Does the DAVINCI CODE Hold the Key to Room Temperature Superconductivity?

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The Road to Room Temperature Superconductivity
Loen, Norway
17-22 June 2007
http://www.w2agz.com/rtsc07.htm

Road2RTS

Abstract for Road to RTSC, Loen, Norway
17 June 2007

Does the Da Vinci Code Hold the Key to Room Temperature Superconductivity

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The year 1957 witnessed what might have been the most important theoretical advance in condensed matter physics of the past century. Bardeen, Cooper and Schreiffer[1] were able to show, based on an elegantly simple proof by Cooper that the degenerate Fermi gas could be gapped by weak lattice vibration-mediated attractive electron-electron interactions, that the transition temperature of superconductors could be semi-quantitatively given by the expression, $T_C = a\theta_D \exp(-1/\lambda)$. Here T_C is the critical temperature, θ_D the phonon Debye temperature, λ the dimensionless electron phonon coupling constant, and a a "gap scaling factor" of order 1-3. Strictly speaking, this simple "BCS relation" holds only for $\lambda < 1$, and $\lambda k\theta_D \ll E_F$, where E_F is the Fermi energy. However, Migdal and Eliashberg[2] later showed modifications of this relation that included higher order attraction terms as well as electron-electron repulsion could accomodate "strong coupling" values of λ in the range 1 – 2 and thus successfully account for the relatively high transition temperatures of the A15 compounds and perhaps the HTSC cuprates as well. The message of BCS is clear: a superfluid state is mediated by the pairing of fermions in a boson field, and its condensation temperature scales both with the characteristic temperature of the boson and the strength of its coupling to the fermions. It is possible that attempts to increase T_C by engineering a rise in the electron-phonon λ, given the known range of Debye temperatures available, may give rise to unphysical material constraints.[3] Even other possible "boson flavors," e.g., "magnons or "spin waves" or "resonating bonds," may not possess characteristic energies large enough to get T_C to room temperature with realistically achievable coupling constants. On the other hand, various sorts of charge polarization bosons, such as excitons, have characteristic energies on the order of 1 eV and in principle could manifest in properly designed structures superconducting transition temperatures on the order of 300 K, even under extremely weak electron-exciton coupling. This opportunity did not go unnoticed and was suggested (before BCS!) by Fritz London[4] as possible in macro-organic molecules, and analytically addressed post-BCS by Davis, Gutfreund and Little,[5] Ginzburg,[6] and Allender, Bray and Bardeen,[7] and was even the subject of a science fiction short story in 1998.[8]

In this lecture, we will review the several model approaches taken in the past in light of their possible incorporation in modern density functional theory employing today's powerful and widely available computational hardware and software applied to novel structures now accessible by "nano-assembly" and "nano-machining" technologies. We will address one of the "devils in the details" of all such models, the required spatial separation of electron transport from the polarization portions of any hypothetical

material embodiment, which often contain quasi-one-dimensional metal chains subject to gapping of their Fermi through commensurate structural distortion. As the title of the lecture hints, there may exist in the wisdom of the ancients some rituals to exorcise this devil.

