Tuesday, Sep 22, 2015

10:00AM New Phases and Emergent Phenomena in Correlated Materials with Strong Spin-Orbit Coupling

Sergey Savrasov (UCD) - *Theory of electron-pohonon superconductivity in Cu doped Bi2Se3 topological insulator*

Theory of electron-pøhonon superconductivity in Cu doped Bi2Se3 topological insulator

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KITP, September 22, 2015

Contents

- **Electron-Phonon Interaction and Unconventional Pairing**
- **Superconductivity in $Cu_xBi_2Se_3$**
- **Calculations of phonons and electron-phonon interactions in $Cu_xBi_2Se_3$**
- **Effects of Coulomb interaction: μ^* and spin fluctuations**
- **Conclusion**

Introduction

▪Recent developments in the theories of TIs have been extended to superconductors described by Bogoluibov-de Genne Hamiltonians:

Such excited phenomena as topologically protected surface states (Majorana modes) have been discussed (Schynder et al. PRB2008, Kitaev, arXiv 2009, Qi et al., PRL 2009). These have potential uses in topologically protected quantum computation

Need for unconventional (non-s-wave like) symmetry of superconducting gap that is now of odd-parity which would realize a topological superconductor.

Not many odd-parity superconductors exist in Nature! One notable example is $SrRu_2O_4$ where not phonons but ferromagnetic spin fluctuations mediate superconductivity.

Why electron-phonon superconductors are all s-wave like?

Are there examples in nature whether electron-phonon coupling can generate a pairing state with l>0 angular momentum?

BCS with General Pairing Symmetry

BCS gap equation for T_c

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} W(\mathbf{k}\mathbf{k}')\Delta(\mathbf{k}')\tanh\left(\frac{\epsilon_{\mathbf{k}'}}{2T_c}\right)/2\epsilon_{\mathbf{k}'}$$

where $W(\mathbf{k}\mathbf{k}')$ is the pairing interaction (always attractive, negative in electron-phonon theory, but can be sign changing in other theories)

To solve it, assume the existence of orthonormalized polynomials at a given energy surface (such, e.g., as spherical harmonics in case of a sphere)

$$\frac{1}{N(\varepsilon)}\sum_{\mathbf{k}} \eta_a(\mathbf{k})\eta_b(\mathbf{k})\delta(\epsilon_{\mathbf{k}} - \varepsilon) = \delta_{ab}$$

Choice of Fermi surface polynomials

Elegant way has been proposed by Allen: Fermi surface harmonics

PHYSICAL REVIEW B VOLUME 13, NUMBER 4 15 FEBRUARY 1976

Fermi-surface harmonics: A general method for nonspherical problems. Application to Boltzmann and Eliashberg equations

Philip B. Allen*
Department of Physics, State University of New York, Stony Brook, New York 11794
(Received 15 October 1975)

Tight-binding harmonics for cubic/hexagonal lattices are frequently used

PHYSICAL REVIEW B VOLUME 37, NUMBER 4 1 FEBRUARY 1988

Stability of anisotropic superconducting phases in UPt_3

W. Putikka and Robert Joynt
Physics Department, 1150 University Avenue, University of Wisconsin-Madison, Madison, Wisconsin 53706
(Received 26 October 1987)

TABLE I. Basis functions for the various representations of D_6. The interaction can be decomposed into sums of products of these functions.

Representation	Function
A_{1g}	$\phi_k=\frac{1}{\sqrt{3}}\cos\left(\frac{ck_z}{2}\right)\left[\cos\left(\frac{\sqrt{3}ak_y}{3}\right)+\cos\left(\frac{ak_x}{2}+\frac{\sqrt{3}ak_y}{6}\right)+\cos\left(\frac{ak_x}{2}-\frac{\sqrt{3}ak_y}{6}\right)\right]$
B_{1g}	$\psi_k=\frac{1}{\sqrt{3}}\sin\left(\frac{ck_z}{2}\right)\left[\sin\left(\frac{\sqrt{3}ak_y}{3}\right)+\sin\left(\frac{ak_x}{2}-\frac{\sqrt{3}ak_y}{6}\right)-\sin\left(\frac{ak_x}{2}+\frac{\sqrt{3}ak_y}{6}\right)\right]$
E_{1g}	$\theta_k=\frac{1}{\sqrt{2}}\sin\left(\frac{ck_z}{2}\right)\left[\sin\left(\frac{ak_x}{2}+\frac{\sqrt{3}ak_y}{6}\right)+\sin\left(\frac{ak_x}{2}-\frac{\sqrt{3}ak_y}{6}\right)\right]$
	$\xi_k=\frac{1}{\sqrt{6}}\sin\left(\frac{ck_z}{2}\right)\left[2\sin\left(\frac{\sqrt{3}ak_y}{3}\right)+\sin\left(\frac{ak_x}{2}+\frac{\sqrt{3}ak_y}{6}\right)-\sin\left(\frac{ak_x}{2}-\frac{\sqrt{3}ak_y}{6}\right)\right]$

Expanding superconducting energy gap and pairing interaction

$$\Delta(\mathbf{k}) = \sum_{\alpha} \Delta_a(\epsilon_{\mathbf{k}})\eta_a(\mathbf{k}) \qquad \Delta_a(\varepsilon) = \frac{1}{N(\varepsilon)} \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}} - \varepsilon)\Delta(\mathbf{k})\eta^*_{\alpha}(\mathbf{k})$$

$$W(\mathbf{k}\mathbf{k}') = \sum_{\alpha\beta} W_{ab}(\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}'})\eta_a(\mathbf{k})\eta_b(\mathbf{k}')$$

$$W_{ab}(\varepsilon\varepsilon') = \frac{1}{N(\varepsilon)N(\varepsilon')} \sum_{\mathbf{k}\mathbf{k}'} \delta(\epsilon_{\mathbf{k}} - \varepsilon)\eta^*_a(\mathbf{k})W(\mathbf{k}\mathbf{k}')\eta_b(\mathbf{k}')\delta(\epsilon_{\mathbf{k}'} - \varepsilon')$$

The gap equation becomes

$$\Delta_a(\varepsilon) = -\int d\varepsilon' \sum_{b} W_{ab}(\varepsilon\varepsilon')\Delta_b(\varepsilon')N(\varepsilon') \tanh\left(\frac{\varepsilon'}{2T_c}\right)/2\varepsilon'$$

In original BCS model pairing occurs for the electrons within a thin layer near Ef

$$\Delta_a(\varepsilon) = \begin{cases} \Delta_a & \text{for } -\omega_D < \varepsilon < +\omega_D \\ 0 & \text{otherwise} \end{cases}$$

$$W_a(\varepsilon\varepsilon') = \begin{cases} W_a & \text{for } -\omega_D < \varepsilon < +\omega_D \\ 0 & \text{otherwise} \end{cases}$$

This reduces the gap equation to (integral is extended over Debye frequency range)

$$\Delta_a = -N(0)\sum_b W_{ab}\Delta_b \int_{-\omega_D}^{+\omega_D} d\varepsilon' \frac{1}{2\varepsilon'} \tanh\left(\frac{\varepsilon'}{2T_c}\right)$$

Assuming crystal symmetry makes $W_{ab}=W_a\delta_{ab}$ and evaluating the integral gives

$$T_c = 1.134\omega_D e^{-1/\lambda_a} \qquad \lambda_a = -N(0)W_a$$

where the average electron-phonon coupling in a given a channel is given by the Fermi surface average of the electron-phonon coupling

$$W_a = \frac{1}{N(0)N(0)}\sum_{\mathbf{kk}'} \delta(\epsilon_{\mathbf{k}})\eta_a(\mathbf{k})W(\mathbf{kk}')\eta_a(\mathbf{k}')\delta(\epsilon_{\mathbf{k}'})$$

Finally, the superconducting state with largest λ_a will be realized.

If mass renormalizations and Coulomb interaction effects are taken into account, the T_c is determined by

$$T_c^{(a)} = 1.14\omega_D \exp\left(-\frac{1}{\lambda_a^{eff}}\right)$$

where the effective coupling constant is weakened by μ^* and renormalized

$$\lambda_a^{eff} = \frac{\lambda_a - \mu_a^*}{1 + \lambda_{s-h}}$$

Due to electronic mass enhancement like in specific heat renormalization

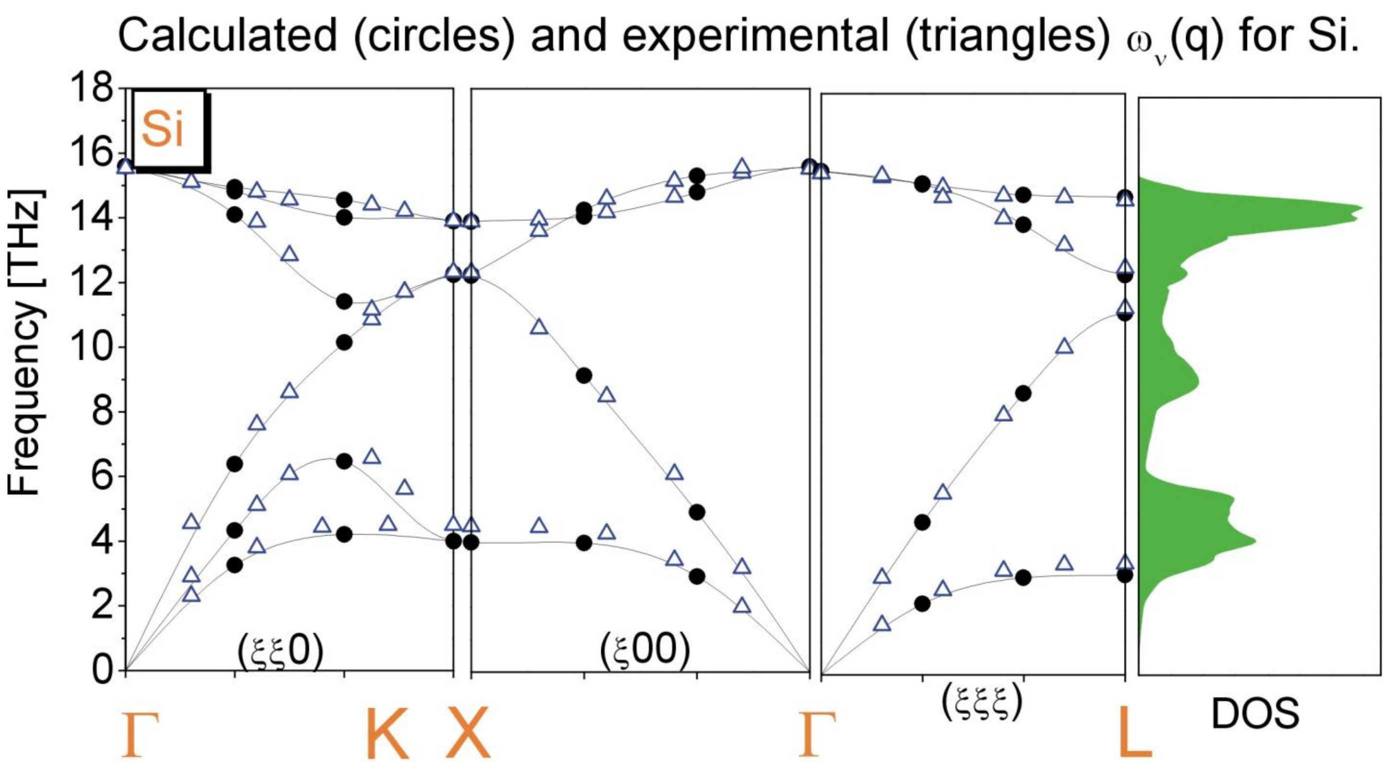
because Fermi surface averaging of the interaction includes bare DOS and $\varepsilon(\mathbf{k})$

$$\lambda_a = -W_a N(0) = -\frac{1}{N(0)} \sum_{\mathbf{k}\mathbf{k}'} \delta(\epsilon_{\mathbf{k}})\eta_a(\mathbf{k}) W(\mathbf{k}\mathbf{k}')\eta_a(\mathbf{k}')\delta(\epsilon_{\mathbf{k}'})$$

The electron-phonon matrix elements $W(\mathbf{k}\mathbf{k}')$ can be found from first principles electronic structure calculations using density functional linear response method (SS, PRL 1992)

