

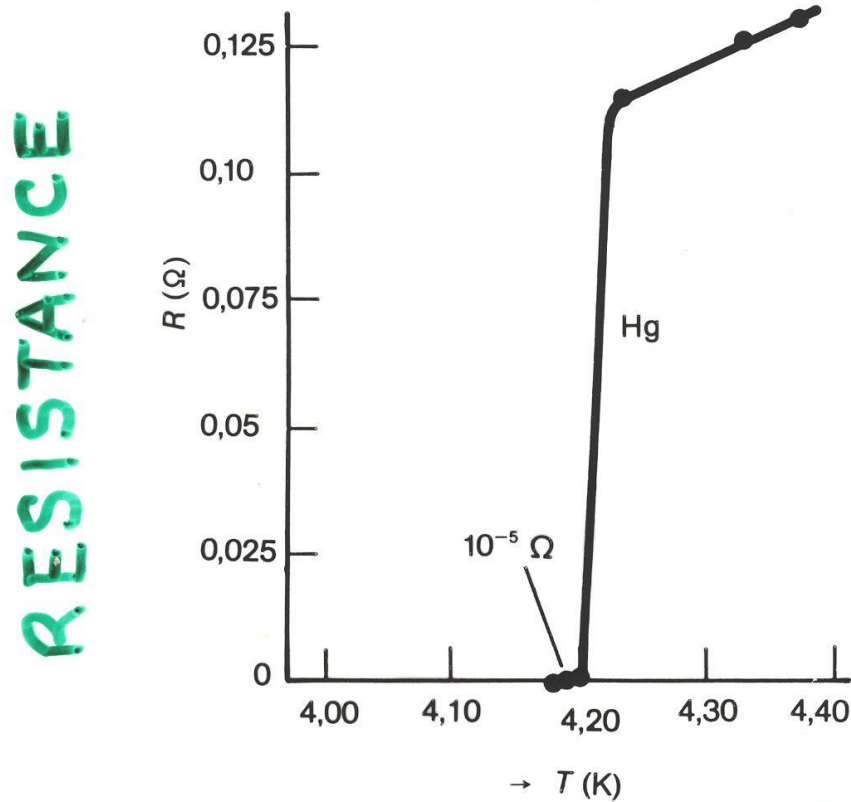
The Evolution of the Theory of Electron-Phonon Induced Pairing and its Limits for Superconducting Systems

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1911

THE FIRST SUPERCONDUCTOR

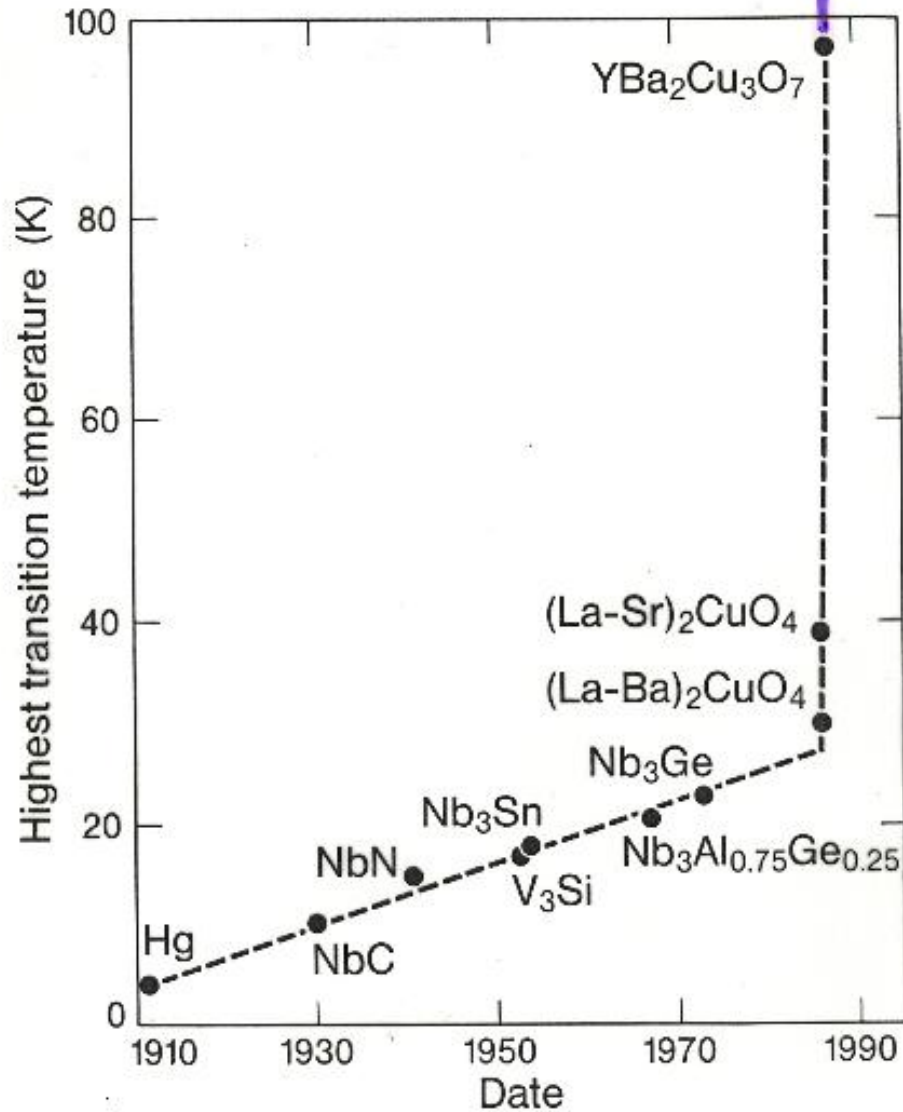


TEMPERATURE

H. KAMERLINGH ONNES

Hg-Ba-Ca-Cu-O → 165K (PRESSURE)

133K
127K



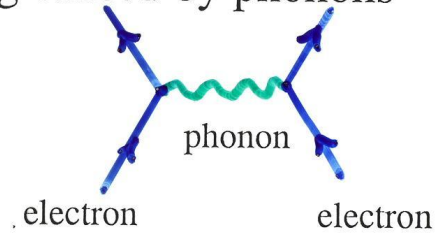
CLASSES OF SUPERCONDUCTORS

CLASS 1: conventional metals, C60,
some organics, doped
semiconductors, MgB₂

CLASS 2: copper oxides, heavy
fermion metals, some organics

BCS Theory (1957)

Overlapping pairs
Pairing caused by phonons



BCS Model (1957) $T_C = 1.13 T_D e^{-1/NV}$

$$NV = \lambda - \mu > 0$$

↑ ↑
attractive phonon repulsive Coulomb
interaction interaction

Improvements (1960's)

$$\lambda \rightarrow \lambda^* = \frac{\lambda}{1 + \lambda} \qquad \mu \rightarrow \mu^* = \frac{\mu}{1 + \mu \ln \frac{E_F}{E_D}}$$

CAN BCS THEORY PREDICT T_c ?

$$T_c \propto T_D \underbrace{e^{-\frac{1}{NV}}}_{\substack{\omega \\ 300K}} \sim 11K$$

$$\text{IF "NV"} \rightarrow 0.03 \quad T_c \rightarrow 10^{-12}$$

NEED TO KNOW "NV" **VERY ACCURATELY**
TO PREDICT T_c

DOPED SEMICONDUCTOR



FIRST SUPERCONDUCTING OXIDE

(COHEN 1963; SCHOOLEY ET AL 1964)

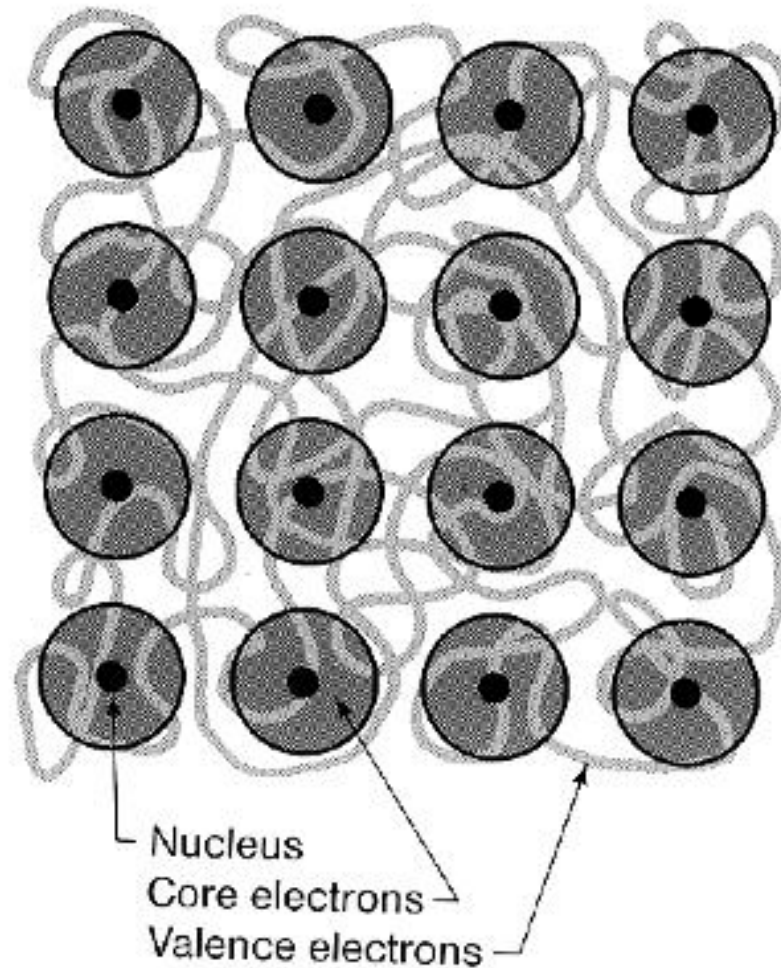
CONCEPTUAL BASIS

ONE CAN ARGUE FOR TWO
MODELS OR “MENTAL
PICTURES” OF A SOLID:

1. INTERACTING ATOMS
MODEL (REDUCTIONISM)
2. ELEMENTARY EXCITATIONS
MODEL (EMERGENCE)

Standard Model

Plane Wave Pseudopotential Method [PWPM]



Plane Wave Pseudopotential Method (Standard Model of Solids)

For a broad class of solids, clusters, and molecules, this method describes ground-state and excited-state properties such as:

electronic structure

crystal structure and structural transitions

structural and mechanical properties

vibrational properties

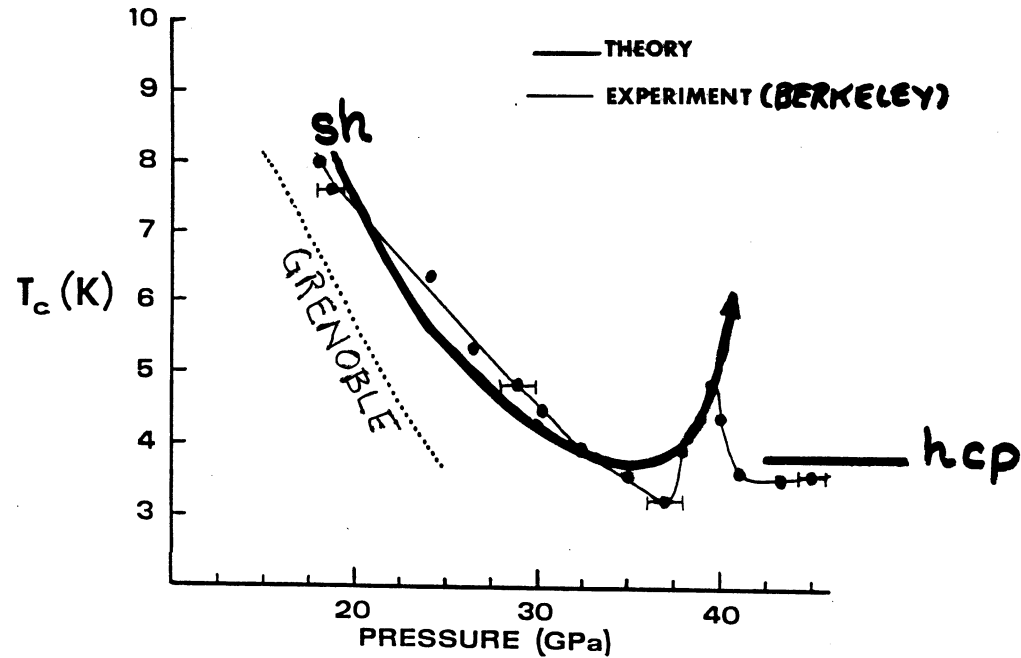
electron-lattice interactions

superconductivity

optical properties

photoemission properties

sh and hcp SILICON T_c (PRESSURE)



THEORY

CHANG, DACROGNAN & COHEN

EXP.