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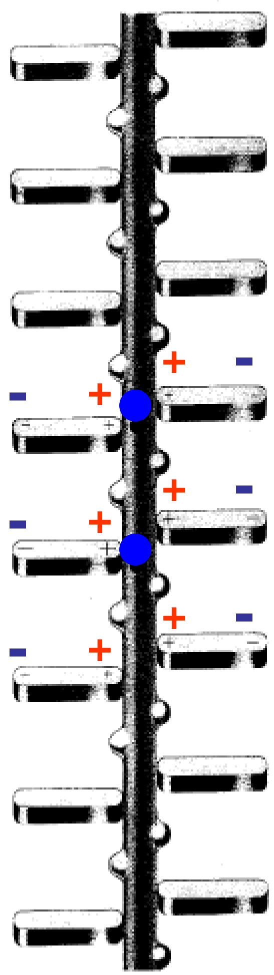
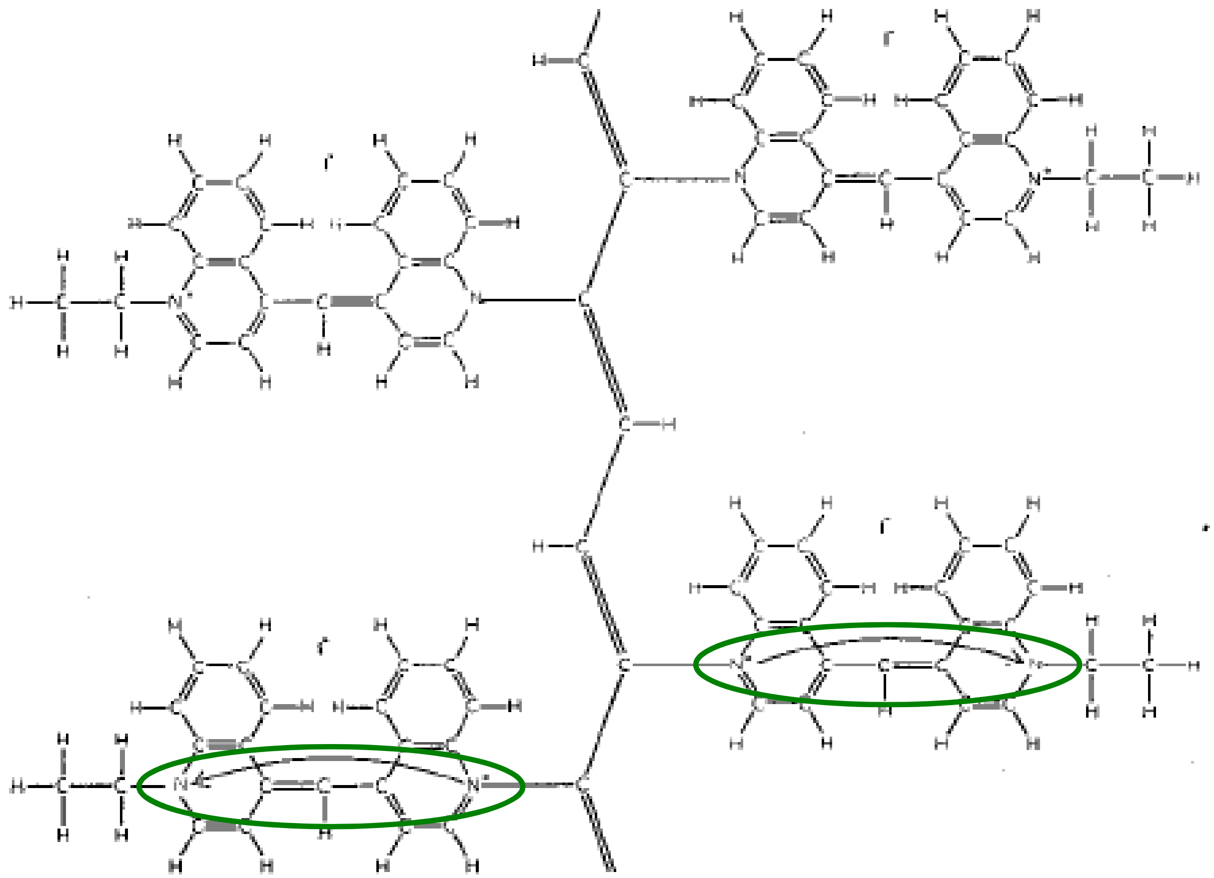
[1] J. Bardeen, L. N. Cooper and J. R. Schrieffer, Phys. Rev. 108, 1175 (1957).
[2] A. B. Migdal, Sov. Phys. JETP 5, 1174 (1958); G. M. Eliashberg, Sov. Phys. JETP 11, 1364 (1959).
[3] M. R. Beasley – This conference
[4] F. London, "Superfluids," (John Wiley & Sons, London, 1950), pp. 8-9.
[5] D. Davis, H. Gutfreund and W. A Little, Phys. Rev. B13, 4766 (1976).
[6] V. L. Ginzburg, Sov. Phys. Usp. 13, 335 (1970).
[7] D. Allender, J. Bray and J. Bardeen, Phys. Rev. B7, 1020 (1973).
[8] P. M. Grant, Physics Today, May 1998.

London (1950)

Little, 1963





Diethyl-cyanine iodide

“Bill Little’s BCS”

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

~~$\lambda k\Theta \square E_F$~~

Where

Θ = Exciton Characteristic Temperature (~ 22,000 K)

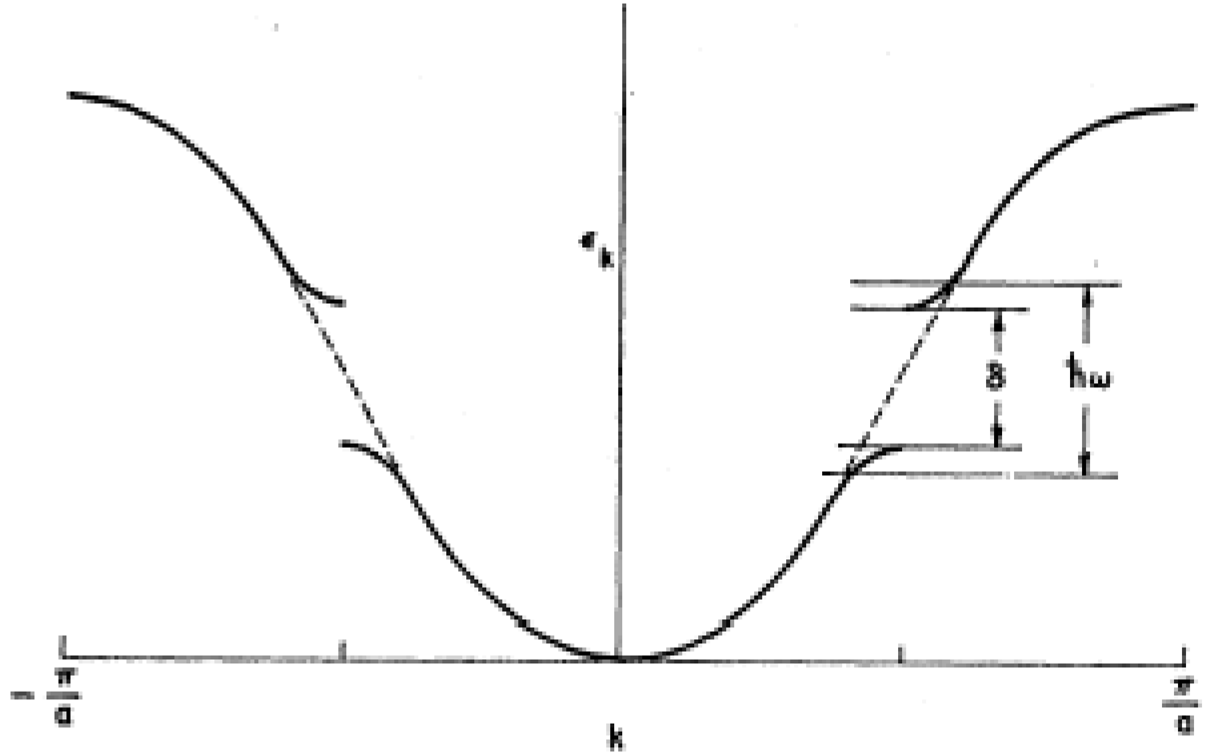
λ = Fermion-Boson Coupling Constant (~ 0.2)