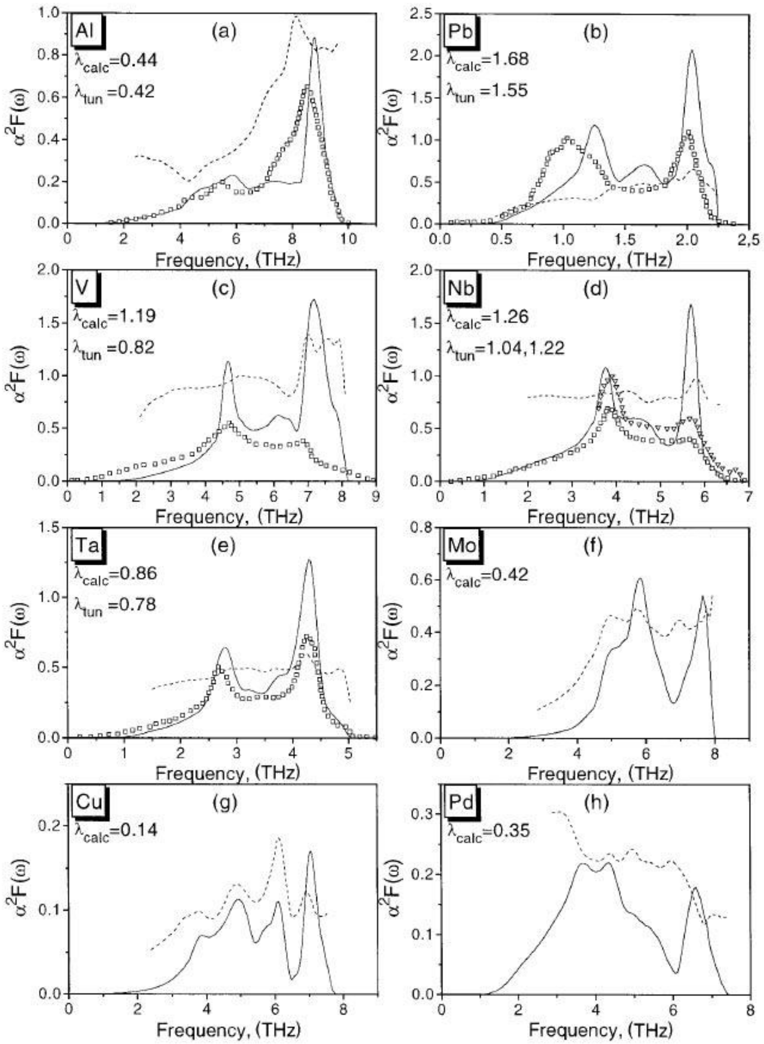
Density Functional Linear Response

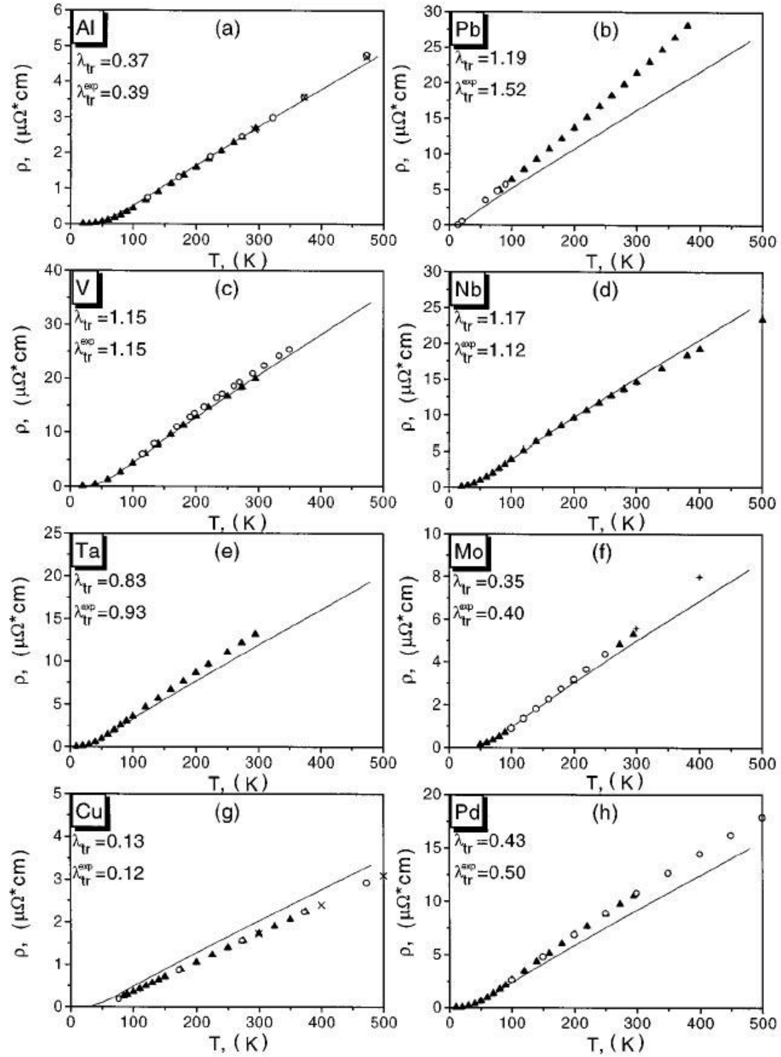
Big progress in ab initio modeling **lattice dynamics** & **electron-phonon interactions** using Density Functional Theory



(SS, PRB 1996)

Superconductivity & Transport in Metals

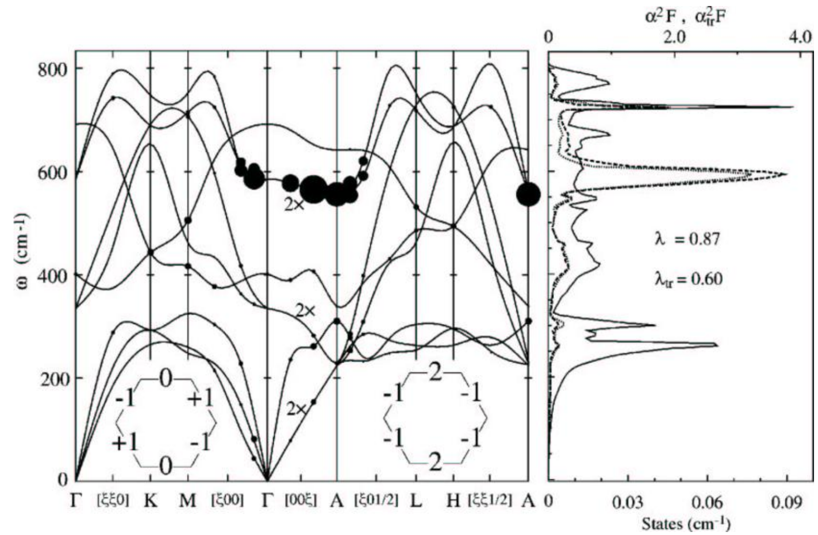




Recent Superconductors: MgB_2, LiBC, etc

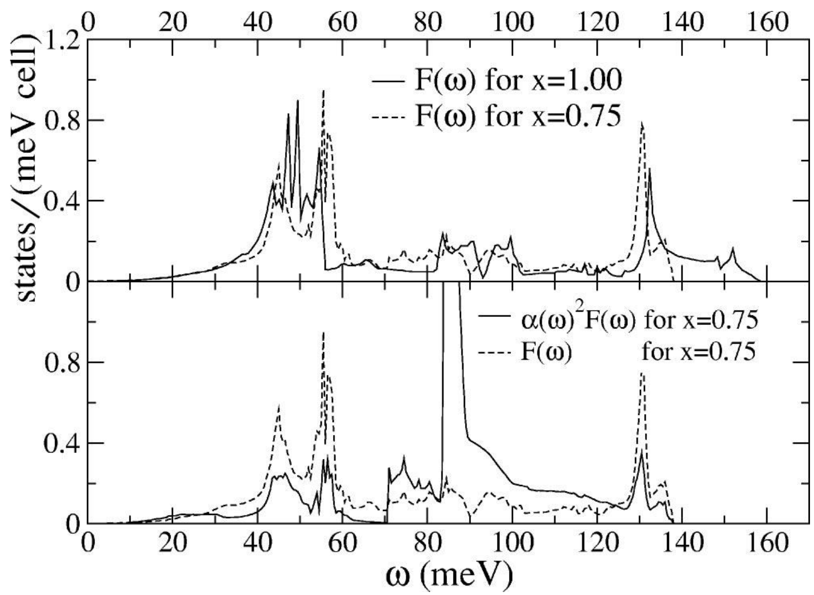
❑ Superconductivity in MgB_2 was recently studied using density functional linear response

(*after O.K. Andersen et.al. PRB **64**, 020501 (R) 2002*)



❑ Doped LiBC is predicted to be a superconductor with T_c~20 K

(*in collaboration with An, Rosner Pickett, PRB **66**, 220602(R) 2002*)



Why electron-phonon superconductors are all s-wave like?

The electron-phonon matrix elements $W(\mathbf{k},\mathbf{k}')$ appeared in the expression for λ

$$\lambda_a = -\frac{1}{N(0)}\sum_{\mathbf{kk}'}\delta(\epsilon_{\mathbf{k}})\eta_a(\mathbf{k})W(\mathbf{kk}')\eta_a(\mathbf{k}')\delta(\epsilon_{\mathbf{k}'})$$

are fairly k-independent!

In the extreme case $W(\mathbf{k},\mathbf{k}') = W_0$ we obtain:

$$\lambda_a = -W_0 N(0)\delta_{a=s-wave}$$

that is only s-wave lambda is larger than zero, all other pairing channels have zero coupling.

Are more exotic pairings possible due to strong anisotropy of electron-phonon interaction? Consider another extreme: an EPI singular at some wavevector $\mathbf{q}_0$

$$W(\mathbf{k},\mathbf{k}') = W_1\delta(\mathbf{k}-\mathbf{k}'-\mathbf{q}_0) = W_1\sum_a \eta_a(\mathbf{k})\eta_a(\mathbf{k}'+\mathbf{q}_0)$$

We obtain

$$\lambda_a = -W_1\sum_{\mathbf{k}}\delta(\epsilon_{\mathbf{k}})\eta_a(\mathbf{k})\eta_a(\mathbf{k}+\mathbf{q}_0) = -W_1 N(0)O_a(\mathbf{q}_0)$$

where the overlap matrix between two polynomials shows up

$$O_a(\mathbf{q}_0) = \frac{1}{N(0)}\sum_{\mathbf{k}}\delta(\epsilon_{\mathbf{k}})\eta_a(\mathbf{k})\eta_a(\mathbf{k}+\mathbf{q}_0)$$

It would be less than unity for non-zero angular momentum index a unless

$\mathbf{q}_0 \Rightarrow 0$

$$\lim_{q_0\to 0} O_a(\mathbf{q}_0) = 1$$

We obtain that λ's become degenerate, $\lambda_a = -W_1 N(0)$, for all(!) pairing channels if electron-phonon coupling gets singular at long wavelenghts!

However, even in this extreme scenario, for the $l>0$ state to win, additional effects such as Coulomb interaction μ*, need to be taken into account.

That is why, practically, in any intermediate case, s-wave symmetry always wins, since it always makes largest electron-phonon λ.

To find unconventional pairing state we have to look for materials with singular EPI and this should occur at small wavevectors (longwavelength limit!)

We predict by first principle calculation that is the case of doped topological insulator Bi2Se3.