GRENOBLE: MIGNOT, CHOUTEAU & MARTINEZ

BERKELEY: ERSKINE & YU

Computational Methods

Atomic numbers of Mg and B



Ab initio pseudopotentials for Mg and B



Density functional theory
(electronic structures of MgB₂)



Frozen-phonon method
(phonon structure)



Atomic masses
of Mg and B



Electron-phonon interactions
(normal-state specific heat)



Eliashberg formalism

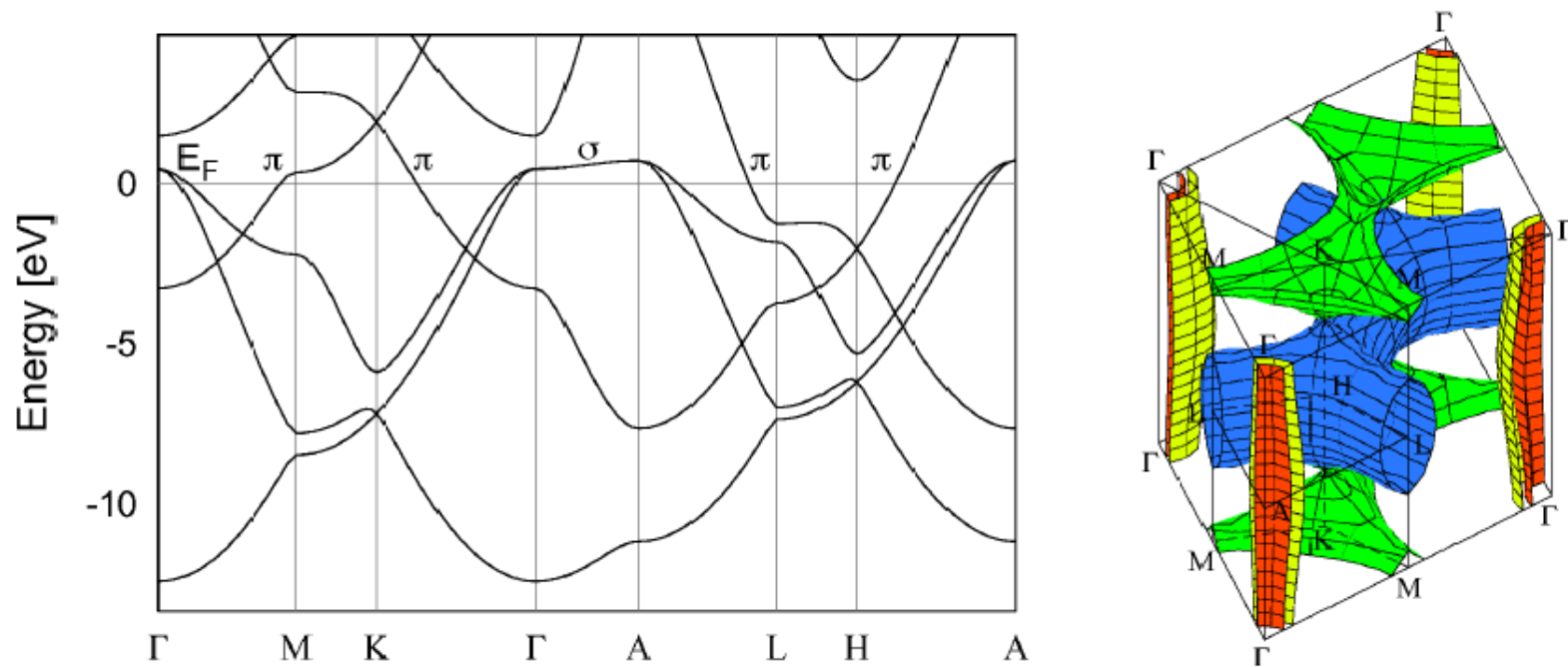


μ^*

(T_c , isotope effect, superconducting gap, specific heat)

Pristine MgB₂: Electronic structures and Fermi surface

- Band structure

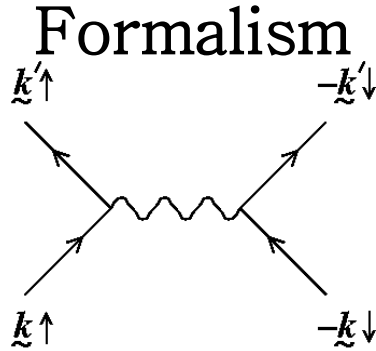


- Fermi surface consists of four sheets:
two from σ -bonding boron $p_{x,y}$ orbitals
and two from π -bonding boron p_z orbitals.

Also: An & Pickett, PRL 2001; Kortus, et al, PRL 2001; Liu, et al, PRL 2001;
Kong, et al, PRB 2001; ...

Superconductivity in the Eliashberg

BCS
Theory



Electron pairing
via phonon
exchange

Main ingredient: momentum- and frequency-
dependent Eliashberg function

$$\alpha^2 F(\vec{k}, \vec{k}', \omega) \equiv N(\epsilon_F) \sum_j |g_{\vec{k}\vec{k}'}^j|^2 \delta(\omega - \omega_{j\vec{q}})$$

where $N(\epsilon_F)$ = density of states per spin at Fermi
level

$g_{\vec{k}\vec{k}'}$ = electron-phonon matrix element

$\omega_{j\vec{q}}$ = frequency of phonon in j th branch

Equivalently:
with $\vec{q} = \vec{k} - \vec{k}'$

$$\lambda(\vec{k}, \vec{k}', n) \equiv \int_0^\infty d\omega \alpha^2 F(\vec{k}, \vec{k}', \omega) \frac{2\omega}{\omega^2 + (2n\pi T)^2}$$

$$\lambda = \langle \lambda(\vec{k}, \vec{k}', 0) \rangle$$

Transition Temperature and Isotope Effect

	harmonic		anharmonic		experiment
	isotropic	anisotropic	isotropic	anisotropic	
T_c	28 K	55 K	19 K	39 K	39 K
α_B	0.42	0.46	0.25	0.32	0.26, 0.30
α_{Mg}	0.04	0.02	0.05	0.03	0.02
λ	0.73		0.61		0.58, 0.62
ω_{ph}	62.7 meV		75.9 meV		75.9, 76.9

$$\mu^*(\omega_c) = 0.12.$$

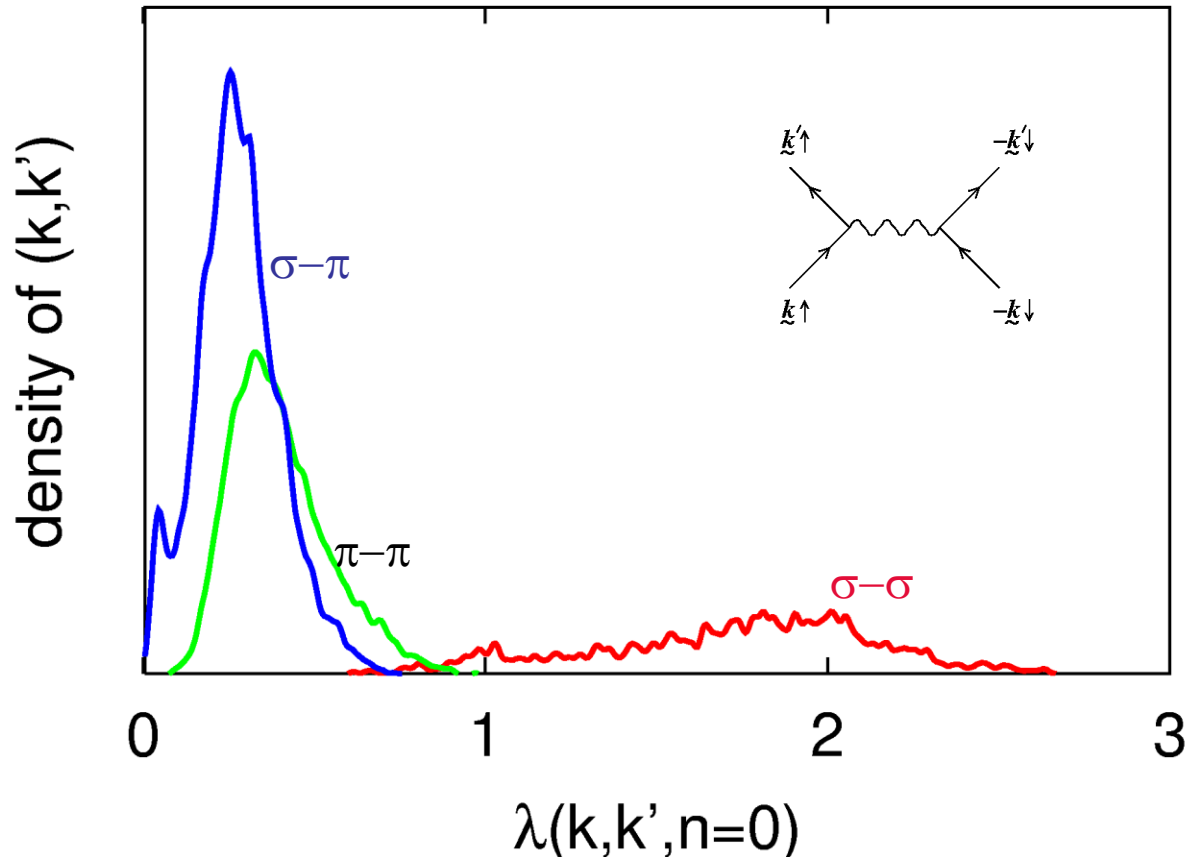
Anharmonicity --> small

λ : averaged electron-phonon coupling.

ω_{ph} : frequency of the in-plane B-B stretching modes (E_{2g}) at Γ .

For $0.10 \leq \mu^*(\omega_c) \leq 0.14$, $41 \text{ K} \geq T_c \geq 37 \text{ K}$

Distribution of Electron-Phonon Couplings

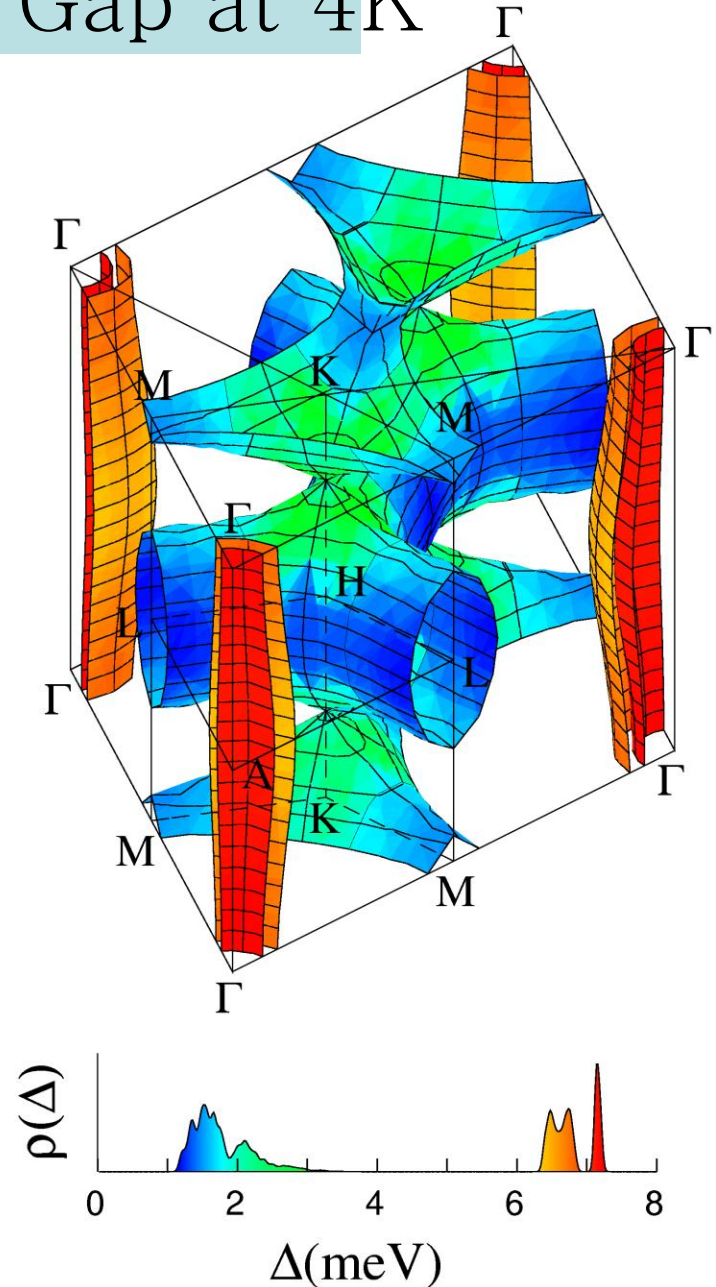


Notes:

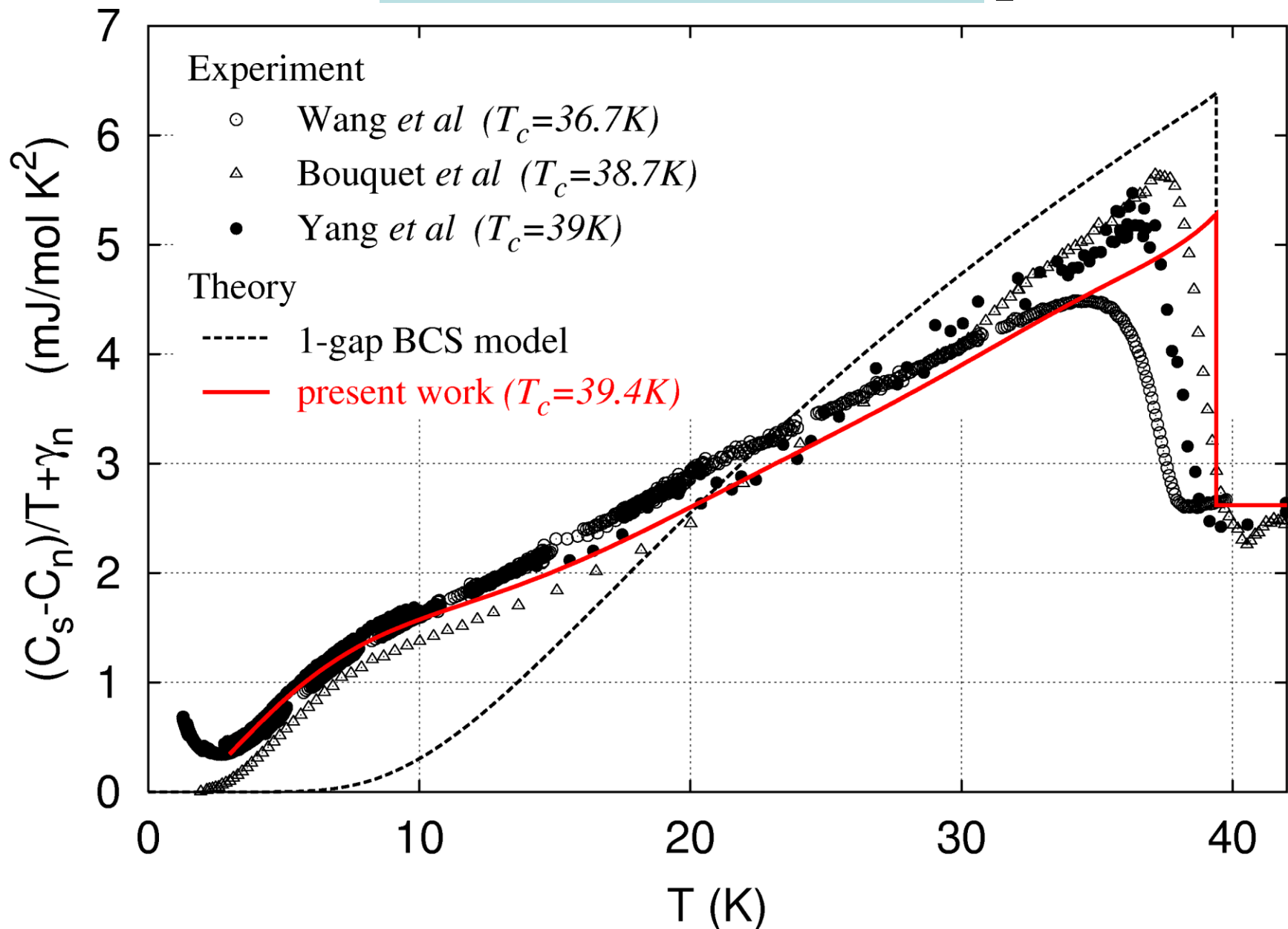
- 1) most metals: $\lambda \sim 0.3 - 0.5$
- 2) MgB_2 : $\langle \lambda \rangle = 0.61$; specific heat data $\lambda = 0.58, 0.62$

Superconducting Gap at 4K

- $\Delta(\mathbf{k})$ on Fermi surface at $T=4$ K
- Large gap on cylindrical σ -sheets
- 2 dominant sets of gap values



Specific Heat of MgB_2



Summary

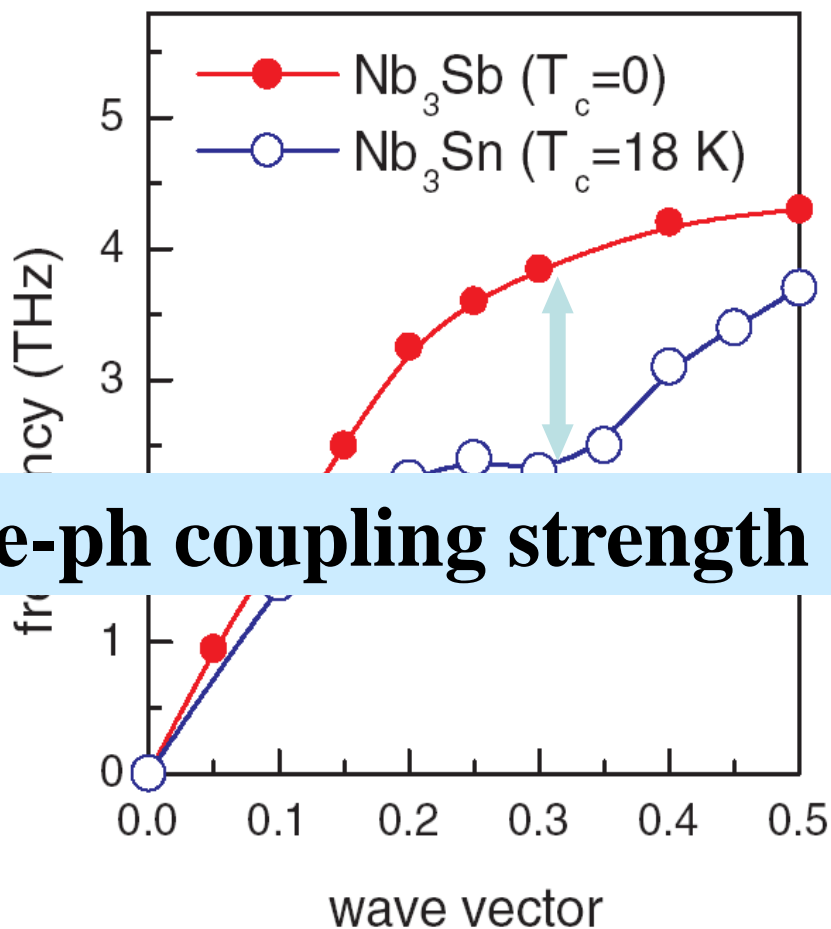
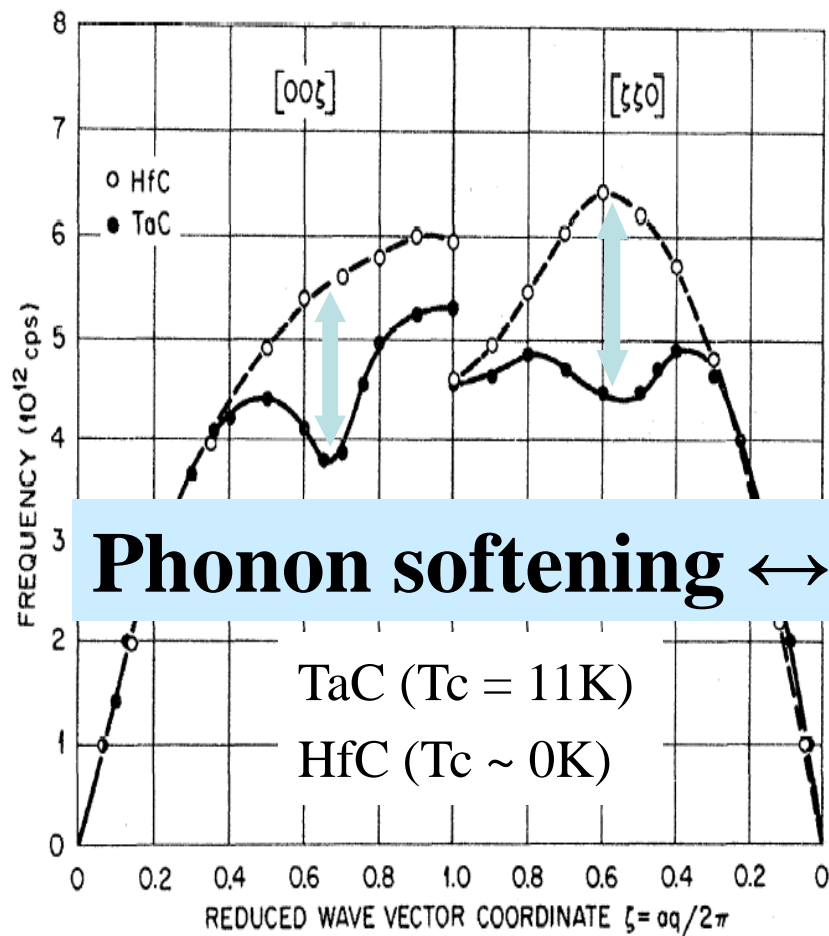
- MgB₂ is a **multi-gap, phonon-mediated** superconductor
- Large electron-phonon coupling of the σ boron states responsible for high T_c
- Need to solve the **k-dependent** Eliashberg equations to obtain the correct T_c and other quantities
- First-principles results explained T_c , specific heat, isotope exponents, photoemission, tunneling, and other data
- Theory predicts at least **2 dominant** superconducting gap values at low temperature, and the two-gap feature is robust against pressure, doping and impurity scattering.

RAISING T_c

WE TRIED TO USE THEORY TO SUGGEST
HOW TO INCREASE THE TRANSITION
TEMPERATURE OF MAGNESIUM DIBORIDE
SIGNIFICANTLY BUT FAILED!

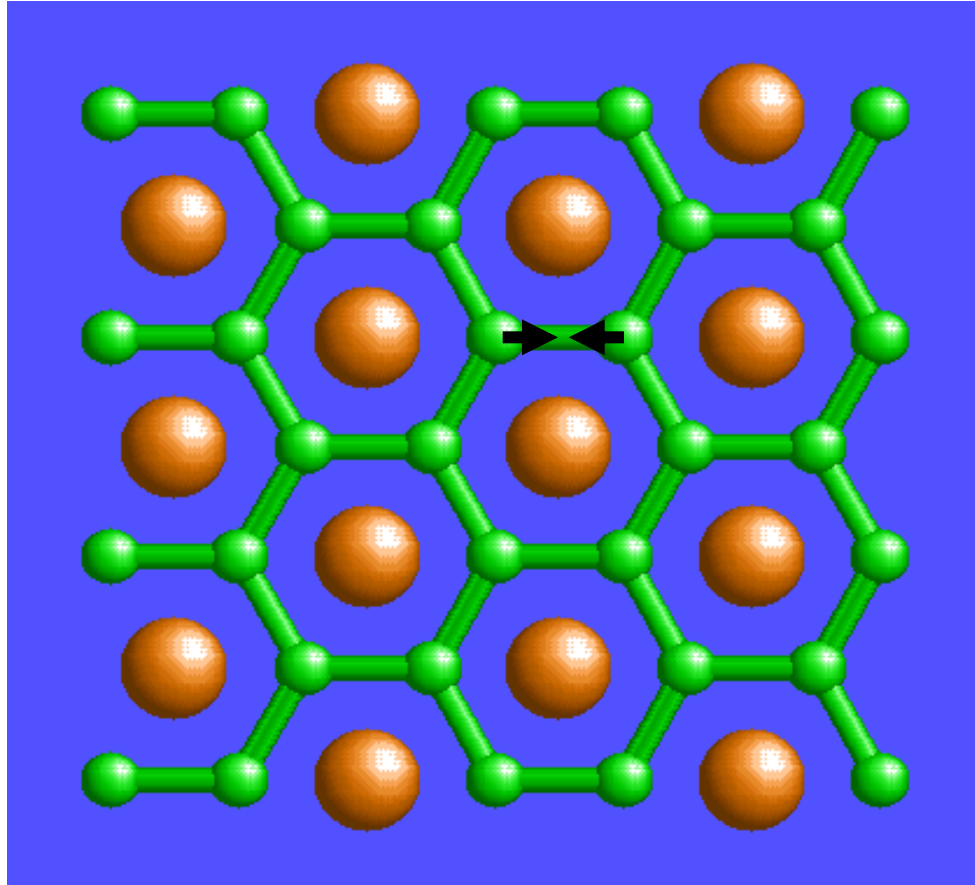
THIS RESULT IS CONSISTENT WITH
EXPERIMENTS UP TO NOW.