μ^* = Fermion-Fermion Repulsion (?)

a = “Gap Parameter, ~ 1-3”

Tc = Critical Temperature, ~ 300 K

Spine is a Semiconductor!



False Alarm:

SUPERCONDUCTING FLUCTUATIONS AND THE PEIERLS INSTABILITY IN AN ORGANIC SOLID*

L.B. Coleman, M.J. Cohen, D.J. Sandman, F.G. Yamagishi, A.F. Garito and A.J. Heeger

Department of Physics and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, Pennsylvania 19174, U.S.A.

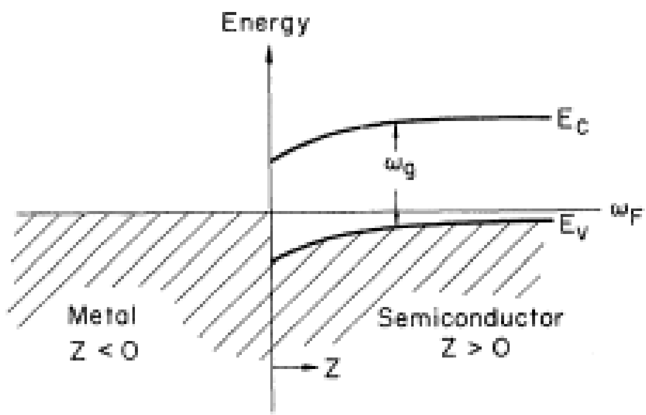
(*Received* 20 *February* 1973 *by E. Burstein*)

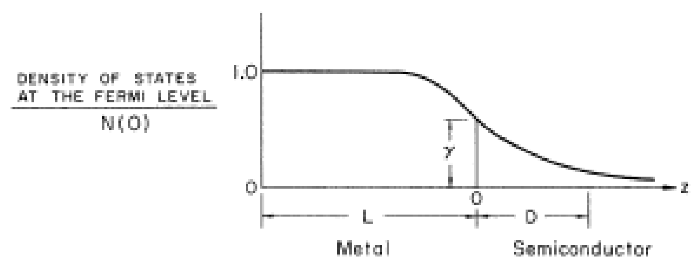
Allender-Bray-Bardeen (1973)

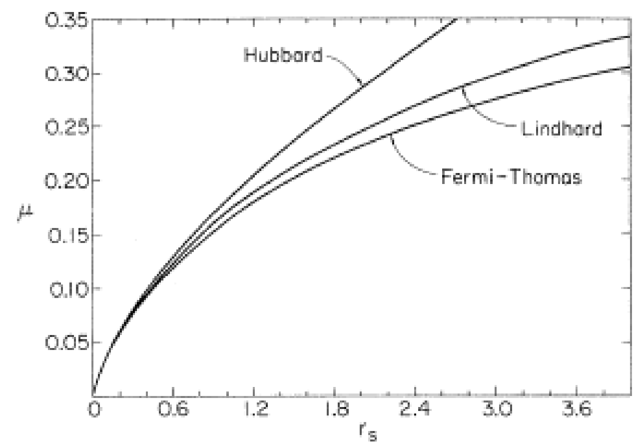
PHYSICAL REVIEW B VOLUME 7, NUMBER 3 1 FEBRUARY 1973

Model for an Exciton Mechanism of Superconductivity*

David Allender,† James Bray, and John Bardeen
Department of Physics and Materials Research Laboratory, University of Illinois, Urbana, Illinois 61801
(Received 7 August 1972)







Electron-Exciton Interaction

Exciton c-a Operators

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

Electron-Exciton Coupling

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

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

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

Davis – Gutfreund – Little (1975)

PHYSICAL REVIEW B VOLUME 13, NUMBER 11 1 JUNE 1976

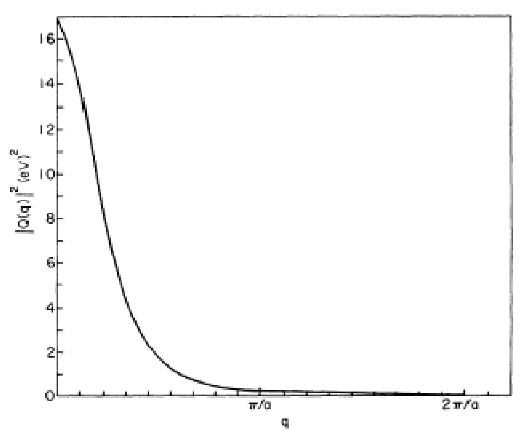
Proposed model of a high-temperature excitonic superconductor*