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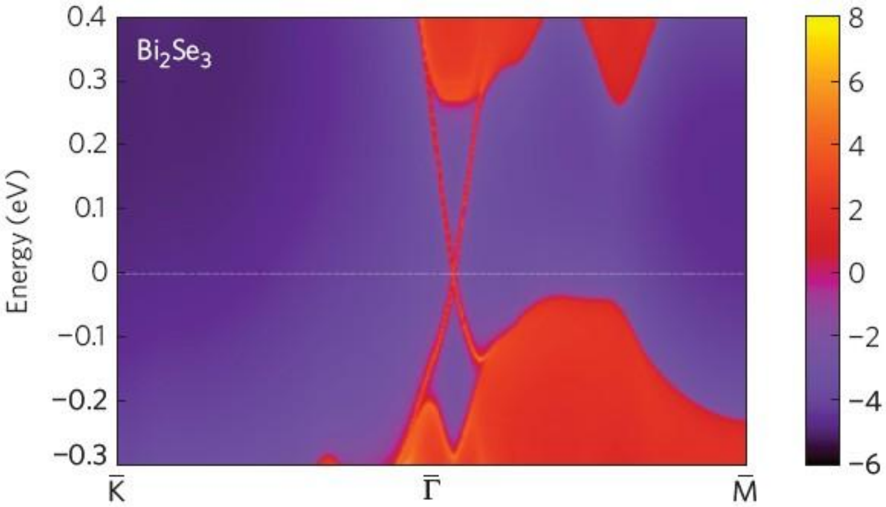
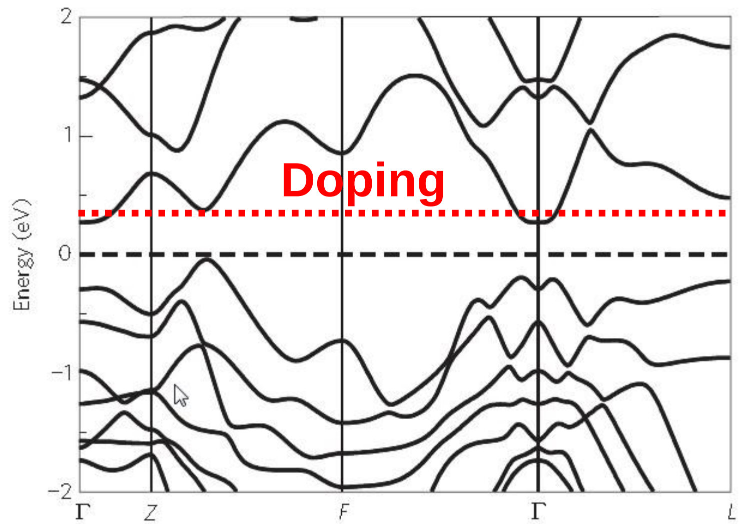
Superconductivity in Doped Topological Insulators

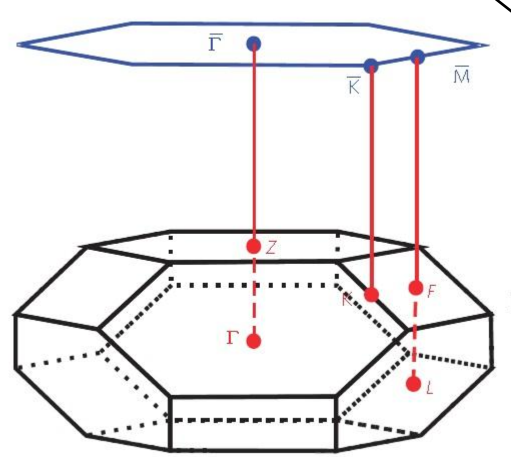
Criterion by Fu and Berg (PRL 2010): a topological superconductor has odd-parity pairing symmetry and its Fermi surface encloses an odd number of time reversal invariant momenta (that are Γ,X,L points of cubic BZ lattices)

Implications for topological insulators: doped topological insulator may realize a topological superconductor

Theory by Fu and Berg (PRL 2010): doping Bi_2Se_3 with electrons may realize odd-parity topological superconductor with conventional electron-phonon couplings:







TRIM point

ARTICLES

PUBLISHED ONLINE: 10 MAY 2009 | DOI: 10.1038/NPHYS1270

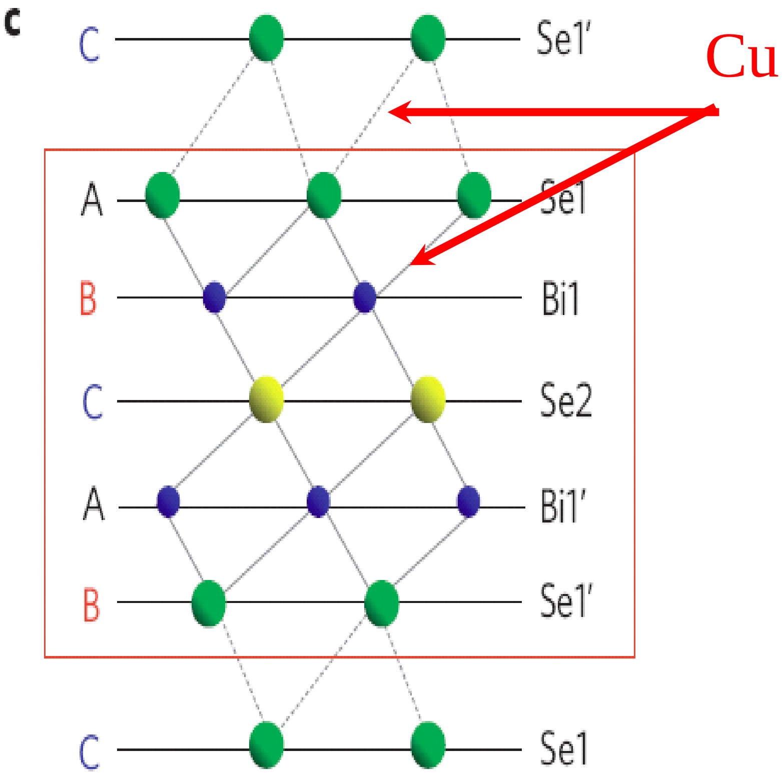
nature physics

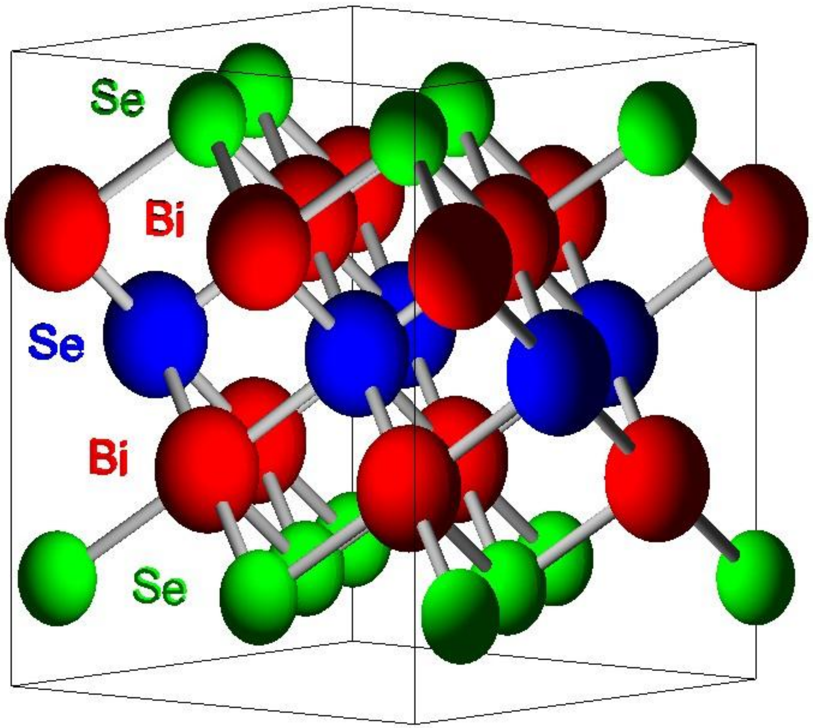
Topological insulators in Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3 with a single Dirac cone on the surface

Haijun Zhang[1], Chao-Xing Liu[2], Xiao-Liang Qi[3], Xi Dai[1], Zhong Fang[1] and Shou-Cheng Zhang[3]*

Superconductivity in $Cu_xBi_2Se_3$

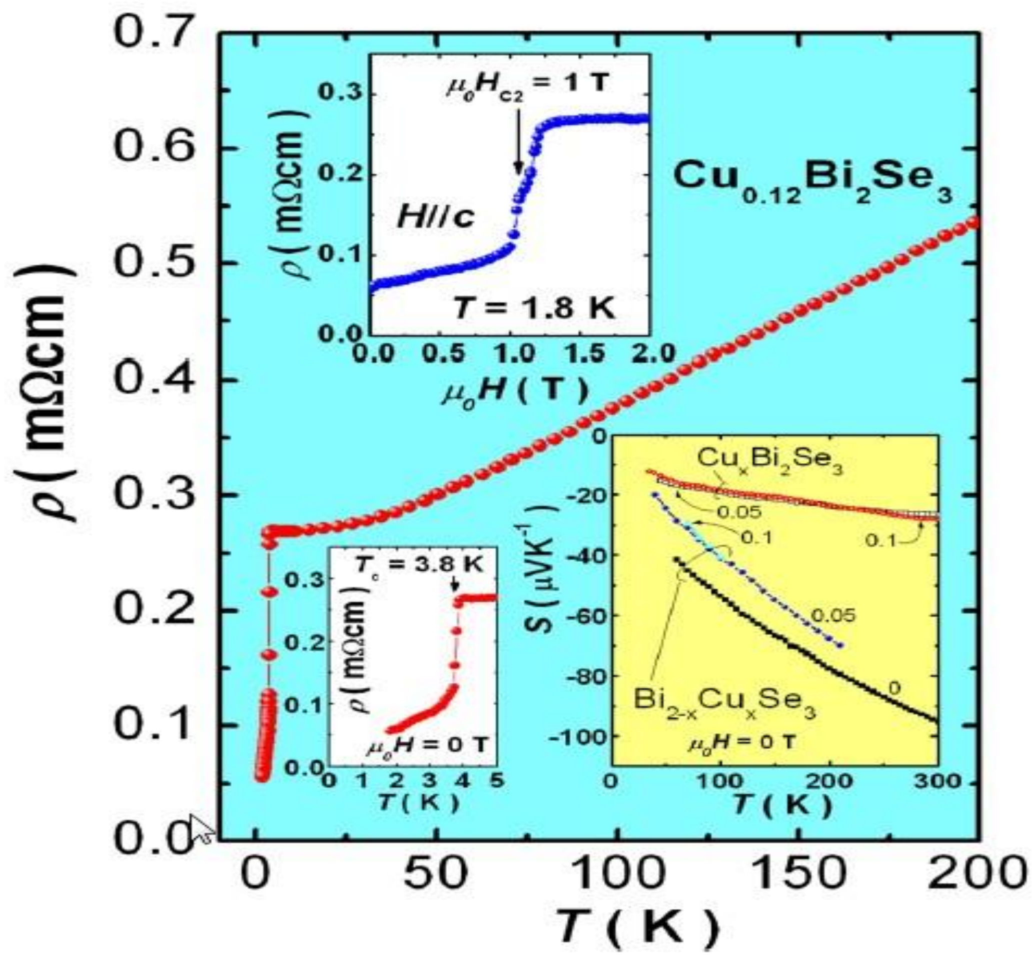
Hor et al, PRL 104, 057001 (2010)





Hor et al, PRL 104, 057001 (2010)

Tc up to 3.8K



Symmetry of Pairing State

- Point-contact spectroscopy: odd-parity pairing in $Cu_xBi_2Se_3$ (Sasaki et.al, PRL 2011) via observed zero-bias conductance

PRL **107,** 217001 (2011) PHYSICAL REVIEW LETTERS week ending 18 NOVEMBER 2011

Topological Superconductivity in $Cu_xBi_2Se_3$

Satoshi Sasaki,[1] M. Kriener,[1] Kouji Segawa,[1] Keiji Yada,[2] Yukio Tanaka,[2] Masatoshi Sato,[3] and Yoichi Ando[1,*]
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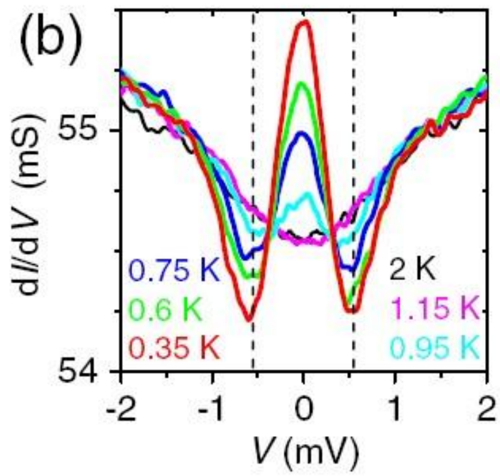
[3]*Instituite for Solid State Physics, University of Tokyo, Chiba 277-8581, Japan*
(Received 2 August 2011; published 14 November 2011)