Phonon softening in superconductors

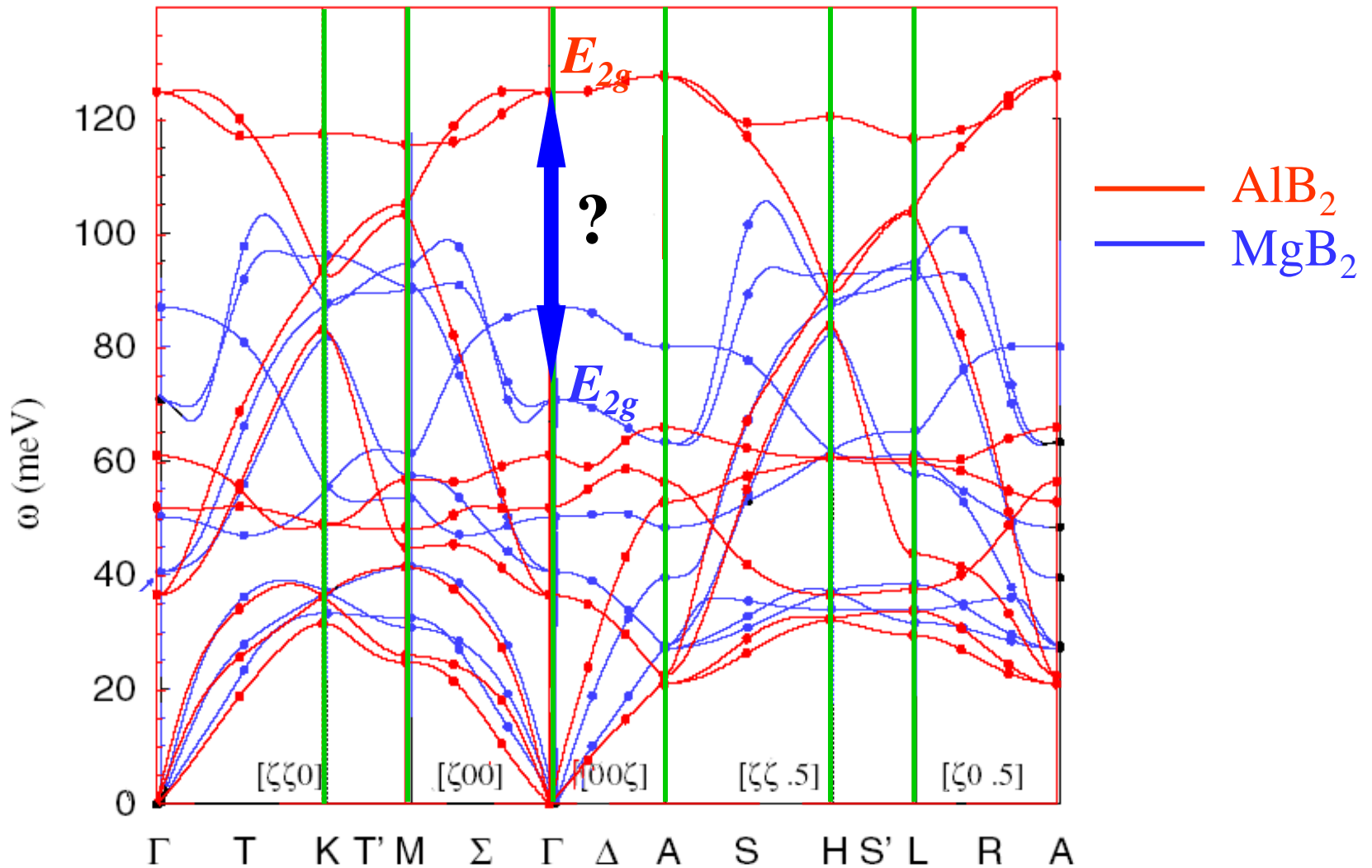


Phonon softening \leftrightarrow e-ph coupling strength

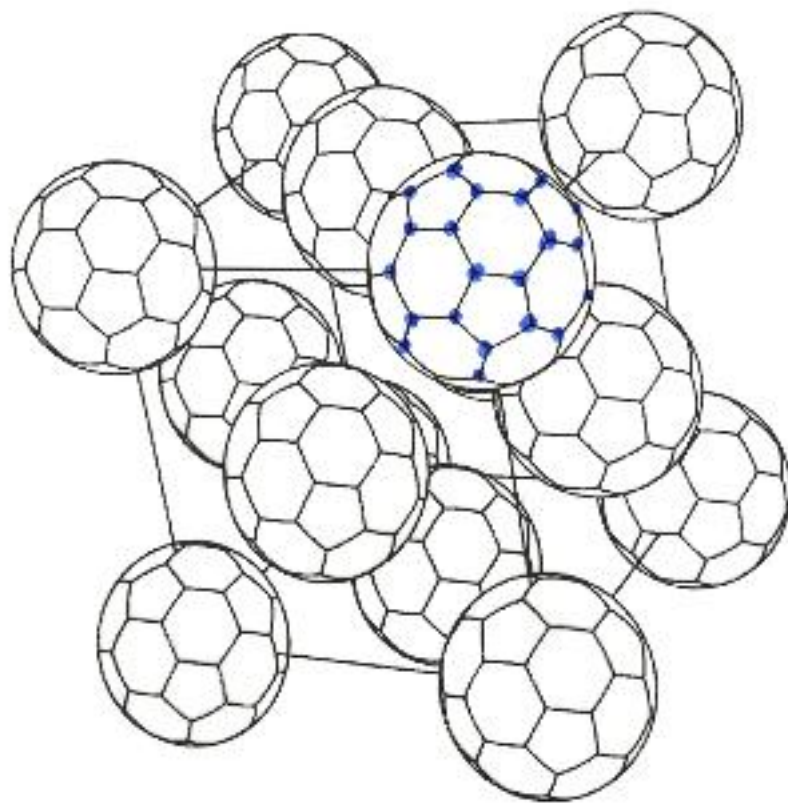
E_{2g} phonon in MgB_2 and AlB_2



E_{2g} phonon in MgB_2 and AlB_2

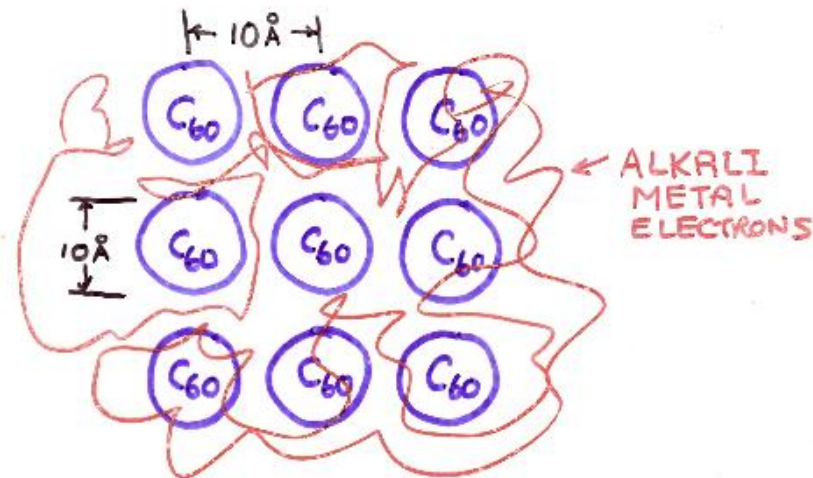


• CARBON ATOMS



SOLID C_{60}

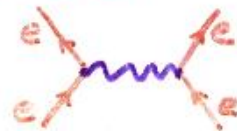
"STANDARD MODEL"



ELECTRON-PHONON SCATTERING



PAIRING



PHONONS
(MOSTLY INTRABALL)

SUPERCONDUCTIVITY (HEBARD *et al*
1991)

$$\frac{2\Delta}{k_B T_c} = 3.53 \quad (\text{BCS})$$

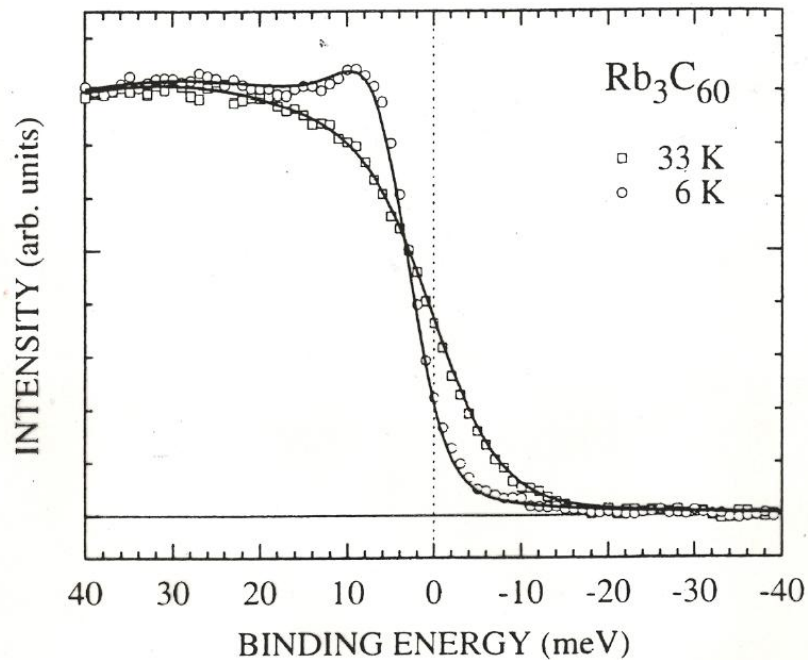


FIG. 4. Photoemission spectra of Rb_3C_{60} at 33 K (squares) and at 6 K (circles). The data are modeled (solid lines) with, respectively, a Fermi-Dirac function at 33 K and a BCS function with a gap $\Delta = 4.4$ meV, broadened by the resolution functions found for the Pt reference.

(SAME FOR K_3C_{60} ; $\Delta = 2.9$ meV)

HESPER ET AL

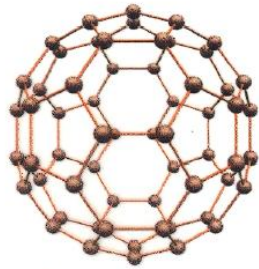
WE FIND THAT FOR C₆₀ THAT THE
ELECTRON-PHONON PARAMETER IN BCS $\lambda \sim NV$

THEREFORE TO GET HIGHER T_c's, WE :

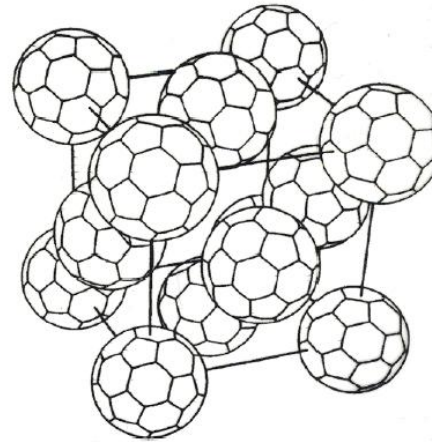
CAN INCREASE "N" WITH CARRIERS BY DOPING OR BAND
STRUCTURE [e.g. S. SAITO USING d-ELECTRON EFFECTS]
OR

CAN INCREASE "V" BY INCREASING THE "CURVATURE"
GRAPHITE → NANOTUBE → C₆₀ → C₃₆ → ?

Possible Crystal Structure



$C_{60} (I_h)$



FCC



$C_{36} (D_{6h})$



<u>Stacking</u>	<u>Structure</u>
ABAB	hexagonal
ABCABC	rhombohedral

PREDICT

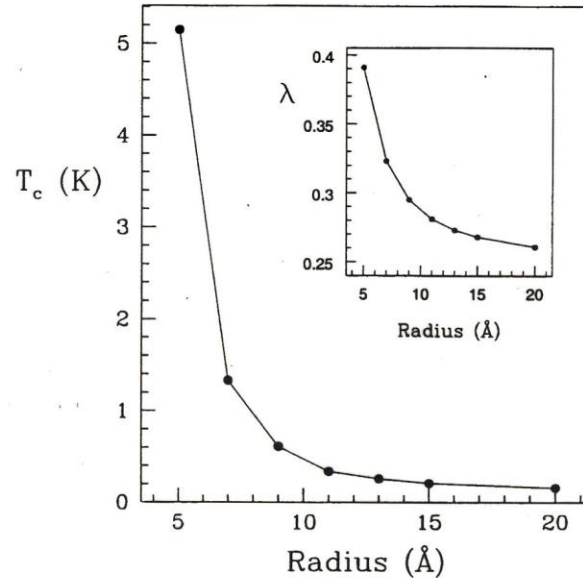
Grossman, Cote, Louie, Cohen, 1998

T_c (K-doped C_{36} solid) $\approx 6 T_c$ (K-doped C_{60} solid)
 $\approx 100K$

Electron-Phonon Coupling and Superconductivity in Carbon Nanotubes

THEORY:

[L. X. Benedict, V. H. Crespi, S. G. Louie and M. L. Cohen, PRB 52, 14935 (1995)]

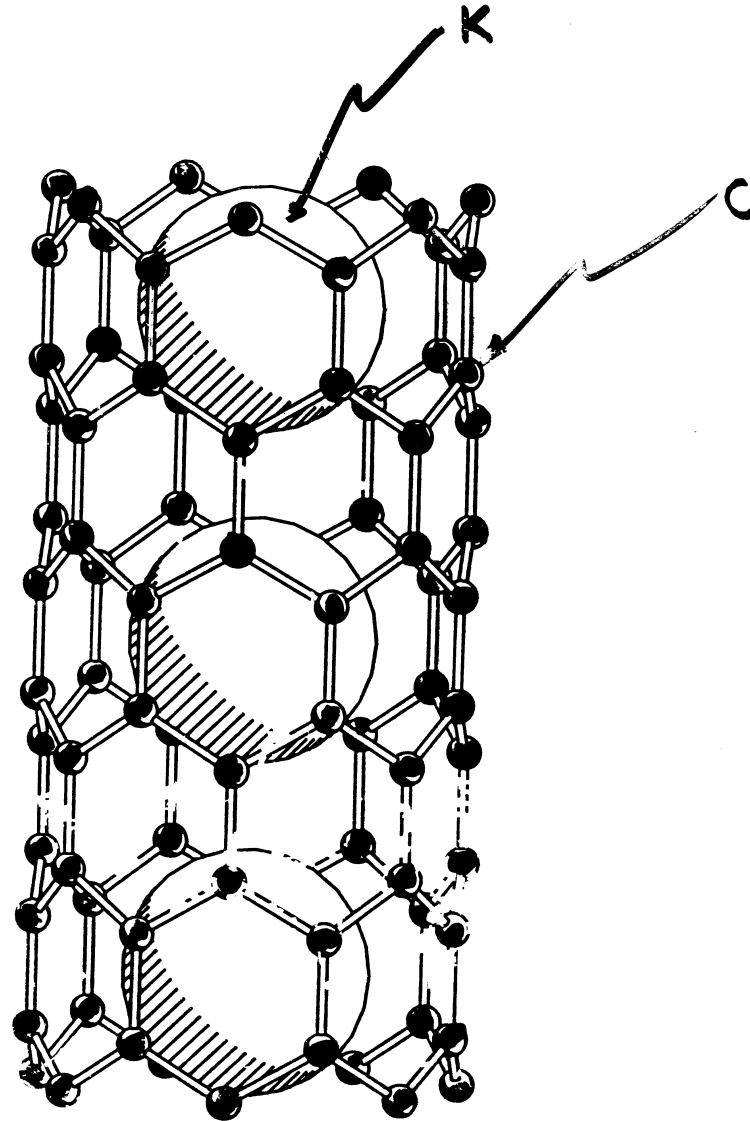


- Large curvature of small diameter tubes leads to enhanced λ .
- T_c can be in the range of 10-20 degrees Kelvin for diameter $d < 5$ Å.