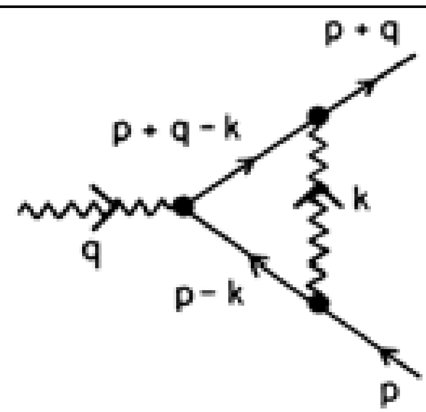
D. Davis,† H. Gutfreund,‡ and W. A. Little
Physics Department, Stanford University, Stanford, California 94305
(Received 16 October 1975)

$$g_{\mathbf{k+q},\mathbf{k}}^{q\nu,mn} \longrightarrow$$

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

$$Q_\alpha(q) = \frac{1}{N^{3/2}}\int\sum_{j,h}\phi^*(r_1 - R_j)\,\phi(r_1 - R_h)e^{i[kR_h-(k-q)R_j]}V(r_1r_2)\sum_{m,l,\nu}[u^{\nu}_{\alpha l}(q) + i\,v^{\nu}_{\alpha l}(q)]\,e^{-iqR_l}\,\Psi^*_{\nu}(R_{ml})\Psi_{00}\,d^3r_1d^3\tau$$