- Scanning-tunneling spectroscopy: fully gapped state in $Cu_xBi_2Se_3$

PRL **110,** 117001 (2013) PHYSICAL REVIEW LETTERS week ending 15 MARCH 2013

Experimental Evidence for *s*-Wave Pairing Symmetry in Superconducting $Cu_xBi_2Se_3$ Single Crystals Using a Scanning Tunneling Microscope

Niv Levy,[1,2] Tong Zhang,[1,2] Jeonghoon Ha,[1,2,3] Fred Sharifi,[1] A. Alec Talin,[1] Young Kuk,[3] and Joseph A. Stroscio[1,*]
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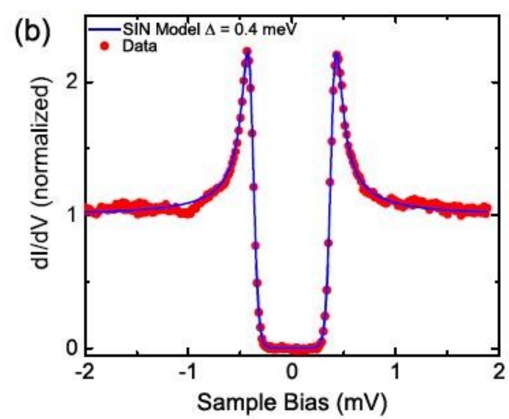
[3]*Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea*
(Received 1 November 2012; published 12 March 2013)



Superconductivity in the Doped Topological Insulator $Cu_xBi_2Se_3$ under High Pressure

T. V. Bay,[1] T. Naka,[2] Y. K. Huang,[1] H. Luigjes,[1] M. S. Golden,[1] and A. de Visser[1,*]

[1]*Van der Waals–Zeeman Institute, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands*

[2]*National Institute for Materials Science, Sengen 1-2-1, Tsukuba, Ibaraki 305-0047, Japan*

(Received 2 September 2011; published 31 January 2012)

We report a high-pressure single crystal study of the topological superconductor $Cu_xBi_2Se_3$. Resistivity measurements under pressure show superconductivity is depressed smoothly. At the same time the metallic behavior is gradually lost. The upper-critical field data $B_{c2}(T)$ under pressure collapse onto a universal curve. The absence of Pauli limiting and the comparison of $B_{c2}(T)$ to a polar-state function point to spin-triplet superconductivity, but an anisotropic spin-singlet state cannot be discarded completely.

DOI: 10.1103/PhysRevLett.108.057001 PACS numbers: 74.70.Dd, 74.25.Op, 74.62.Fj

Pressure-Induced Unconventional Superconducting Phase in the Topological Insulator Bi_2Se_3

Kevin Kirshenbaum,[1] P. S. Syers,[1] A. P. Hope,[1] N. P. Butch,[2] J. R. Jeffries,[2] S. T. Weir,[2] J. J. Hamlin,[3] M. B. Maple,[3] Y. K. Vohra,[4] and J. Paglione[1,*]

[1]*Department of Physics, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, Maryland 20742, USA*

[2]*Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, Livermore, California 94550, USA*

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(Received 26 February 2013; published 20 August 2013)

Simultaneous low-temperature electrical resistivity and Hall effect measurements were performed on single-crystalline Bi_2Se_3 under applied pressures up to 50 GPa. As a function of pressure, superconductivity is observed to onset above 11 GPa with a transition temperature T_c and upper critical field H_{c2} that both increase with pressure up to 30 GPa, where they reach maximum values of 7 K and 4 T, respectively. Upon further pressure increase, T_c remains anomalously constant up to the highest achieved pressure. Conversely, the carrier concentration increases continuously with pressure, including a tenfold increase over the pressure range where T_c remains constant. Together with a quasilinear temperature dependence of H_{c2} that exceeds the orbital and Pauli limits, the anomalously stagnant pressure dependence of T_c points to an unconventional pressure-induced pairing state in Bi_2Se_3 that is unique among the superconducting topological insulators.

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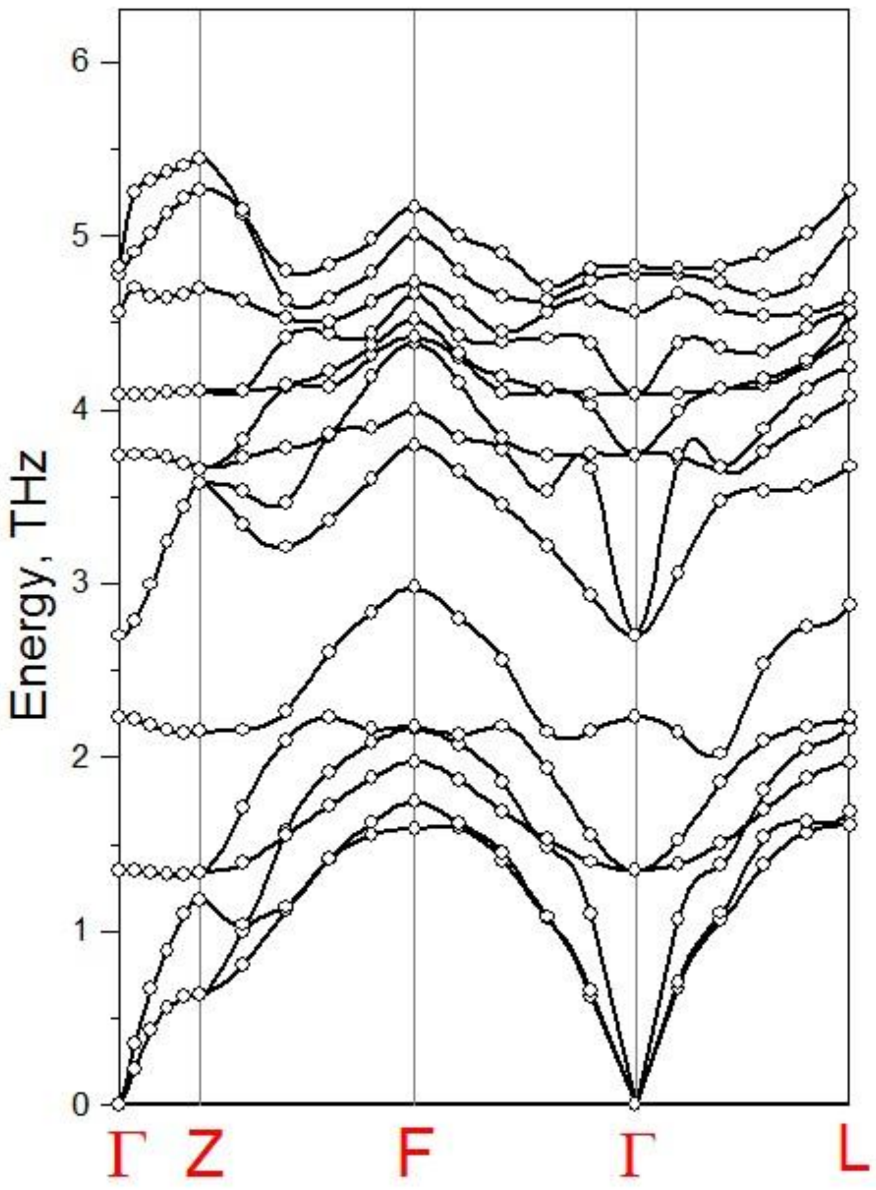
- ❑ **Calculations of phonons and electron-phonon interactions in $Cu_xBi_2Se_3$**
- ❑ Effects of Coulomb interaction: μ* and spin fluctuations
- ❑ Conclusion

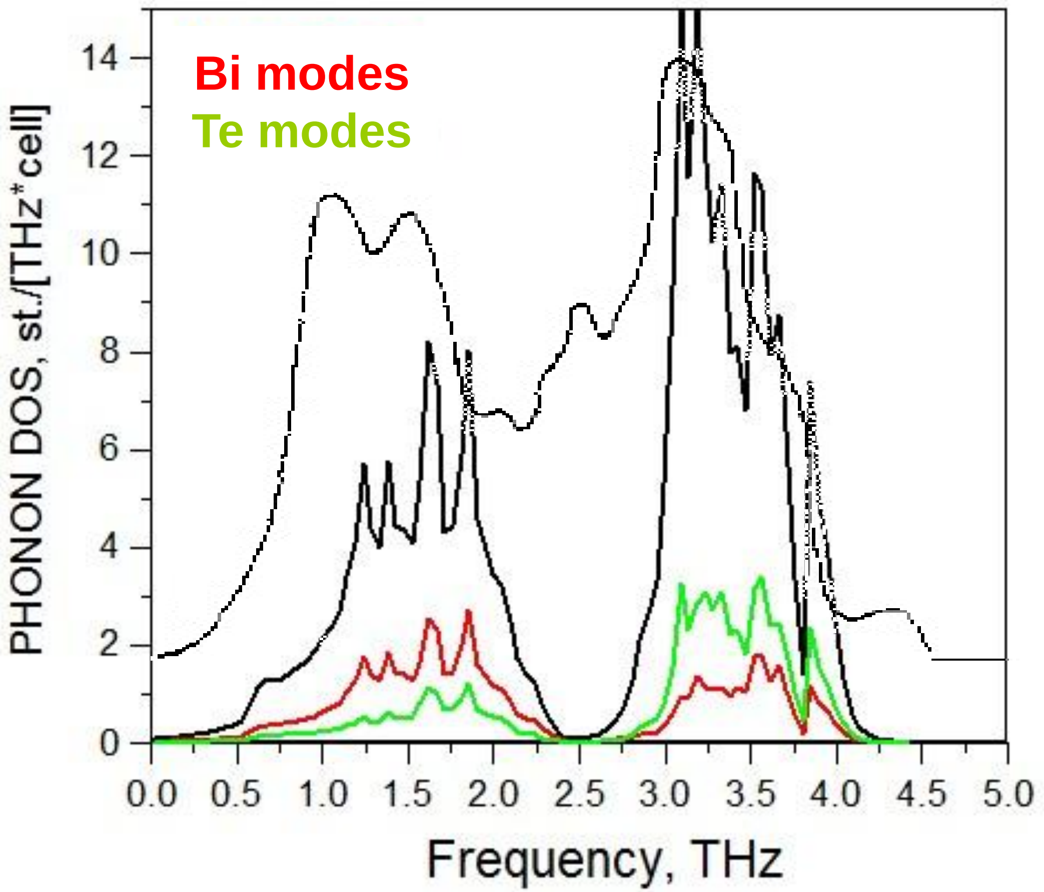
Phonon Spectrum for Bi_2Se_3

Calculated phonon spectrum with density functional linear response approach (SS, PRL 1992)

Local Density Approximation, effects of spin orbit coupling and the basis of linear muffin-tin orbitals is utilized.



