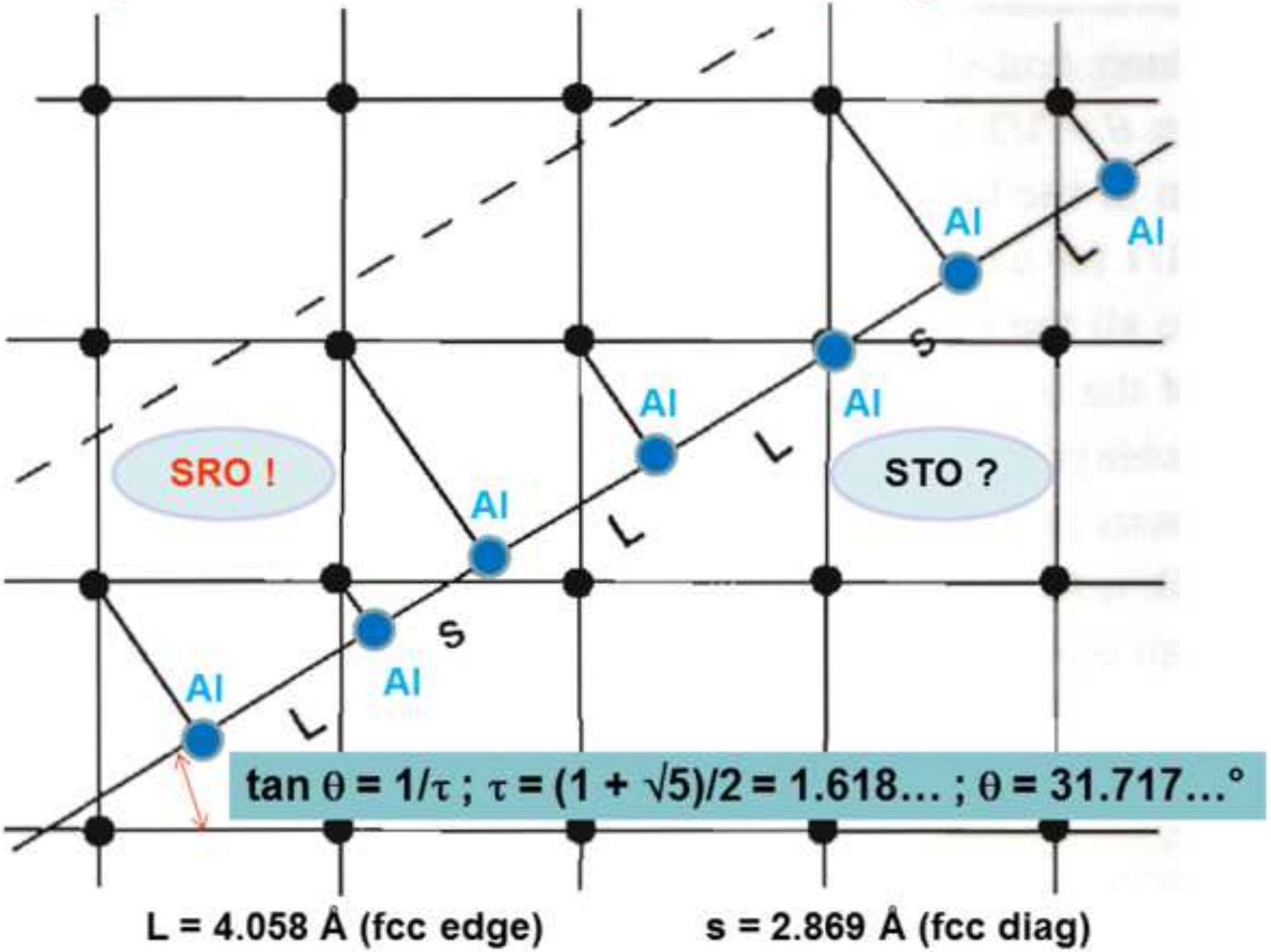
to be "inter-atomic n-n distances,"

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

Where c is a "scaling" parameter.

A Fibonacci fcc "Dislocation Line"