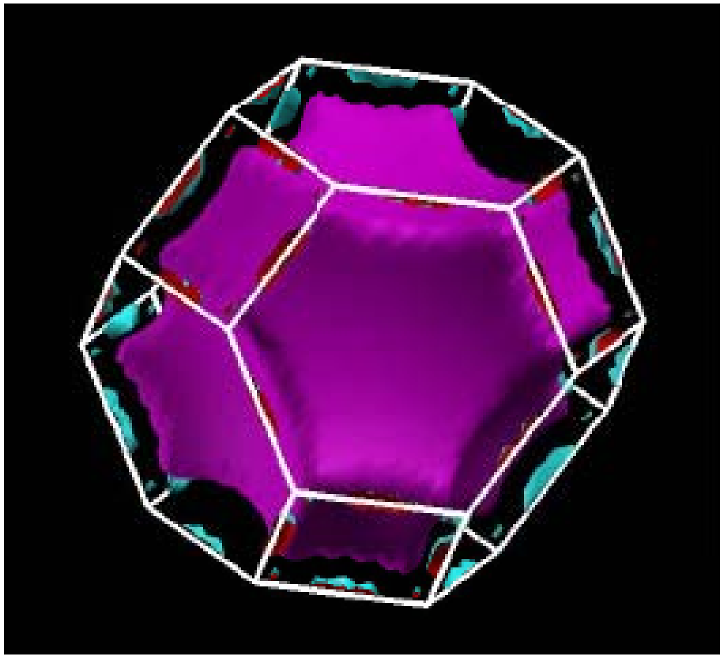


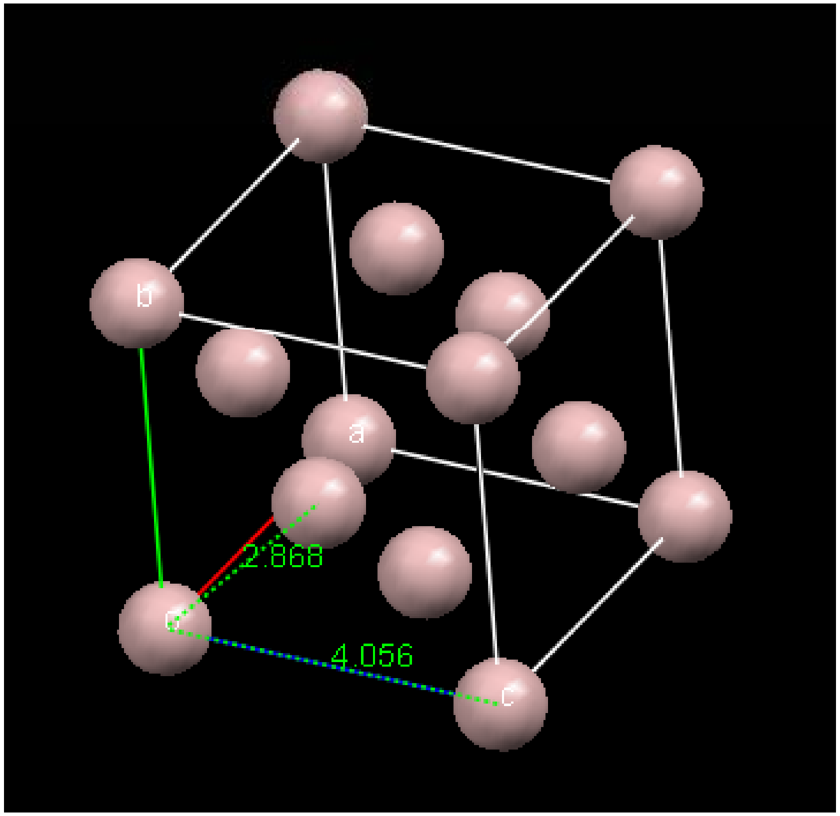


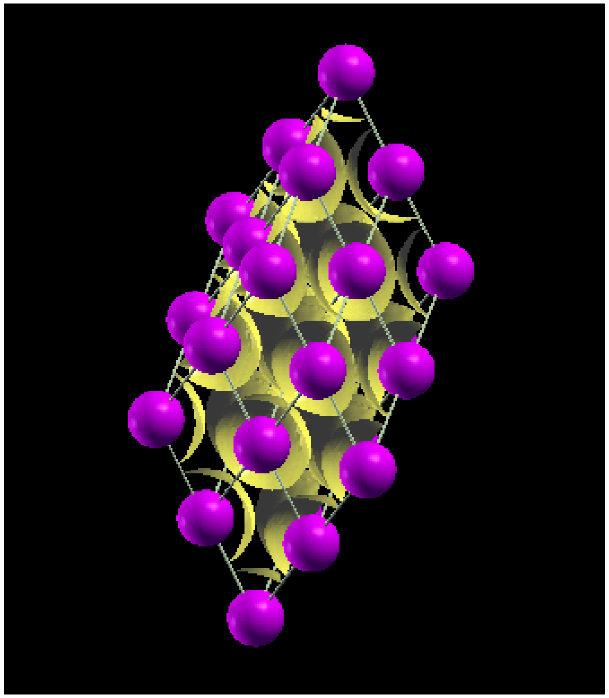
Migdal Issues:

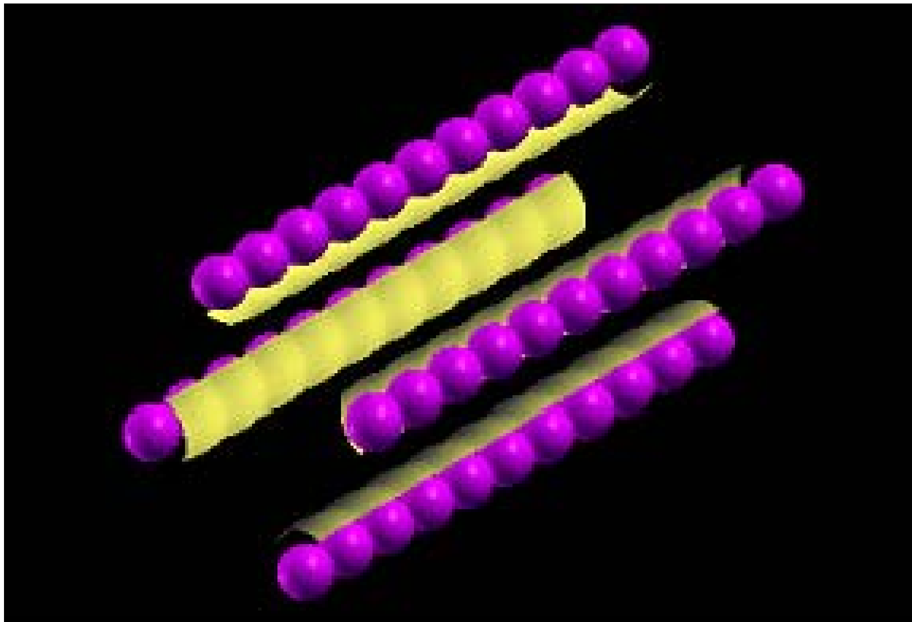
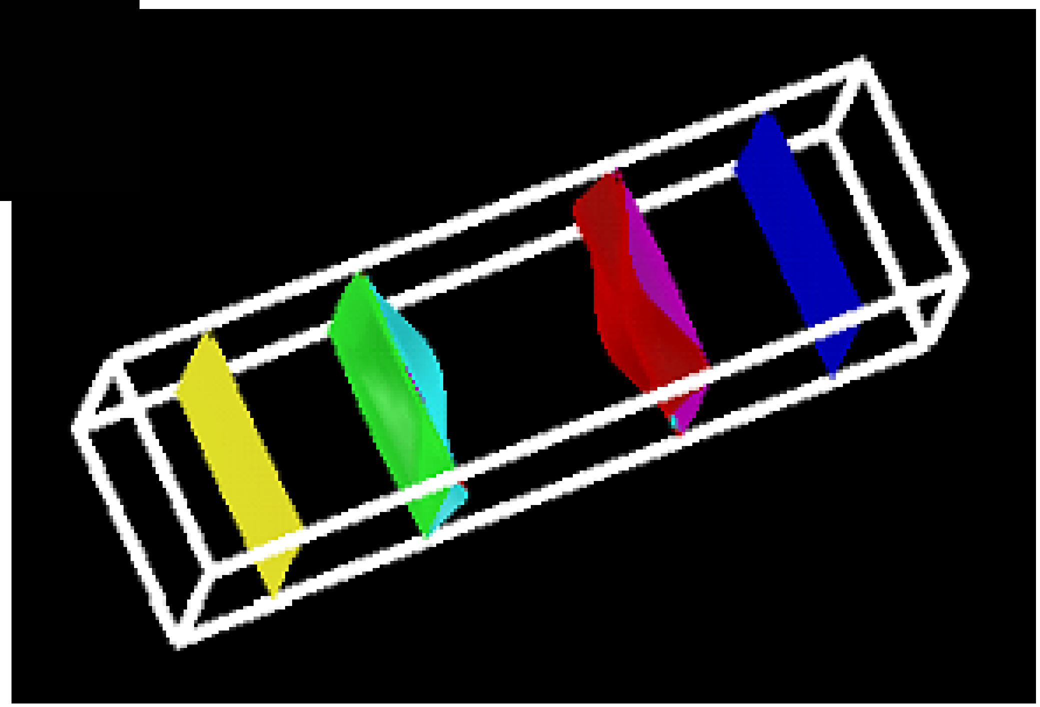
- Only small exciton q's, $v_q > v_F$, couple to the electrons.
- Thus vertex corrections are of order λ^2/θ and we're OK.
- DGL claim this is NOT the case for ABB.
- IMHO, this is an item amenable to numerical analysis.