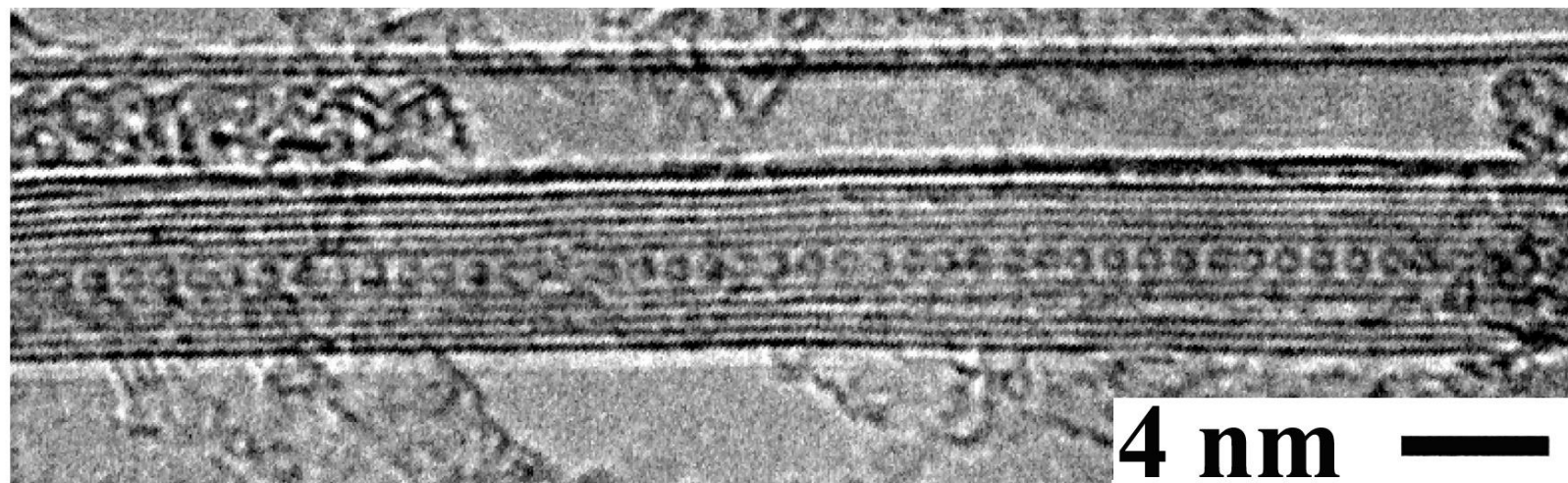
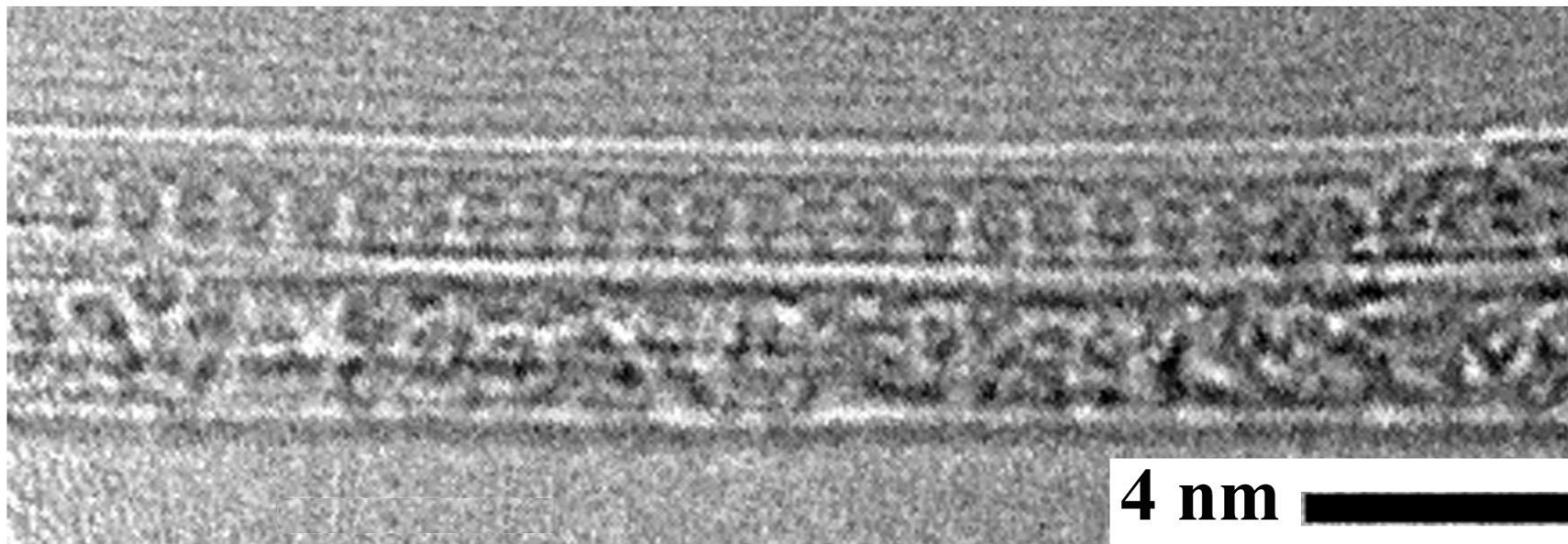
EXP:

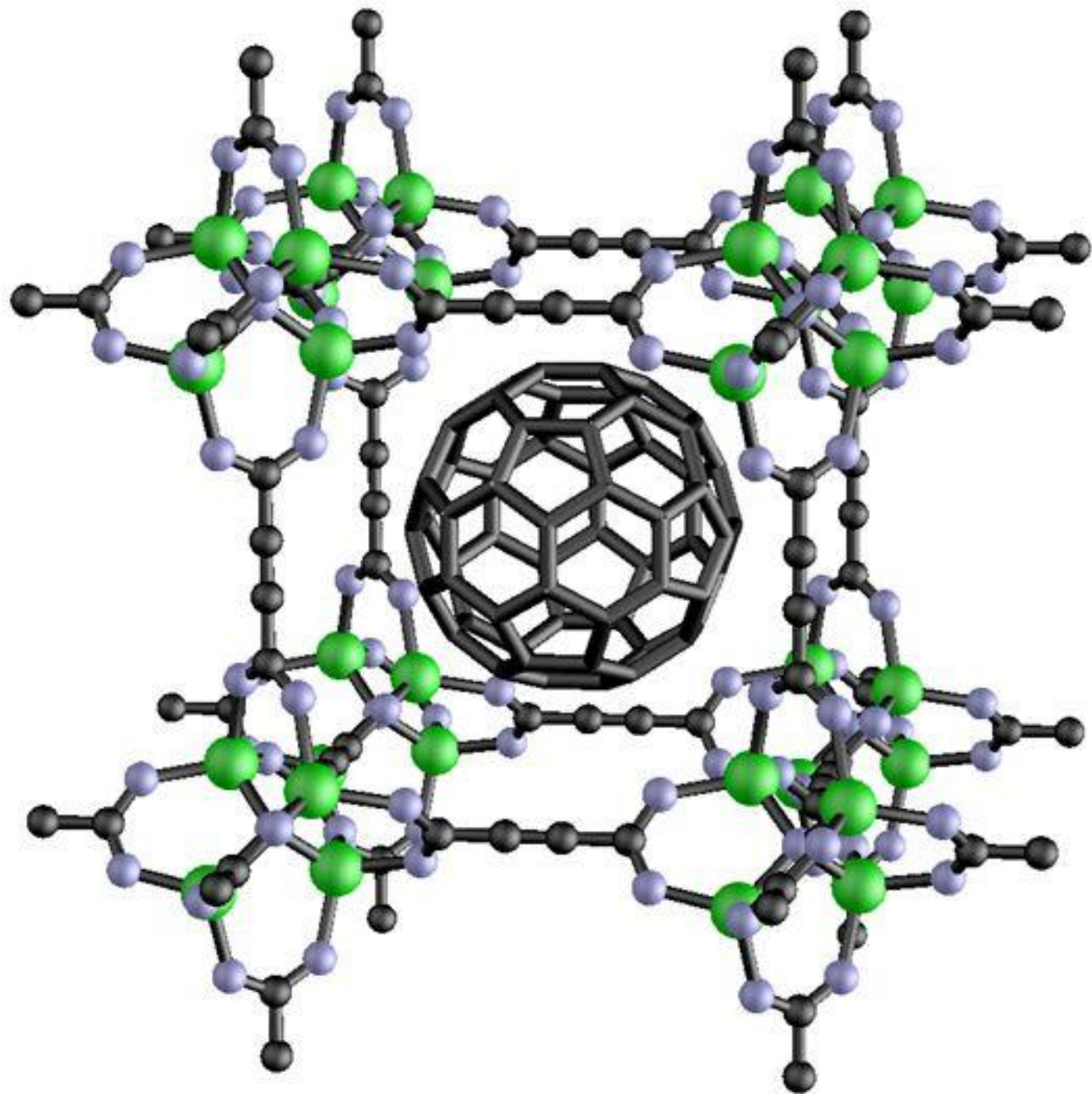
Z.K. TANG *et al*, Science 292, 2462 (2001)

K IN NANOTUBE



BN/C₆₀ Peapods





T_c formulas

$$T_c = 1.14 \omega_{ph} \exp\left(\frac{-1}{N(0)V}\right) \quad \text{BCS, 1957}$$

$$T_c = \frac{T_D}{1.45} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right) \quad \text{McMillan, 1968}$$

$$T_c = \frac{\langle \omega \rangle_{\log}}{1.20} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right) \quad \text{for } \lambda < 1.5$$

$$T_c = 0.183 \sqrt{\lambda \langle \omega^2 \rangle} \quad \text{for } \lambda > 10, \mu^* = 0 \quad \text{Allen and Dynes, 1975}$$

$$\lambda \equiv 2 \int_0^{\omega_{\max}} \alpha^2 F(\omega) \omega^{-1} d\omega$$

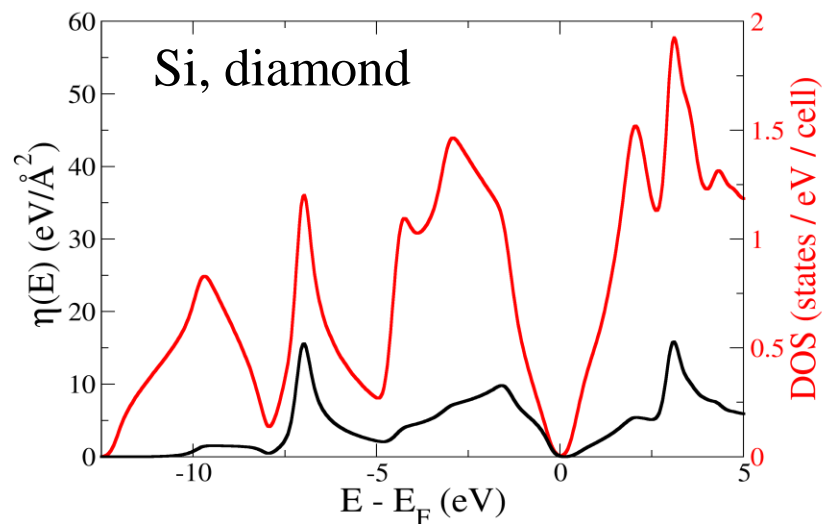
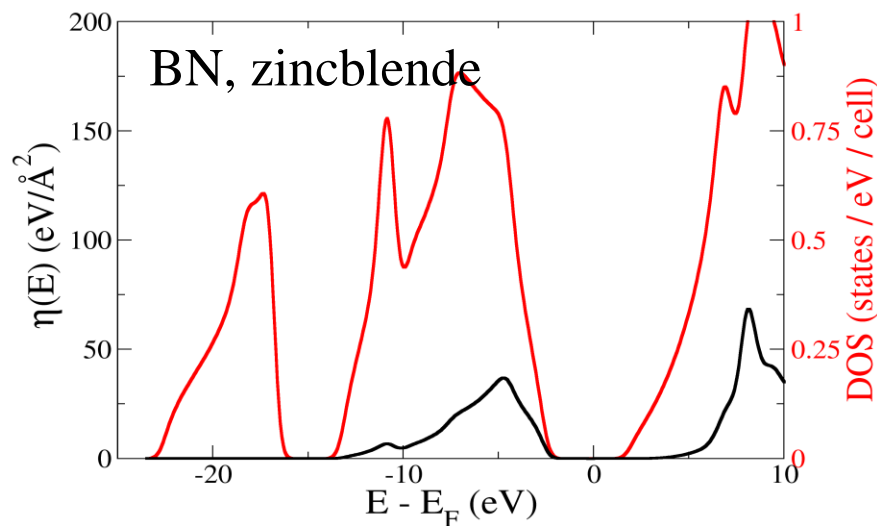
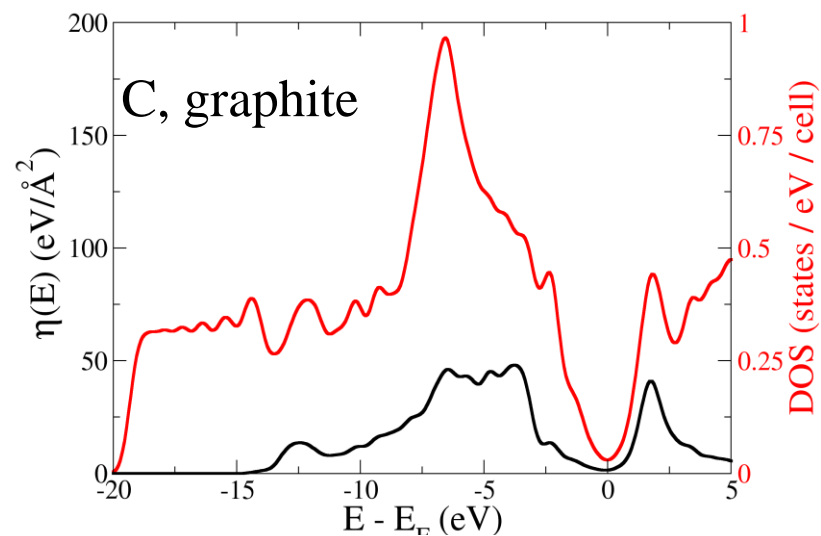
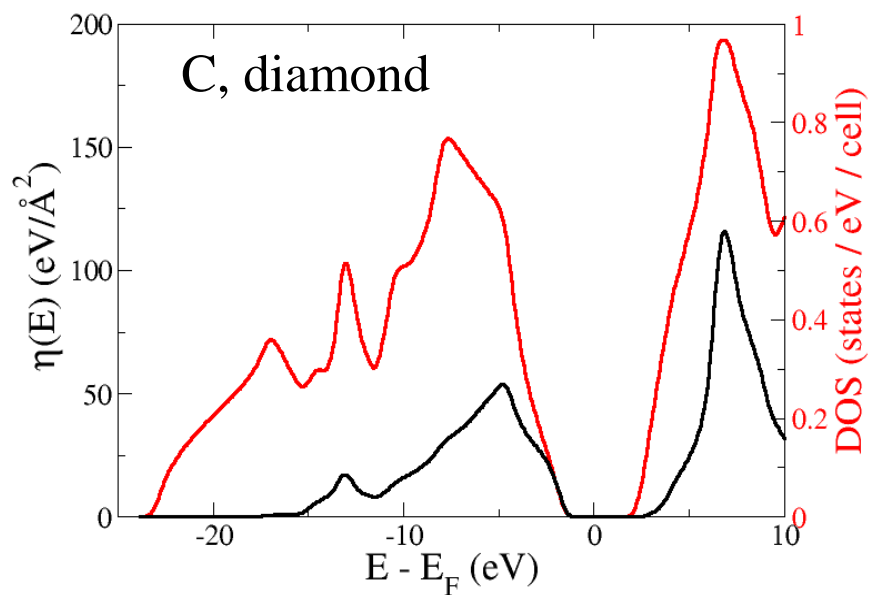
+ anisotropic electrons, anharmonic phonons, etc...