Calculated Phonon Density of States for Bi_2Se_3



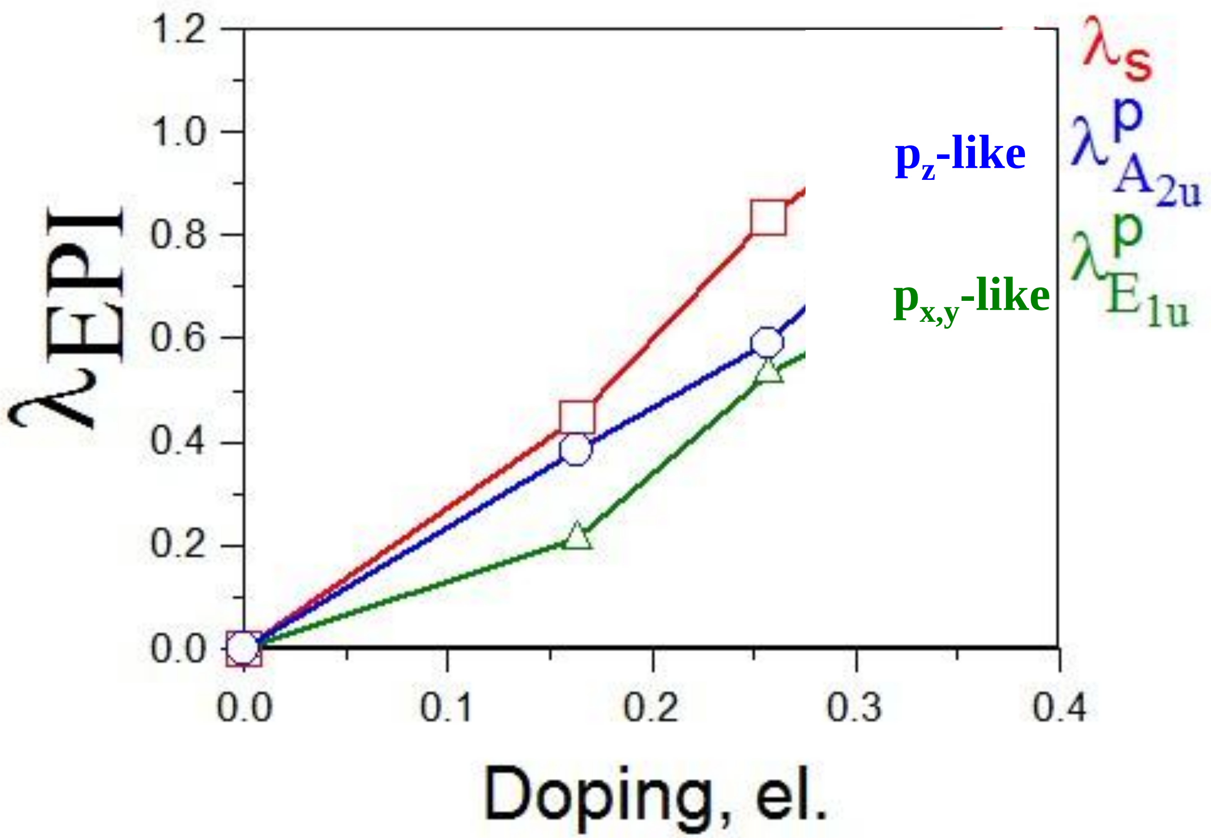
INS Data from Rauh et.al, J Phys C. 1981

Phonons at Γ point for Bi_2Se_3

LDA+SO calculations, in cm^{-1}

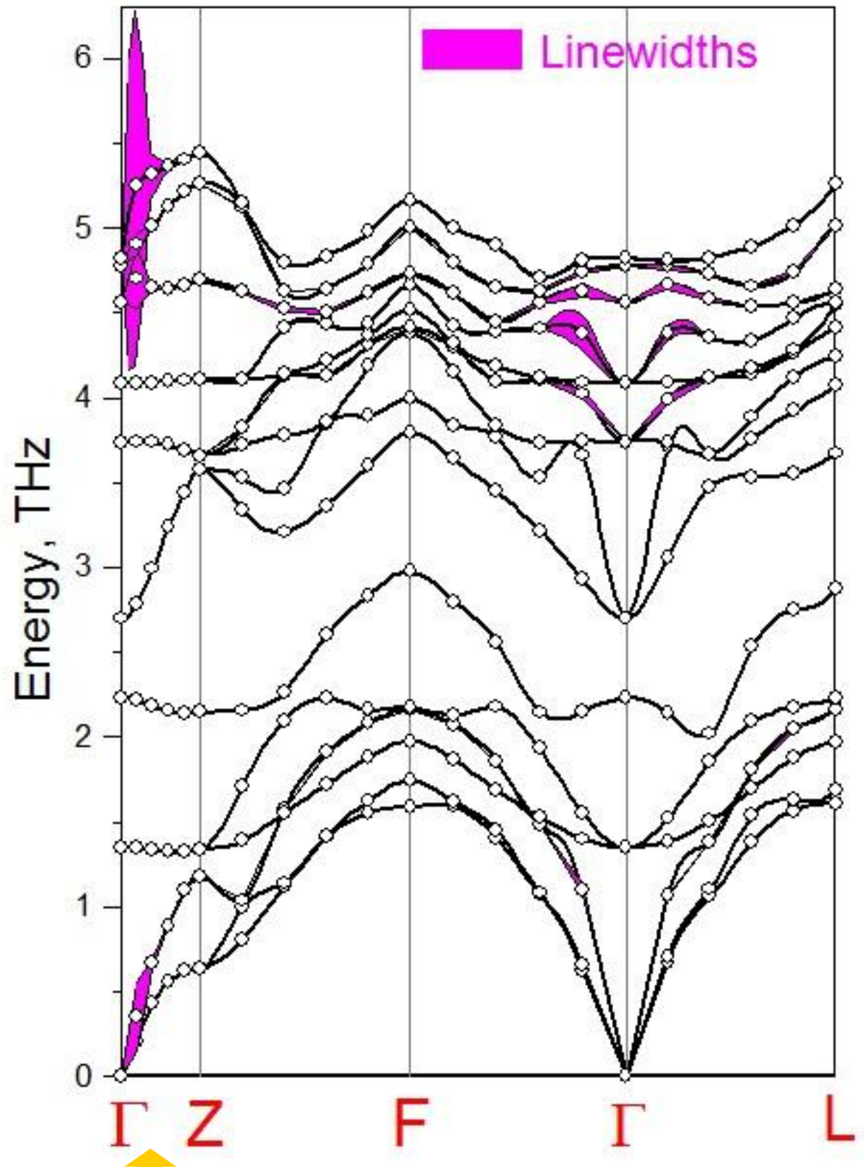
Grid	$2xE_g$	$1xA_g$	$2xE_u$	$2xE_g$	$2xE_u$	$1xA_u$	$1xA_u$	$1xA_g$
10-10-10	45	74	90	124	136	152	150	160
8-8-8	44	48	91	125	136	136	153	164
6-6-6	44	48	91	125	136	136	154	164
Exp (Richter 77)	---	72	65??	131	134	--	---	174
Exp (PRB84,195118)	38.9	73.3	--	132	---	--	---	175
LDA(PRB83,094301)	41	75	80	137	130	137	161	171
GGA(PRB83,094301)	38	64	65	124	127	137	155	166
LDA(APL100,082109)	41	77	80	138	131	138	161	175

Large Electron-Phonon Interaction in $Cu_xBi_2Se_3$



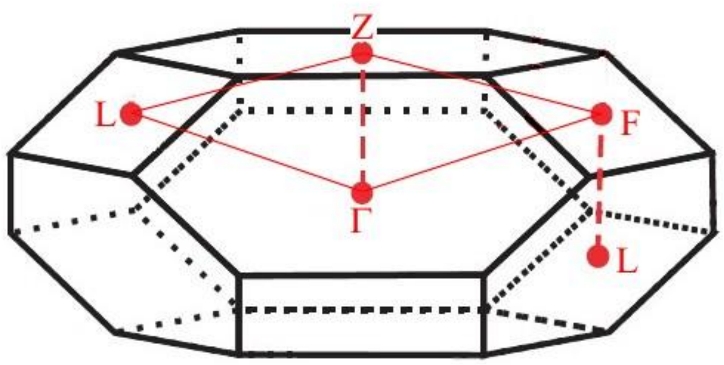
S-wave shows largest coupling. P-wave is also very large!

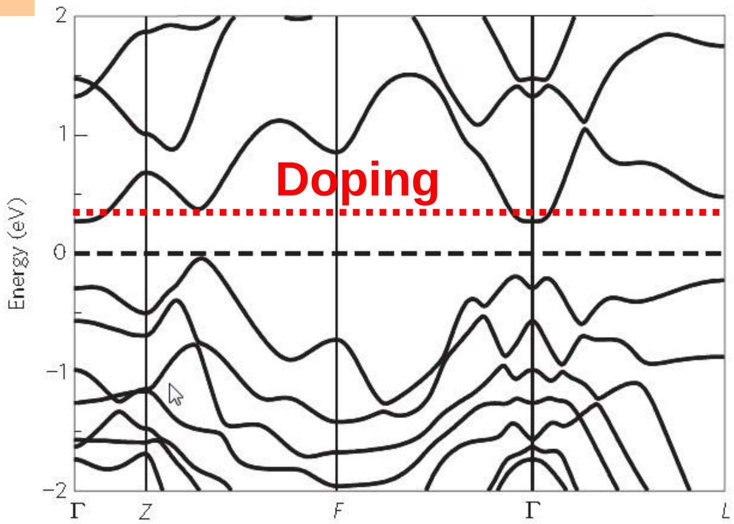
Calculated phonon linewidths in doped Bi_2Se_3

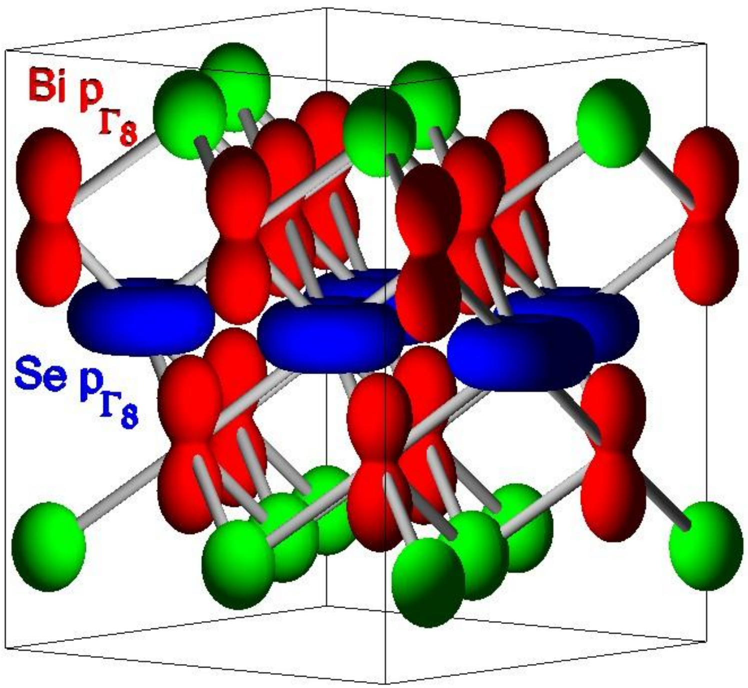


Electron-phonon coupling is enormous at $\mathbf{q}_0 \sim (0,0,0.04)2\pi/c$

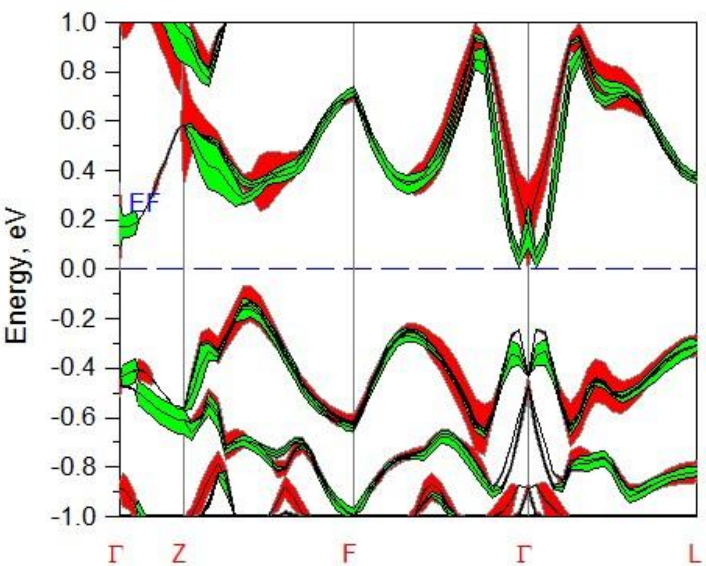
Energy Bands in $Cu_xBi_2Se_3$



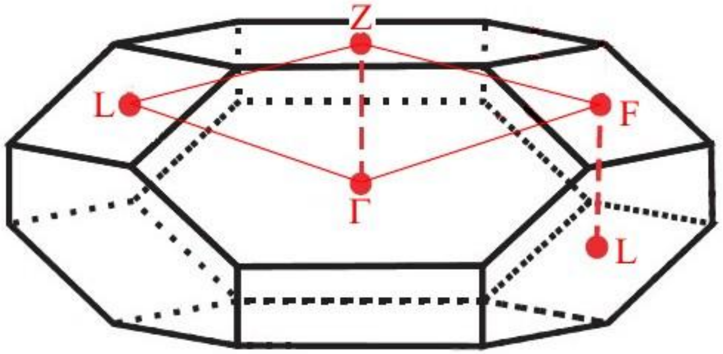




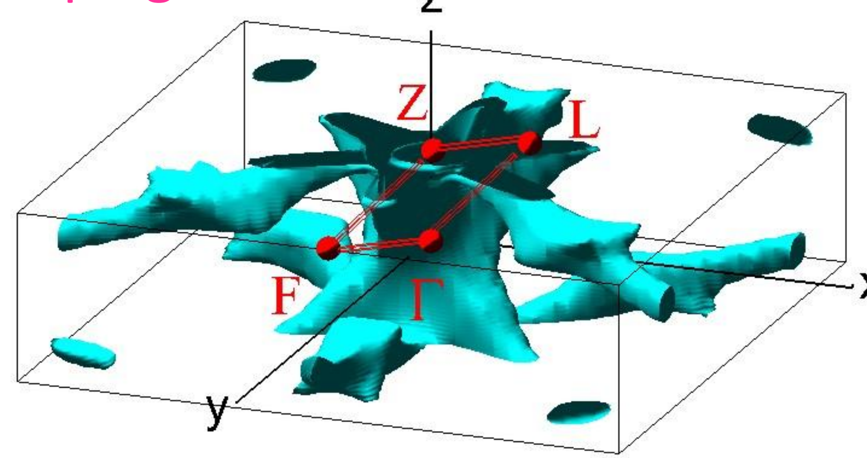
Bi2@2-j3/2::6p{G8-1}; Se3@5-j3/2::4p{G8-3};