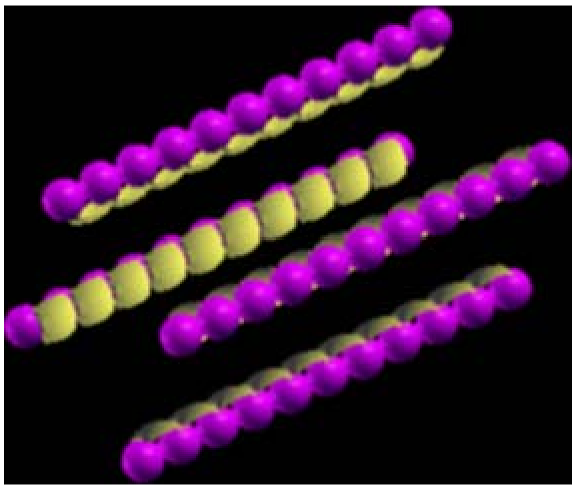
“3-D”Aluminum

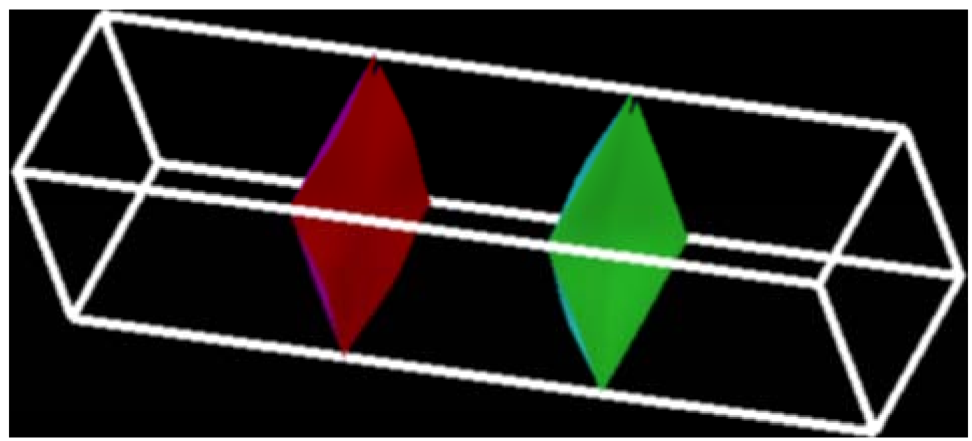










“Not So Famous Danish Kid Brother“

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:

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

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:

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

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

Rigid Ion Approximation

$$V(x) \equiv V_a(x) \otimes s(x)$$

$$s(x) = \sum_{n=-\infty}^{\infty} \delta(x - x_n)$$

$$x_n = na + b\cos\frac{2\pi na}{L}$$

$$s(x) = \sum_{\ell=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} (-i)^{\ell} J_{\ell}\left[2\pi b\left(\frac{m}{a} + \frac{\ell}{L}\right)\right] e^{i2\pi\left(\frac{m}{a}+\frac{\ell}{L}\right)x}$$

Plane Wave Representation

$$\left|k\right\rangle = e^{ikx}$$

$$V(x) = \sum_{K} U(K) e^{iKx}$$

$$E(k) = \frac{\hbar^2 k^2}{2m} + U(0) + \sum_{K \neq 0} \frac{\left|U(K)\right|^2}{\frac{\hbar^2}{2m}\left[k^2 - \left(k-K\right)^2\right]} + \ldots$$

$$V(x) = \sum_{n=-N}^{N} U(n) e^{i \frac{2\pi}{a} r_n x}, \quad r_n \text{ rational}$$