ELECTRON-PHONON COUPLING

$$\lambda \langle \omega^2 \rangle = \sum_i \frac{\eta_i}{M_i}$$

SO λ CAN BE VIEWED AS THE RATIO OF AN ELECTRONIC SPRING CONSTANT η AND A LATTICE SPRING CONSTANT

Numerical results



Values of η

	η (eV/Å ²)	$0.183\sqrt{\lambda\langle\omega^2\rangle}$ (K)	EXP
C (diamond)*	54	290	~ 10
C (graphite)*	48	270	?
BN*	36	240	?
Si*	10	82	~10

*at peak of $\eta(E)$

Strong coupling limit

$$T_c \leq 0.183 \sqrt{\lambda \langle \omega^2 \rangle}$$

electron-phonon coupling strength

Or the electronic spring constant / ionic mass

$$\lambda \sim \frac{\Omega_{ph}^2 - \omega_{ph}^2}{\omega_{ph}^2}$$

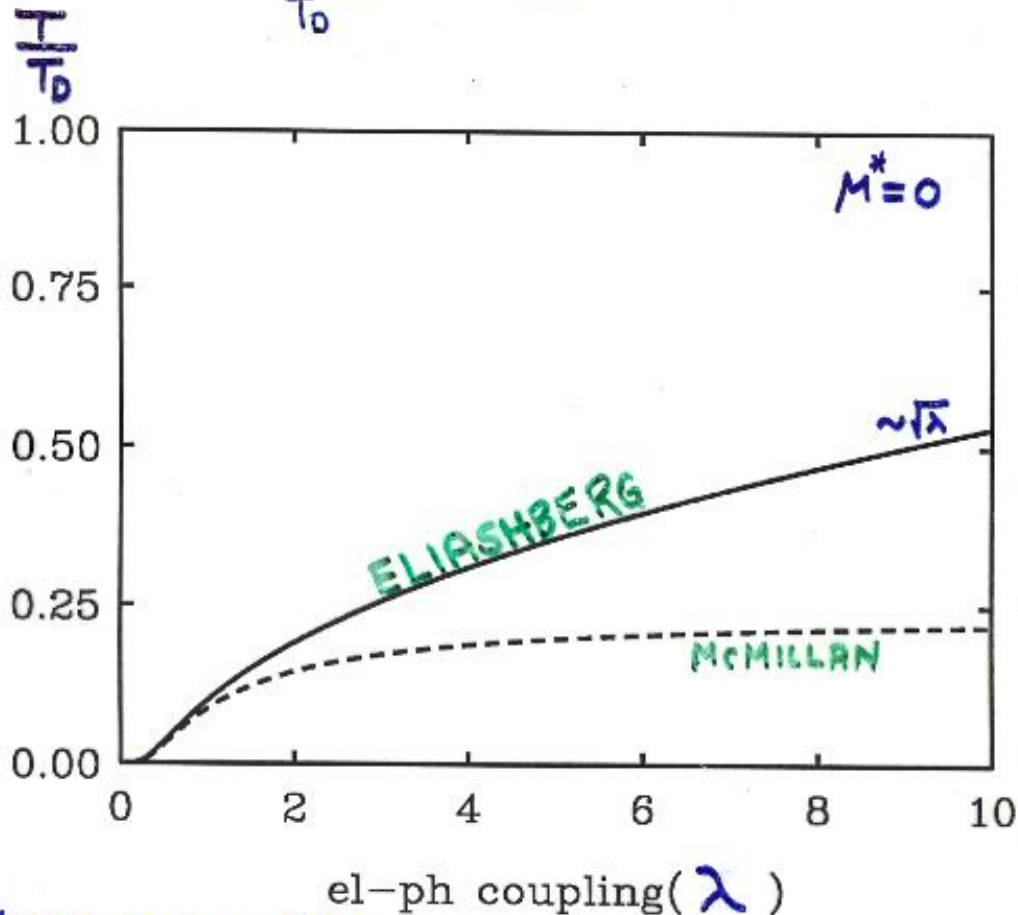
$$\frac{\eta}{M}$$

$$T_c \leq \alpha \sqrt{\Omega_{ph}^2 - \omega_{ph}^2} \leq \alpha \Omega_{ph}$$

stability of bare lattice

McMILLAN 1968

$$\frac{T_c}{T_0} \approx 0.69 e^{-\frac{1}{\lambda^* - \mu^*}}$$



Kresin-Barbee-Cohen

$$\frac{T_c}{\langle \omega \rangle} = 0.26 (e^{2/\lambda} - 1)^{-1}$$

BEYOND BCS MODEL (FREQUENCY DEPENDENCE)

$\Delta, V, N \dots$ are \mathbf{k} and ω dependent

$$\Delta(\epsilon) = - \int_{-\infty}^{\infty} \frac{\Delta(\epsilon') K(\epsilon, \epsilon') \tanh \beta \frac{\epsilon'}{2}}{\epsilon'} d\epsilon'$$

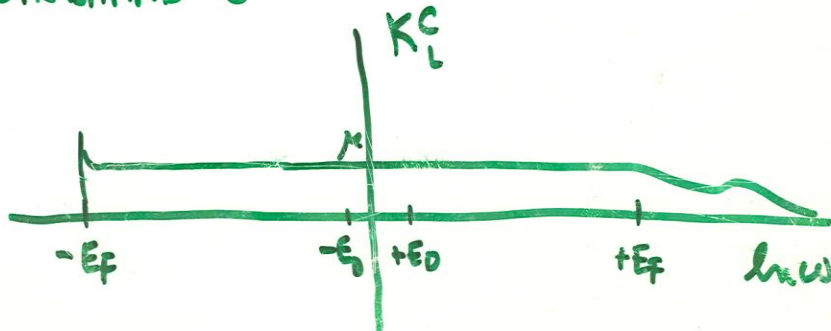
$$K(\epsilon, \epsilon') = \frac{\Omega}{2(2\pi)^2} \frac{m}{\hbar^2 k_F} \int_{q_{\min}}^{q_{\max}} q V(q, \omega) dq$$

$$[K] = [NV] = [\lambda] - [\mu]$$

REPULSIVE COULOMB INTERACTION

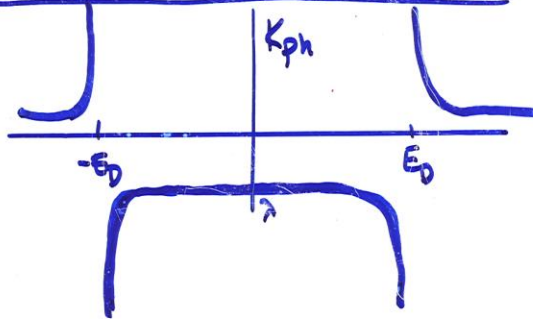
$$K^C = [\mu] \sim \Omega \int q \cdot \frac{4\pi e^2}{\Omega q^2 \epsilon(q, \omega)} dq$$

LINDHARD ϵ

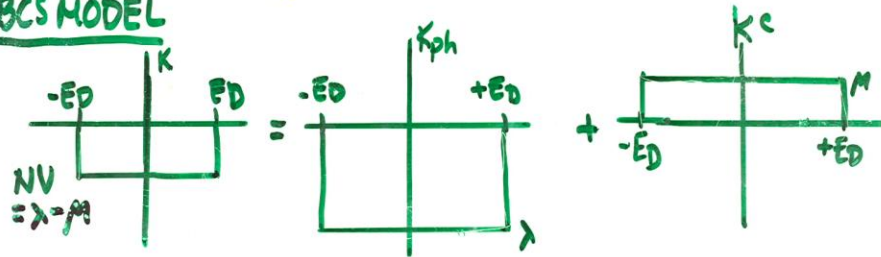


BEYOND BCS MODEL (CONT'D) (FREQUENCY DEPENDENT)

ATTRACTIVE PHONON INTERACTION

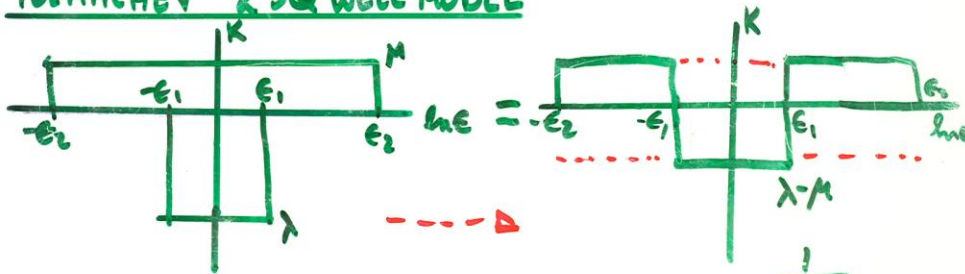


BCS MODEL



NOT APPROPRIATE FOR K_c ; GET $T_c \sim T_D e^{-\frac{1}{\lambda - M}}$

TOLMACHEV 2 SQ WELL MODEL



$E_1 \sim E_D$
 $E_2 \sim E_F$

GET $T_c \sim T_D e^{-\frac{1}{\lambda - M^*}}$
 $M^* = \frac{M}{1 + \mu \ln \epsilon_2 / \epsilon_1}$

BEYOND BCS MODEL (CONT'D) (FREQUENCY DEPENDENCE)

ISOTOPE EFFECT

BCS MODEL $T_c \sim T_D \underbrace{e^{-\frac{1}{\lambda \mu^*}}}_{\text{const}} \sim \frac{1}{T_M}$

$$T_c \sim M^{-\alpha} \quad \alpha = \frac{1}{2} \quad \text{BCS MODEL}$$

2 SQ WELL MODEL

$$T_c \sim T_D e^{-\frac{1}{\lambda \mu^*}}$$

$$\alpha = \frac{1}{2} \left[1 - \left(\frac{\mu^*}{\lambda \mu^*} \right)^2 \right] \Rightarrow \alpha \leq \frac{1}{2}$$

FOR $\mu^* = \frac{\lambda}{2}$; $\alpha = 0$

WAVEVECTOR DEPENDENCE

TOTAL DIELECTRIC FUNCTION

$\epsilon_T(q, \omega)$ can include electron-electron and electron-phonon effects

e.g. $\frac{V_{\mathbf{q}}}{k_{\mathbf{q}}} = \frac{V_{\mathbf{q}}}{\epsilon_T(q, \omega)} = \frac{4\pi e^2}{R q^2} \frac{1}{\epsilon_e + \epsilon_p}$

$$\frac{1}{\epsilon_e + \epsilon_p} = \frac{1}{\epsilon_e} - \frac{\epsilon_p}{\epsilon_e(\epsilon_e + \epsilon_p)}$$