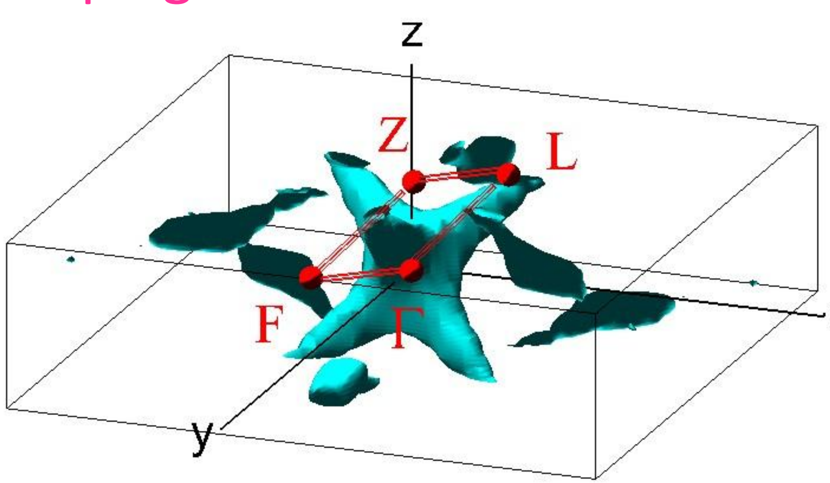
Fermi Surfaces of $Cu_xBi_2Se_3$



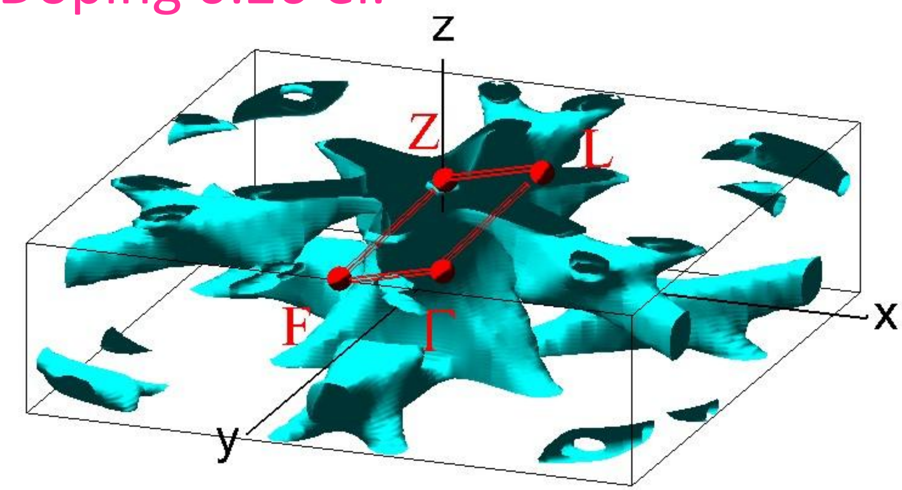
Doping 0.16 el.



Doping 0.07 el.



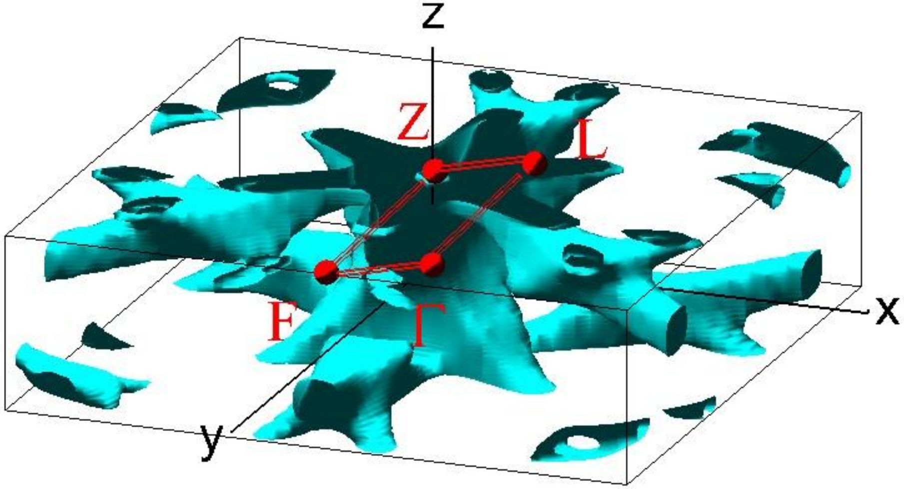
Doping 0.26 el.

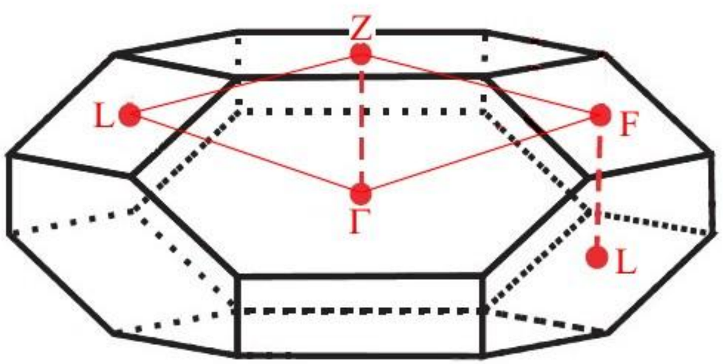


Nesting Function

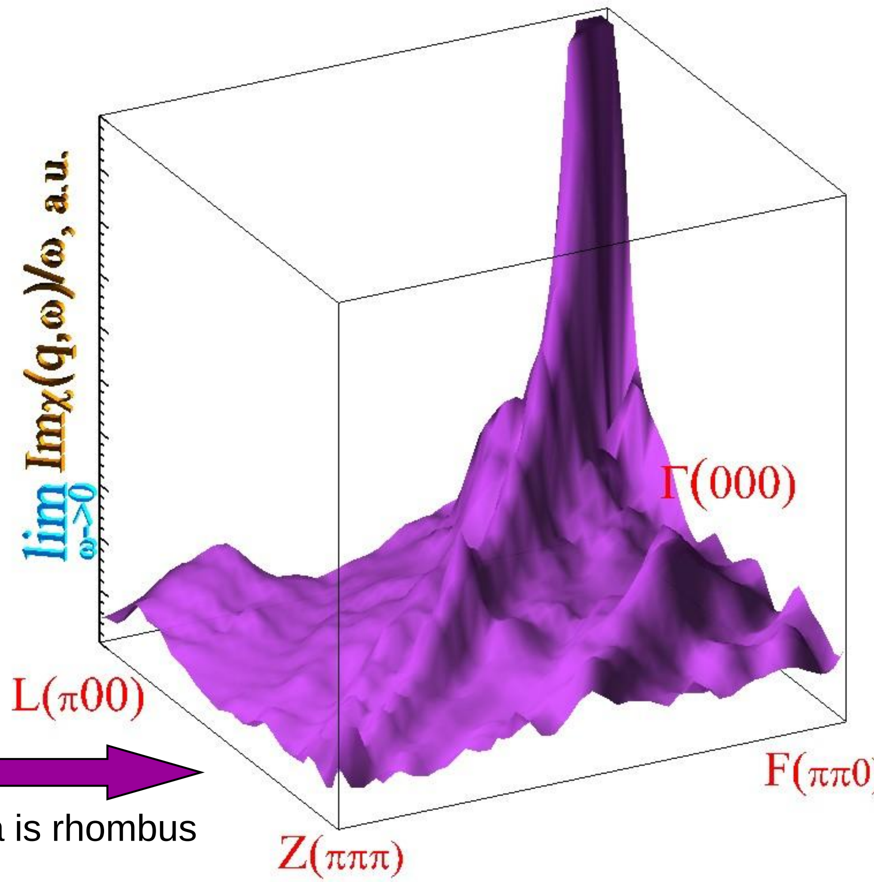
$$\chi(\mathbf{q}) = \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}})\delta(\epsilon_{\mathbf{k+q}})$$

Doping 0.16 el.





Basal area is rhombus

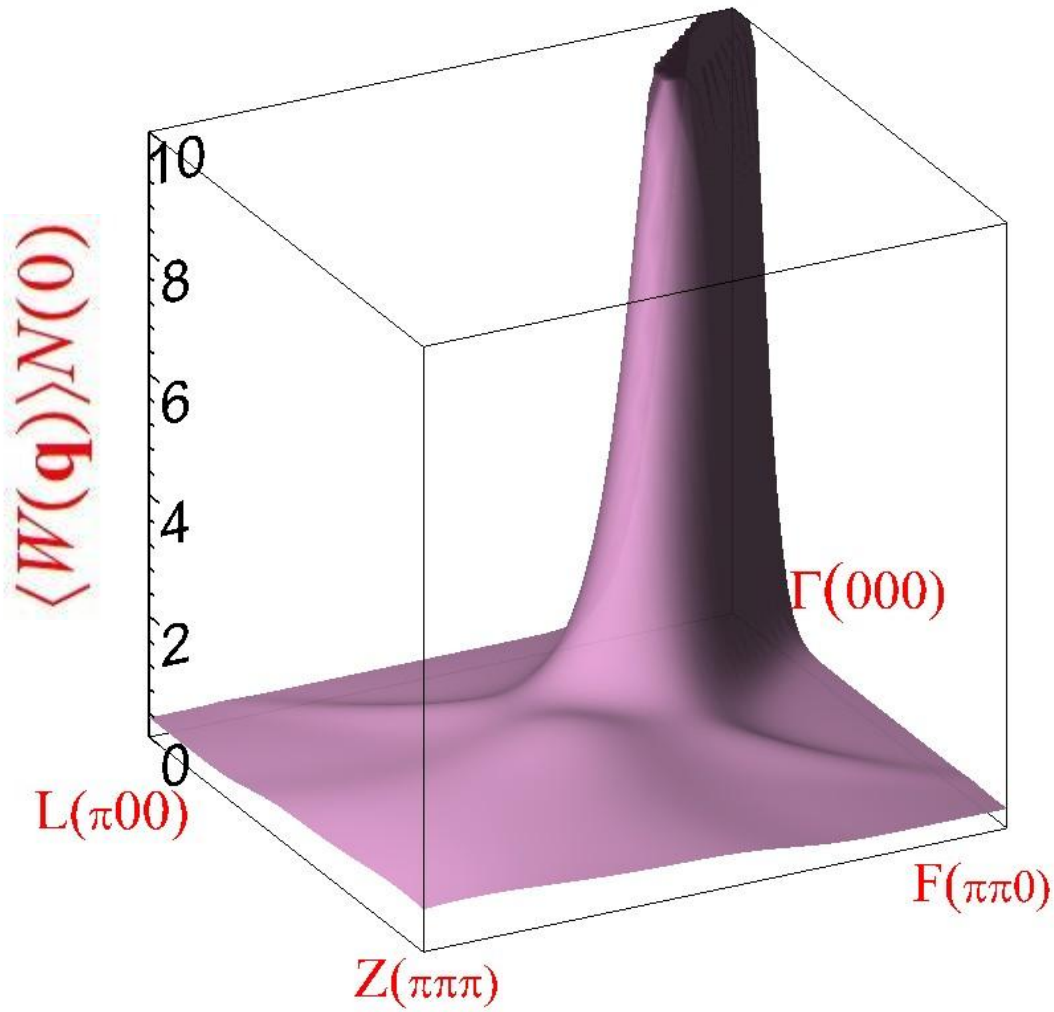


Shows a strong ridge-like structure along ΓZ line at small q's due to quasi 2D features of the Fermi surface.