$$\{r_n\} = \{\mu_n / \nu\}, \quad \{\mu_n\} \in I, \quad \nu = LCD$$

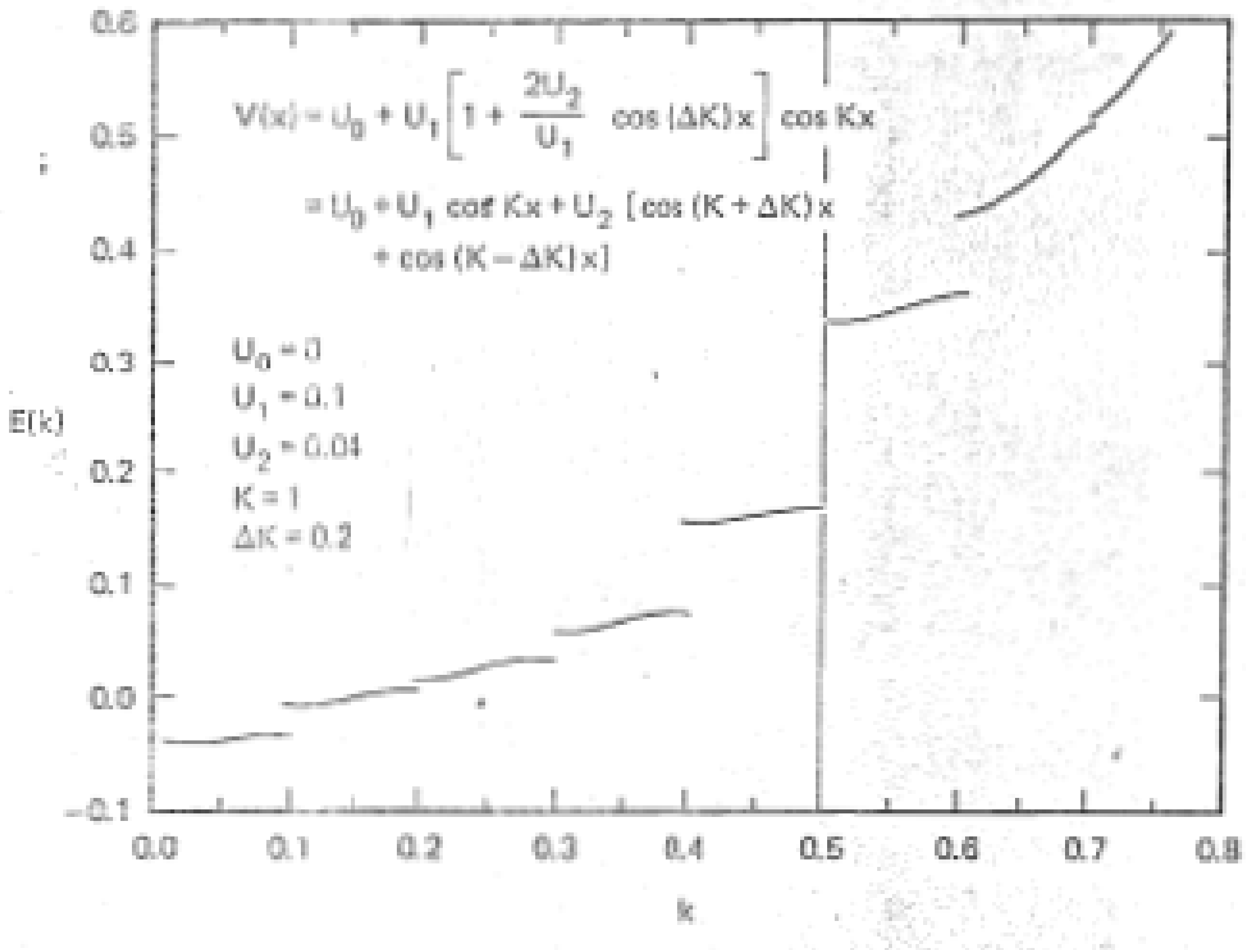
$$\psi_k(x) = \frac{2\pi}{\nu a} \sum_{-\infty}^{\infty} \chi(n) e^{i \frac{2\pi n}{\nu a} x} e^{ikx}, \quad \{n\} \in I$$

$$\lim_{\nu \to \infty} \frac{2\pi}{\nu a} \sum_{n=-\infty}^{\infty} \chi(n) e^{i \frac{2\pi n}{\nu a} x} e^{ikx} \Rightarrow \int_{-\infty}^{\infty} \chi(k' - k) e^{ik'x} dk'$$

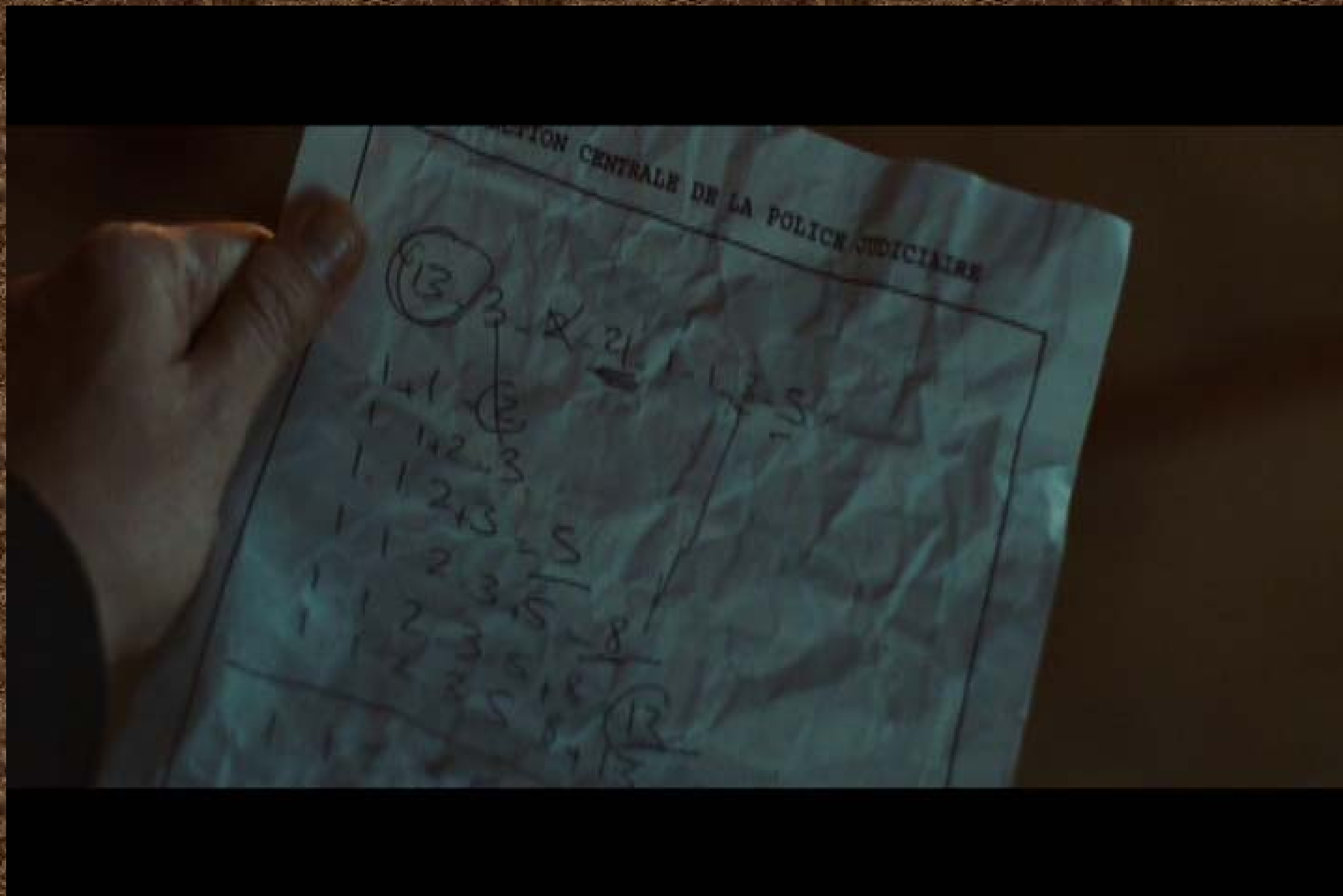
APF "Band Structure"