↑ ↑

COULOMB

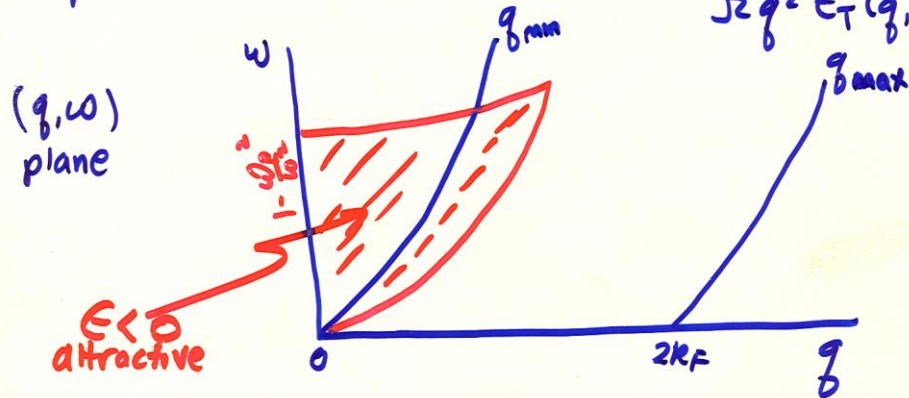
e.g. BARDEEN-PINES



BEYOND BCS MODEL (WAVEVECTOR AND FREQUENCY DEPENDENCE)

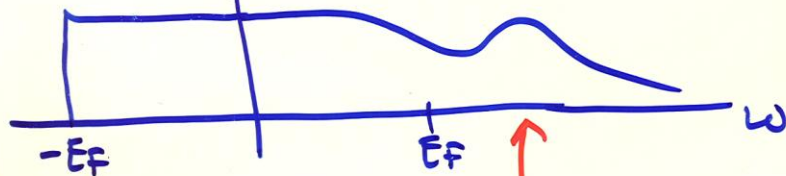
$$K(\omega) \sim \int_{q_{\min}}^{q_{\max}} q V(q, \omega) dq$$

$V(q, \omega)$ can be total interaction = $\frac{4\pi e^2}{\int q^2 \epsilon_T(q, \omega)}$

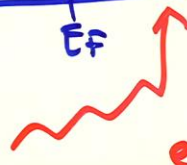


$\hbar\omega = |\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}|$ energy transfer
 $\vec{q} = \vec{k}' - \vec{k}$ "momentum" transfer

FOR $\epsilon_{\text{LINDHARD}}$ $K(\omega) > 0$ (repulsive) for all ω



plasmon



in FEG plasmon exchange is ineffective

$$\frac{\text{HIGH } T_c \Rightarrow}{T_c \sim E_0 f(\lambda_0)}$$

WEAK COUPLING

E_0 large
 $f(\lambda_0)$ small

(electronic
mechanisms)

STRONG COUPLING

E_0 small
 $f(\lambda_0)$ large

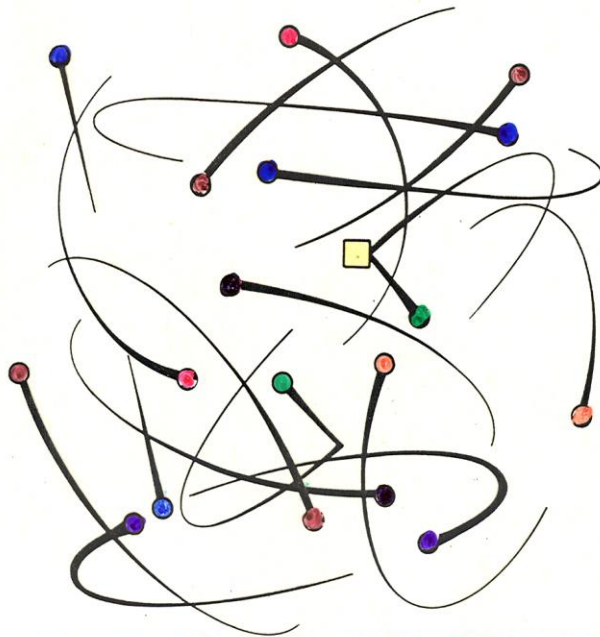
(phonon
and
low ω
mechanisms
spin fluctuations)

IMPORTANT TO KNOW
(FROM EXPERIMENT) WHICH
MODEL APPLIES

exp: $\frac{2\Delta}{kT_c}$, tunneling, $C_v(T)$...

PAIRING

BCS PAIRS : $\frac{d_{\text{PAIR MATES}}}{d_{\text{PAIRS}}} \gg 1$



"BOSON" LIKE PAIRS $\frac{d_{\text{PAIR MATES}}}{d_{\text{PAIRS}}} \ll 1$



FOR Y-Ba-Cu-O
PERHAPS? $\frac{d_{\text{PAIR MATES}}}{d_{\text{PAIRS}}} \sim 1$

Superconductivity in diamond

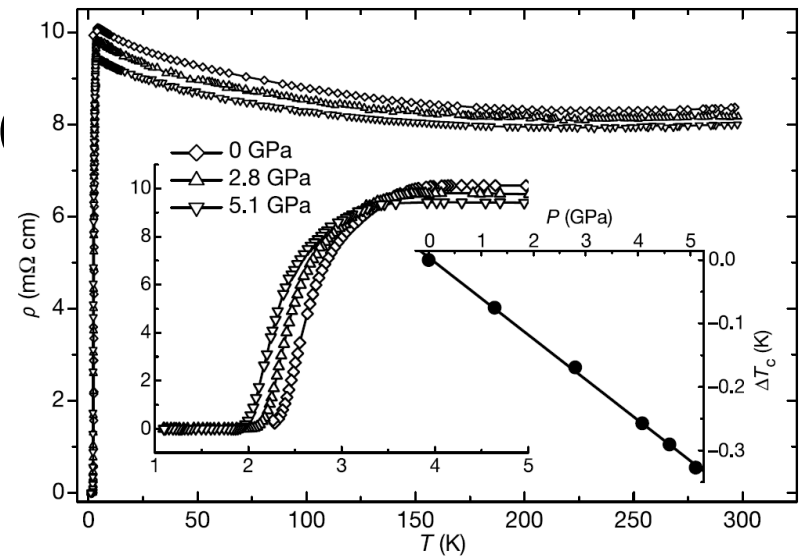
E. A. Ekimov¹, V. A. Sidorov¹, E. D. Bauer², N. N. Mel'nik³, N. J. Curro²,
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ARTICLES

Quasiparticle dynamics in graphene

AARON BOSTWICK¹, TAISUKE OHTA^{1,2}, THOMAS SEYLLER³, KARSTEN HORN² AND ELI ROTENBERG^{1*}

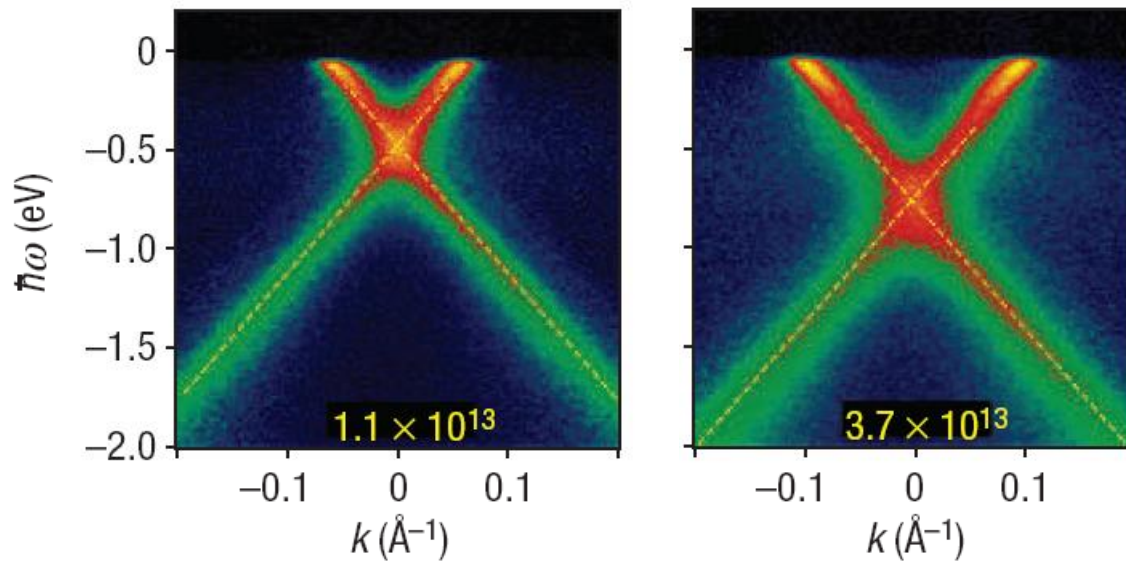
¹Advanced Light Source, E. O. Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

²Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

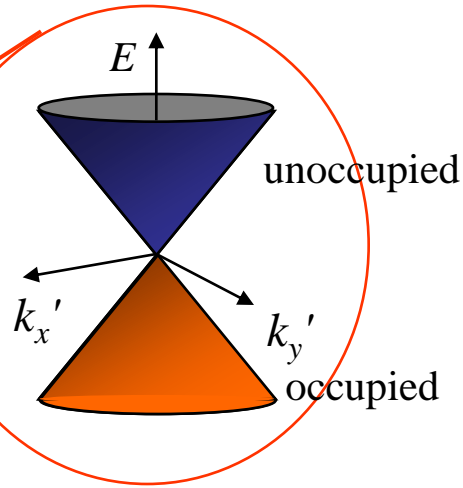
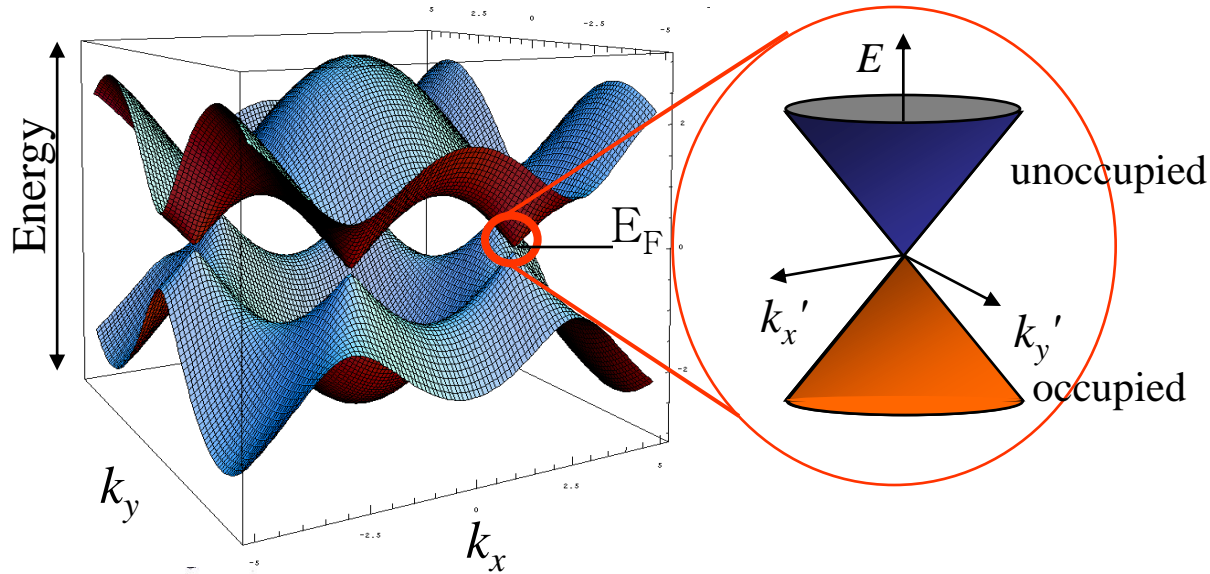
³Institut für Physik der Kondensierten Materie, Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Straße 1, D-91058 Erlangen, Germany

*e-mail: erotenberg@lbl.gov

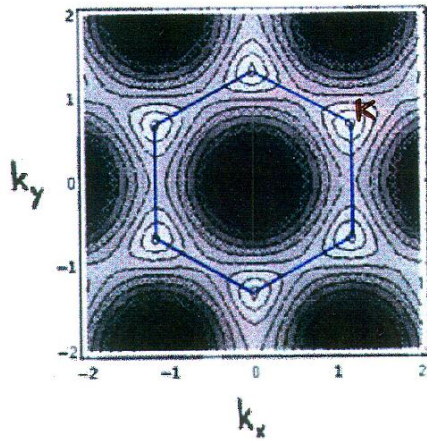
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Graphene Electronic Structure