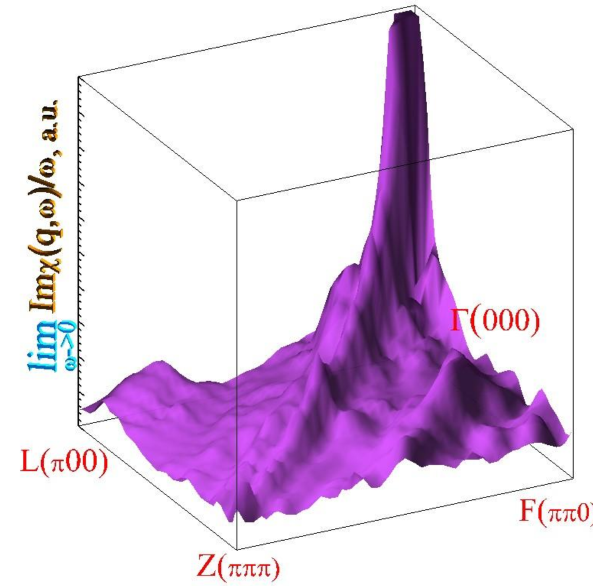
Calculated electron-phonon matrix elements

Define average electron-phonon matrix element (squared) as follows

$$\langle W(\mathbf{q})\rangle = \frac{\sum_{\mathbf{k}} W(\mathbf{k},\mathbf{k}+\mathbf{q})\delta(\epsilon_{\mathbf{k}})\delta(\epsilon_{\mathbf{k+q}})}{\sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}})\delta(\epsilon_{\mathbf{k+q}})}$$

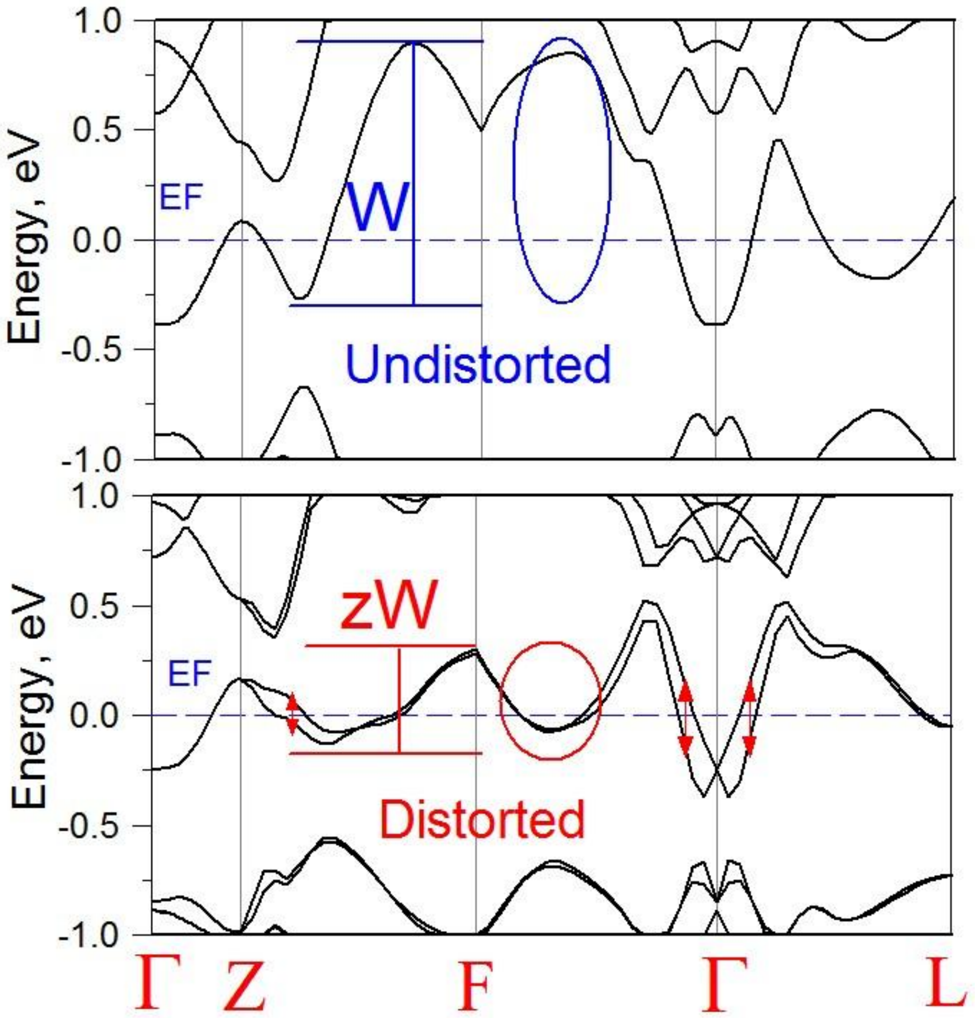


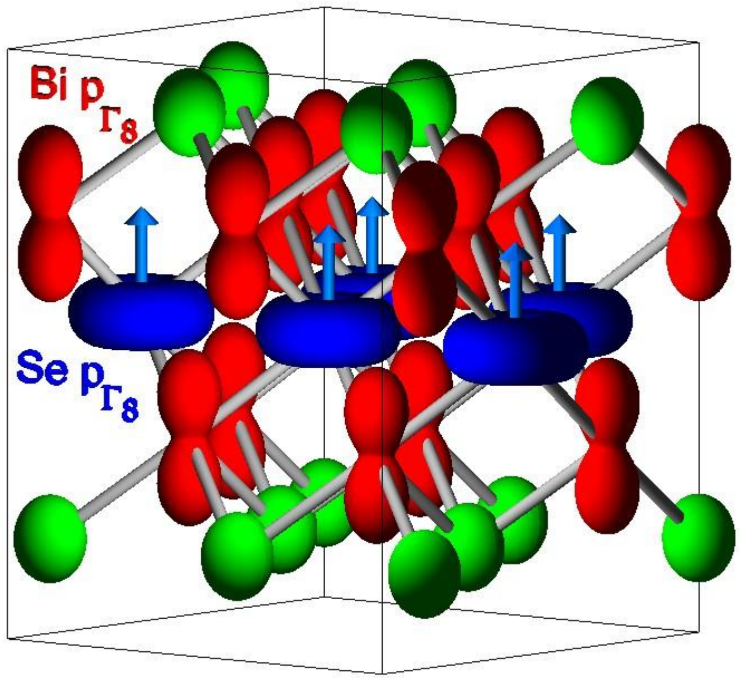
This eliminates all nesting-like features of $\chi(\mathbf{q}) = \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}})\delta(\epsilon_{\mathbf{k+q}})$



Still $\langle W(\mathbf{q})\rangle$ **shows almost singular behavior for** $\mathbf{q}_0 \sim (0,0,0.04)2\pi/c$

Calculated deformation potentials at long wavelengths





Large electron-phonon effects are found due to splitting of two-fold spin-orbit degenerate band by lattice distortions breaking inversion symmetry.
The role of spin-orbit coupling is unusual!

Implications of singular EPI for BCS Gap Equation

For almost singular electron-phonon interaction that we calculate

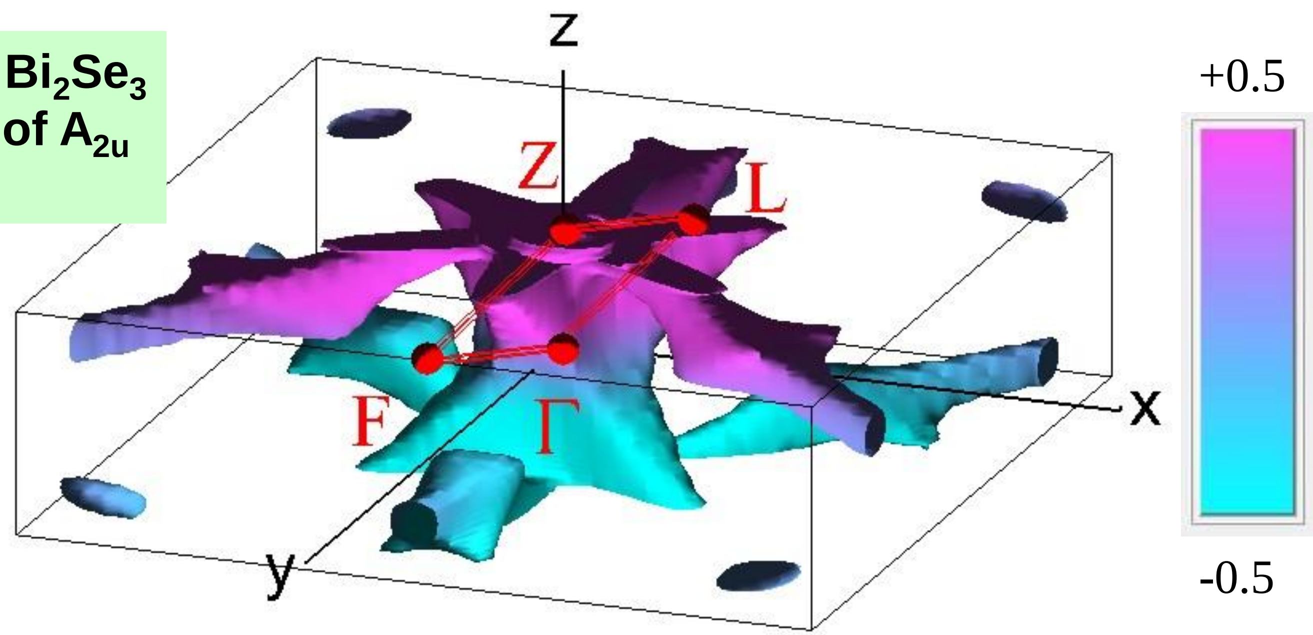
$$W(\mathbf{k},\mathbf{k}') = W_0\delta(\mathbf{k}-\mathbf{k}'-\mathbf{q}_0)$$

with $\mathbf{q}_0$~(0,0,0.04)2π/c, **(**W_0 **is attractive, negative) the BCS gap equation**

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} W(\mathbf{k}\mathbf{k}')\Delta(\mathbf{k}')\tanh\left(\frac{\epsilon_{\mathbf{k}'}}{2T_c}\right)/2\epsilon_{\mathbf{k}'}$$

yields $\Delta(\mathbf{k})\sim\Delta(\mathbf{k}+\mathbf{q}_0)$ **compatible with both s-wave and p-wave symmetries!**

Fermi surface of doped Bi_2Se_3 colored by the gap $\Delta(\mathbf{k})$ of A_{2u} (p_z-like) symmetry.



Contents

Can μ^* suppress s-wave?