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

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



DA VINCI CODE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Fibonacci Chains

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

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

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

Where $G_1 = a,\ G_2 = ab$

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

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

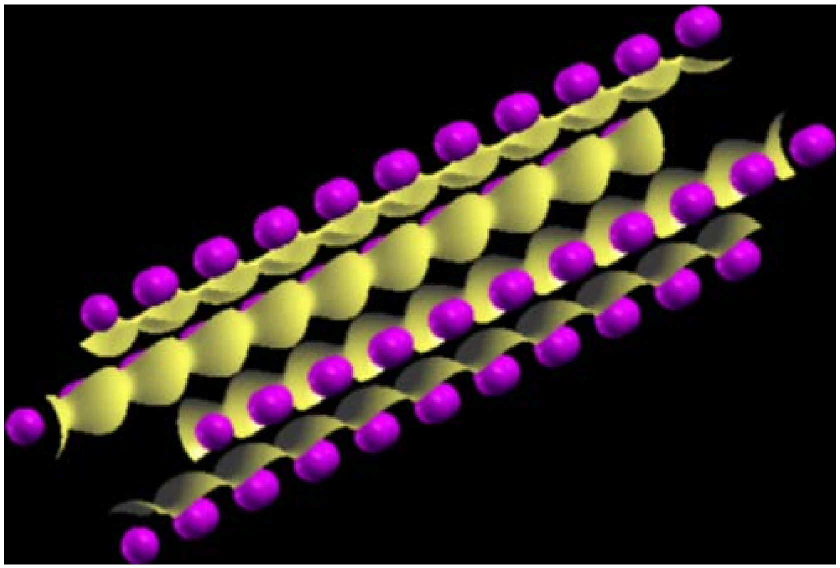
Let $a = c\tau b$, subject to $\langle a, b \rangle$ invariant,

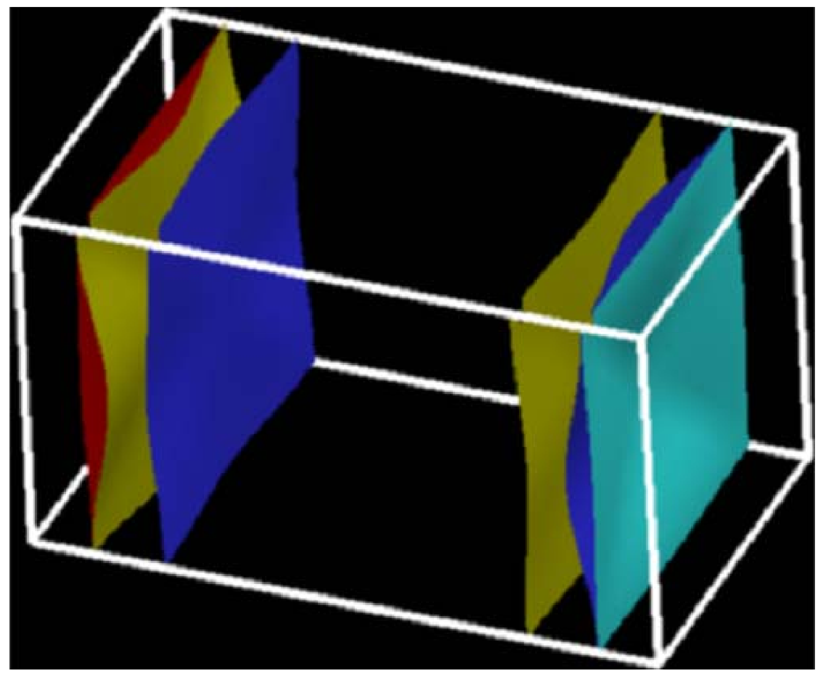
And take a and b

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

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

Where c is a "scaling" parameter.





64 = 65