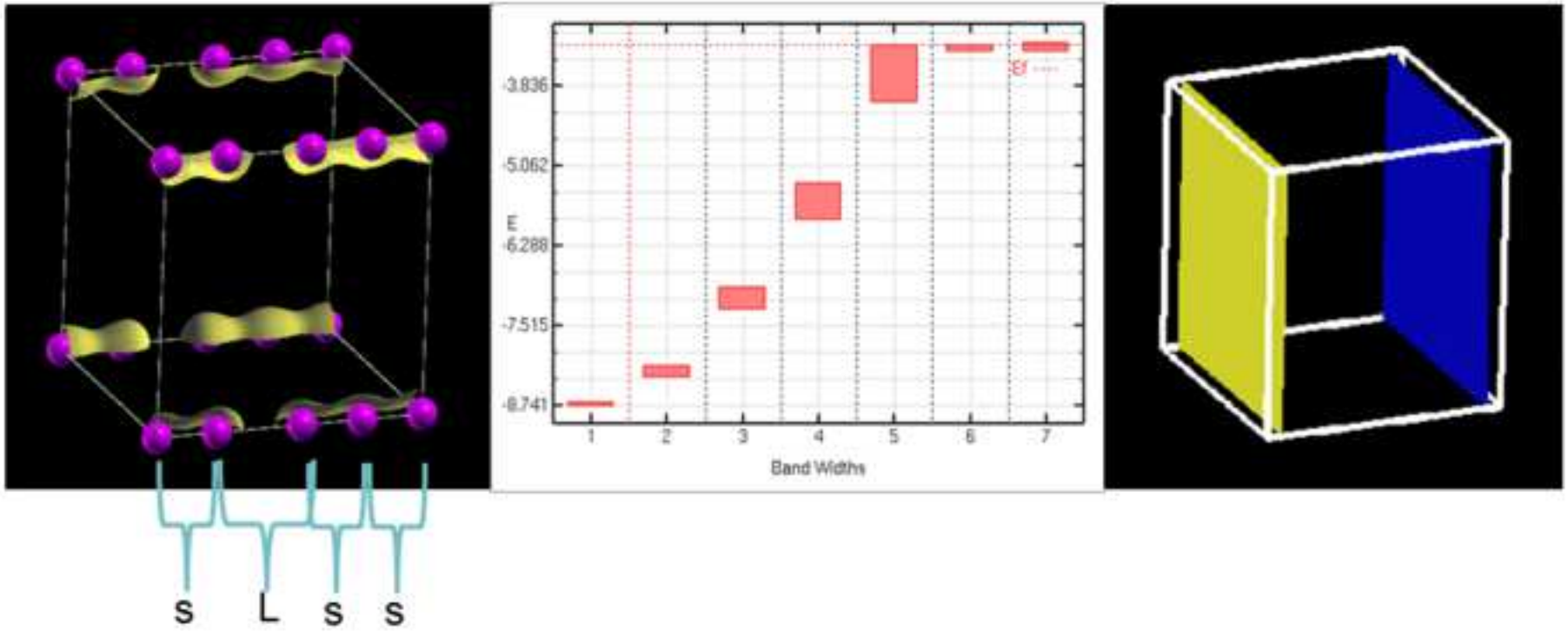
...or maybe Na on Si?...in other words..."a proxy Little model!"



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)



(a) (b) (c)

Davis – Gutfreund – Little (1975)

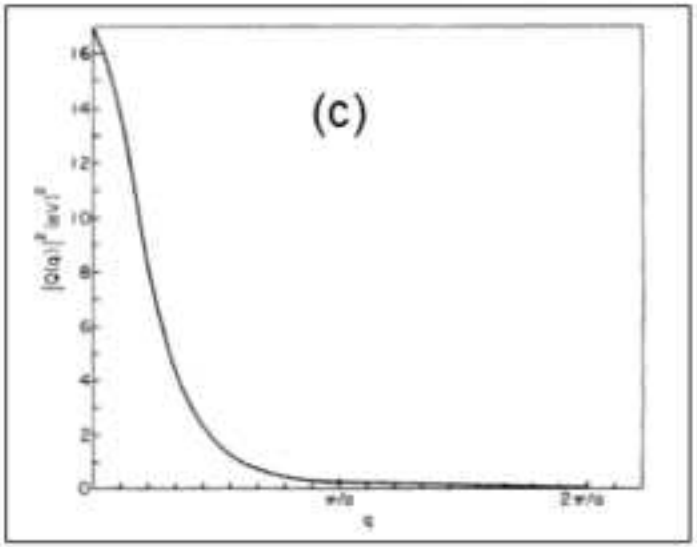
PHYSICAL REVIEW B VOLUME 13, NUMBER 11 1 JUNE 1976

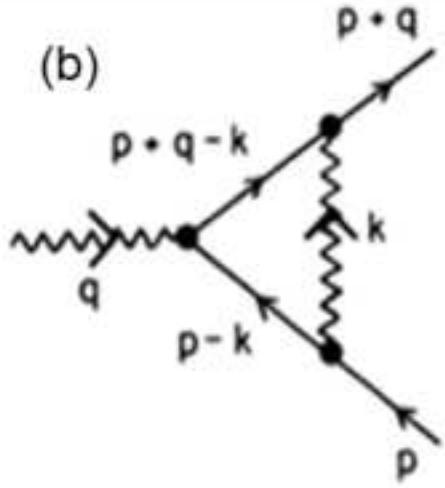
Proposed model of a high-temperature excitonic superconductor*

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

(a)

$$Q_\alpha(q) = \frac{1}{N^{3/2}} \int \sum_{j,k} \phi^*(r_1 - R_j)\,\phi(r_1 - R_k) e^{i[kR_k - (k-q)R_j]} V(r_1 r_2) \sum_{m,l,\nu} \left[u^\nu_{\alpha l}(q) + i v^\nu_{\alpha l}(q)\right] e^{-iqR_l}\, \Psi^*_\nu(R_{ml}) \Psi_{00}\, d^3r_1 d^3\tau$$





Migdal Issues:

- Only small exciton q's, $v_q > v_f$, couple to the fermion carriers.
- Thus vertex corrections are of order λ^2/Θ and we're OK.
- DGL claim such is NOT the case for ABB.