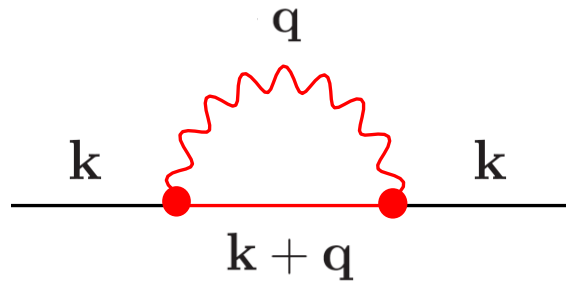
$$E = \pm v_F |k'|$$



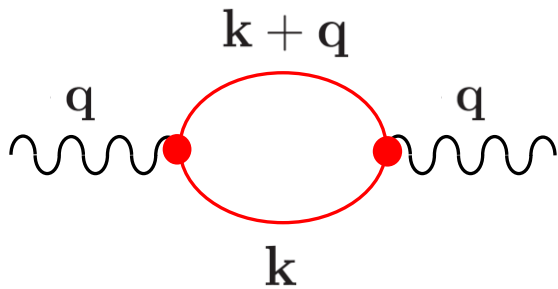
$$E^2 = p^2 c^2$$

2D massless Dirac fermion system

Electron and Phonon Selfenergy



$$\Sigma = i \int \frac{d^2}{(2\pi)^4} |g(1, 2)|^2 D(1 - 2) G(2)$$



$$\Pi = -2i \int \frac{d^1}{(2\pi)^4} |g(1, 2)|^2 G(1) G(2)$$

Wannier Representation

$$g_{mn}^\nu(\mathbf{k}, \mathbf{q}) = \langle m\mathbf{k} + \mathbf{q} | \Delta V_{\mathbf{q}\nu} | n\mathbf{k} \rangle$$

$$|n\mathbf{k}\rangle = \frac{1}{N_e} \sum_{m\mathbf{R}_e} e^{i\mathbf{k}\cdot\mathbf{R}_e} U_{mn,\mathbf{k}}^\dagger |m\mathbf{R}_e\rangle$$

$$\Delta_{\mathbf{q}\nu} V(\mathbf{r}) = \sum_{\mathbf{R}_p} \exp(i\mathbf{q}\cdot\mathbf{R}_p) \sum_{\kappa\alpha} M_\kappa^{-\frac{1}{2}} e_{\mathbf{q}\nu}(\kappa\alpha) \Delta_{\kappa\alpha,\mathbf{R}_p} V(\mathbf{r})$$

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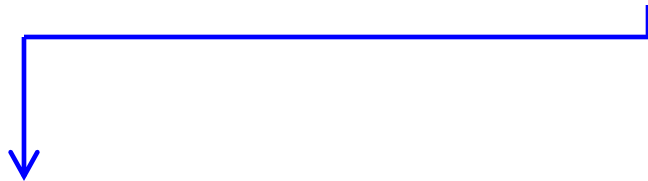
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$$\underbrace{g(\mathbf{k}, \mathbf{q})}_{\text{Bloch}} = \sum_{\mathbf{R}_e, \mathbf{R}_p} e^{i\mathbf{k} \cdot \mathbf{R}_e} e^{i\mathbf{q} \cdot \mathbf{R}_p} u_{\mathbf{q}} U_{\mathbf{k}+\mathbf{q}} \underbrace{g(\mathbf{R}_e, \mathbf{R}_p)}_{\text{Wannier}} U_{\mathbf{k}}^\dagger$$

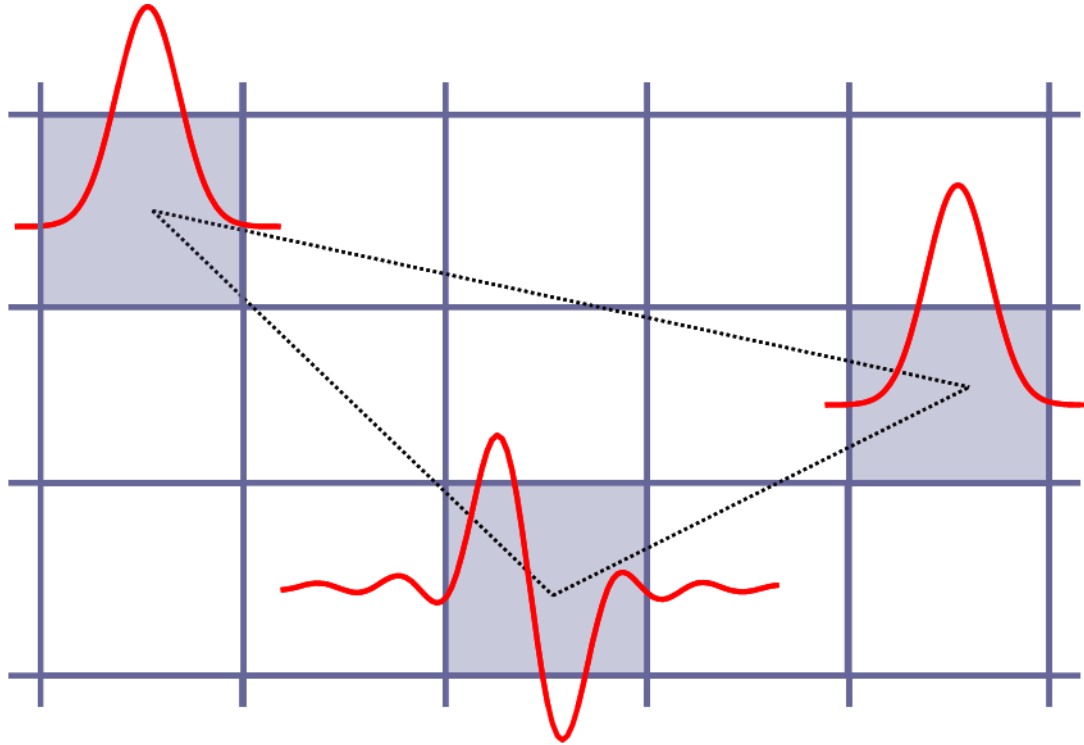
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$$\langle m\mathbf{0}_e | \Delta_{\kappa\alpha, \mathbf{R}_p} V(\mathbf{r}) | n\mathbf{R}_e \rangle$$

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HAROLD WEINSTOCK

JAN 28, 2007

I have proposed that we take steps to videotape the entire workshop.

My colleagues are of 2 minds regarding this suggestion: one is that people will keep their best ideas to themselves; the other is that with a recording of our deliberations, there will be unambiguous proof of the genesis of any idea that leads us to the Promised Land. I clearly support the latter view, but I welcome your comments on this issue.

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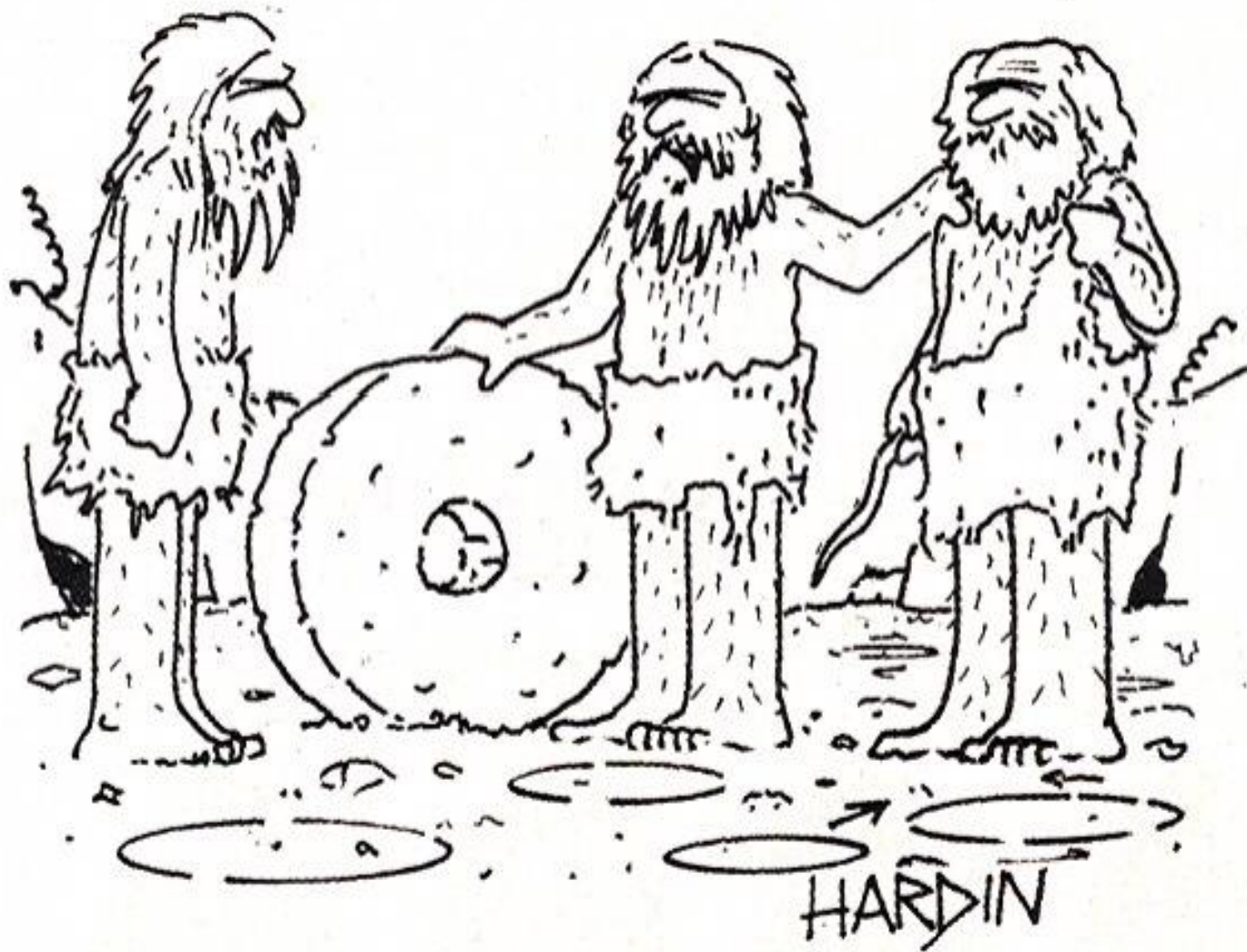
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UNLIKE MOSES, I’M GOING IN WITH THEM!



“To be honest, I never would have invented the wheel if not for Urg’s groundbreaking theoretical work with the circle.”

World Year of Physics 2005

Einstein in the 21st Century



Help make 2005 another *Miraculous Year!*

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www.physics2005.org

Einstein's Thesis Proposals

1. Proposed method for measurement of “c”, using interferometer. Proposed to Prof. Dr. Weber (1900)

(Comment: This was later done by A. A. Michelson who did the experiment and became the first American to be awarded the Nobel Prize [1907])

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REJECTED

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(Comment: very important for electronics)

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3. Performed theoretical work on the thermal conductivity of solids. Wrote up as dissertation. Submitted to Prof. Dr. Weber.

(Comment: again important for electronics and heat applications)

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REJECTED (written on wrong kind of paper?)

4. Performed theoretical work on extension of intermolecular forces from liquids to gases. Wrote up as dissertation. Presented to Prof. Dr. Kleiner.

(Comment: a fundamental theory of how matter behaves)

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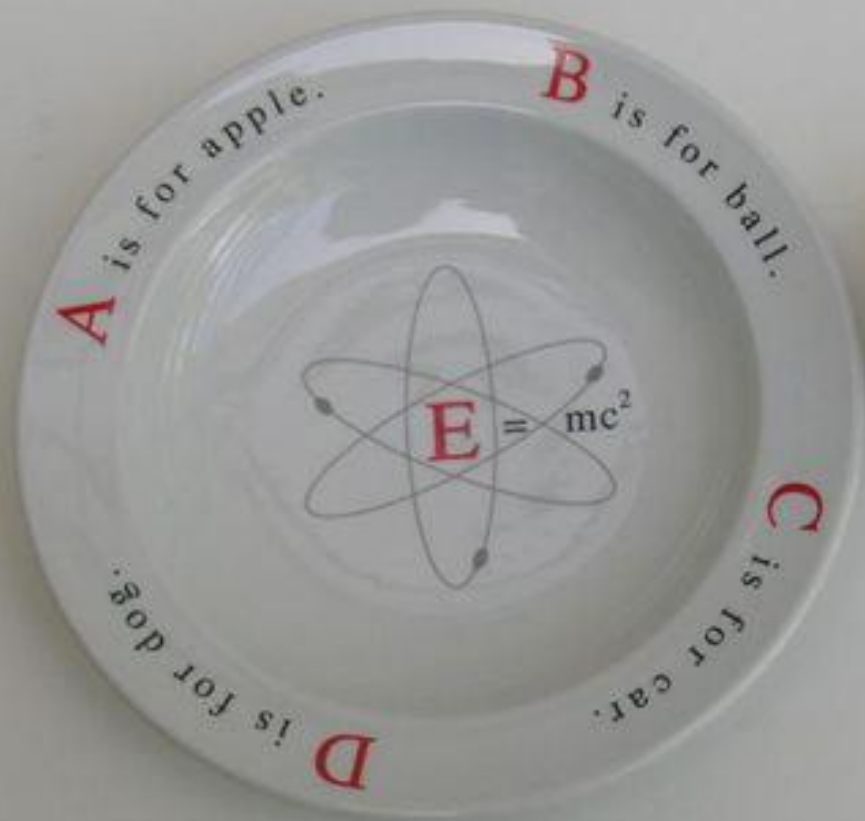
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(Comment: this later led to Einstein's famous equation)



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6. Performed theoretical work on measuring the molecular dimensions of sugar molecules. Wrote up as dissertation. Submitted to Profs. Kleiner and Burkhardt.

(Comment: important to prove the existence of atoms and molecules)

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REJECTED (too short, 17 pages)

7. Added **one sentence** and resubmitted theoretical work on measuring the molecular dimensions of sugar molecules. Submitted to Profs. Kleiner and Burkhardt.

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ACCEPTED (1905) !

ALBERT EINSTEIN

"The most valuable tool of the theoretical physicist is his wastebasket."

THE END