The T_c includes Coulomb pseudopotential μ^*

$$T_c^{(l)} = 1.14\omega_D \exp\left(-\frac{1}{\lambda_l^{eff}}\right)$$

$$\lambda_l^{eff} = \frac{\lambda_l - \mu_l^*}{1+\lambda_{s-h}} \qquad \mu_l^* = \frac{\mu_l}{1+\mu_l \ln \epsilon_F/\omega_D}$$

where μ_l is the Fermi surface average of some screened Coulomb interaction

$$\mu_l = \frac{1}{N(0)}\sum_{\mathbf{k}\mathbf{k}'}\langle \mathbf{k}-\mathbf{k}|U|\mathbf{k}'-\mathbf{k}'\rangle \delta(\epsilon_{\mathbf{k}})\delta(\epsilon_{\mathbf{k}'})\eta_l(\mathbf{k})\eta_l(\mathbf{k}')$$

Assuming Hubbard like on-site Coulomb repulsion

$$\langle \mathbf{k}-\mathbf{k}|U|\mathbf{k}'-\mathbf{k}'\rangle = U$$

μ^* will affect s-wave pairing only

$$\mu_{l=s} = UN(0) \qquad \mu_{l>s} = 0$$

Alexandrov (PRB 2008) studied a model with Debye screened Coulomb interaction

$$U(\mathbf{q}) = \frac{4\pi e^2}{q^2 + \kappa_D^2}$$

and arrived to similar conclusions that

$$\mu_s >> \mu_{l>s}$$

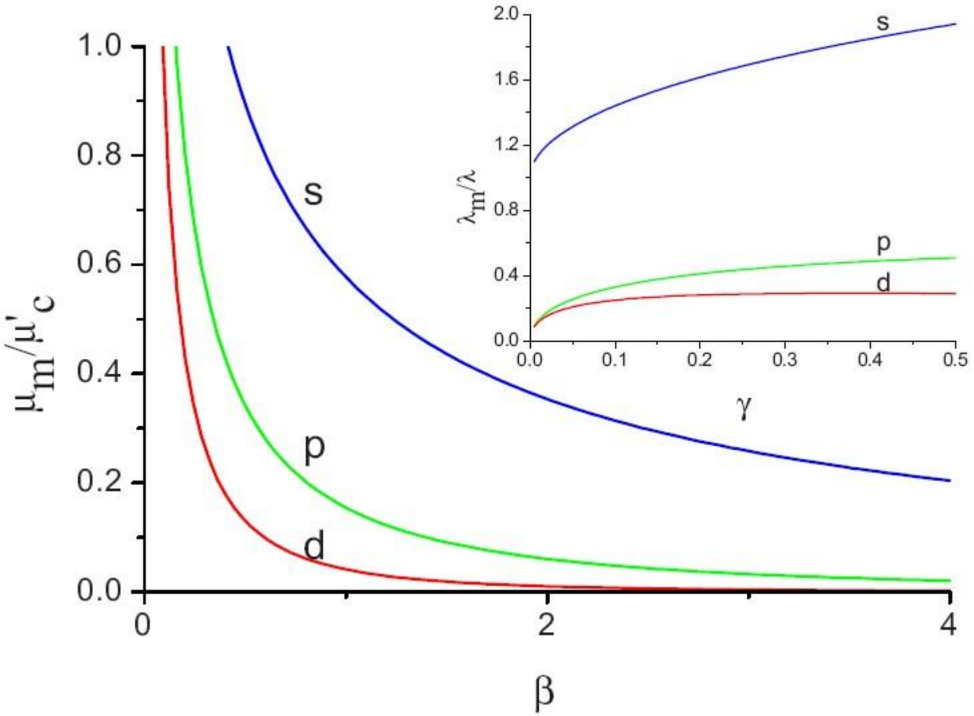


FIG. 1. (Color online) The Coulomb repulsion μ_m as a function of the ratio of the electron wavelength to the screening length squared ($\beta = q_S^2/2k_F^2$), and the electron-phonon coupling constant λ_m as a function of the ratio of the electron wavelength to the inter-plane distance squared, $\gamma = \pi^2/2d^2k_F^2(1+\alpha)$ for $\alpha=4$ (inset) in s, p, and d pairing channels. Here, $\mu'_c = \mu_c\tilde{\gamma}$.

Estimates with μ^*

For doped Bi_2Se_3 we obtain the estimate

$$\omega_D \sim 100K$$

$$\varepsilon_F \sim 2000 - 5000K$$

and

$$\mu_s^* = 0.1$$

For doping by 0.16 electrons we get the estimates

S-wave

$$\lambda_s^{EPI} = 0.45$$

$$\mu_s^* = 0.1$$

P-wave

$$\lambda_{A_{2u}}^{EPI} = 0.39$$

$$\mu_{l>s}^* \sim 0$$

Effective coupling λ-μ^* for p-wave pairing channel wins!

Estimates for spin fluctuations

Spin fluctuations suppress s-wave electron-phonon coupling

VOLUME 17, NUMBER 8 PHYSICAL REVIEW LETTERS 22 AUGUST 1966

EFFECT OF FERROMAGNETIC SPIN CORRELATIONS ON SUPERCONDUCTIVITY*

N. F. Berk and J. R. Schrieffer
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania
(Received 24 June 1966)

and can induce unconventional (e.g. d-wave) pairing

PHYSICAL REVIEW B VOLUME 34, NUMBER 11 1 DECEMBER 1986

d-wave pairing near a spin-density-wave instability

D. J. Scalapino, E. Loh, Jr.,* and J. E. Hirsch†
Institute for Theoretical Physics, University of California, Santa Barbara, California 93106
(Received 23 June 1986)

PHYSICAL REVIEW B VOLUME 34, NUMBER 9 1 NOVEMBER 1986

Spin-fluctuation-mediated even-parity pairing in heavy-fermion superconductors

K. Miyake,* S. Schmitt-Rink, and C. M. Varma
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
(Received 27 June 1986; revised manuscript received 11 August 1986)

$$\lambda_l^{eff} = \frac{\lambda_l^{EPI} - \mu_l^* + \lambda_l^{SF}}{1 + \lambda_{s-h}^{EPI} + \lambda_{s-h}^{SF}}$$

Coupling Constants due to Spin Fluctuations

Evaluate coupling constants in various channels

$$\lambda_l^{(sf)} = \frac{1}{N(0)} \sum_{\mathbf{k}\mathbf{k}'} \langle \mathbf{k} - \mathbf{k} | V | \mathbf{k}' - \mathbf{k}' \rangle \delta(\epsilon_{\mathbf{k}}) \delta(\epsilon_{\mathbf{k}'}) \eta_l(\mathbf{k}) \eta_l(\mathbf{k}')$$

with the effective interaction for singlet pairing

$$V^{(S=0)}(\mathbf{q},\omega) = \frac{1}{2}[U + \frac{U\pi(\mathbf{q},\omega)U}{1 - U\pi(\mathbf{q},\omega)}] + \frac{3}{2}[U - \frac{U\pi(\mathbf{q},\omega)U}{1 + U\pi(\mathbf{q},\omega)}]$$

and for triplet pairing

$$V^{(S=1)}(\mathbf{q},\omega) = \frac{1}{2}[U + \frac{U\pi(\mathbf{q},\omega)U}{1 - U\pi(\mathbf{q},\omega)}] - \frac{1}{2}[U - \frac{U\pi(\mathbf{q},\omega)U}{1 + U\pi(\mathbf{q},\omega)}]$$

Spin fluctuational mass renormalizations:

$$\lambda_{s-h}^{SF} = \frac{1}{N(0)} \sum_{\mathbf{k}\mathbf{k}'} \langle \mathbf{k}\mathbf{k}' | V^{eff} | \mathbf{k}'\mathbf{k} \rangle \delta(\epsilon_{\mathbf{k}}) \delta(\epsilon_{\mathbf{k}'})$$

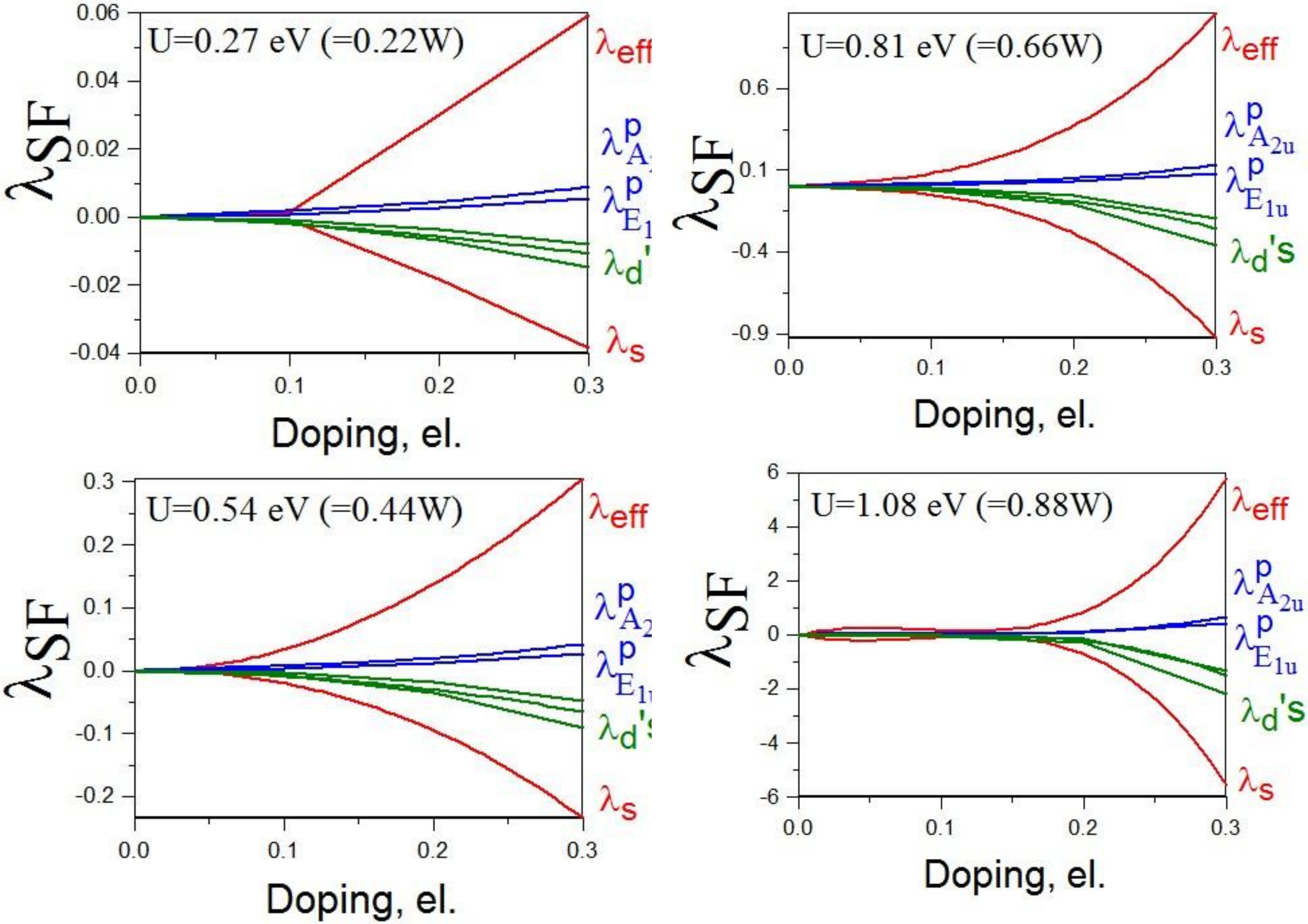
$$V^{eff}(\mathbf{q},\omega) = -U + \frac{1}{2} \frac{U\pi(\mathbf{q},\omega)U}{1 - U\pi(\mathbf{q},\omega)} + \frac{3}{2} \frac{U\pi(\mathbf{q},\omega)U}{1 + U\pi(\mathbf{q},\omega)} - U\pi(\mathbf{q},\omega)U$$

Stoner Instability in doped Bi_2Se_3

Stoner criterion provides some estimates for the upper bounds of U

Doping (el)	N(0), st/eV	Critical U (eV)
0.1	0.8	1.2
0.2	1.5	0.7
0.3	1.8	0.54

FLEX Coupling Constants



Resulting Coupling Constants

For doping by 0.16 electrons we get the estimates (negative is repulsion)

S-wave

$$\lambda_s^{EPI} = 0.45$$

$$\mu_s^* = 0.1$$

$$\lambda_s^{SF} = -0.05$$

$$\lambda_s^{Total} = 0.30$$

P-wave

$$\lambda_{A_{2u}}^{EPI} = 0.39$$

$$\mu_{l>s}^* \sim 0$$

$$\lambda_{A_{2u}}^{SF} = +0.02$$

(positive, attractive!)

$$\lambda_{A_{2u}}^{Total} = 0.41$$

$$U = 0.5eV$$

$$W = 1.2eV$$

Effective coupling λ^{EPI}-$\mu^*+\lambda^{SF}$ **(note sign convention!) for p-wave pairing of A_{2u} symmetry may be largest one!**

$$\lambda_{A_{2u}}^{eff} = \frac{0.41}{1+0.45+0.05} = 0.27, T_c = 1.14\omega_D e^{-1/\lambda_{A_{2u}}^{eff}} \approx 3K$$

Similar consequences are seen at other doping levels where the difference between electron-phonon λ_s and λ_p is between 0.1 and 0.2.

Conclusion

- **Large electron-phonon coupling is found for $Cu_xBi_2Se_3$**
- **Not only s-wave but also p-wave pairing is found to be large due to strong anisotropy and quasi-2D Fermi surfaces. $\lambda_s \sim \lambda_p$**
- **Coulomb interaction and spin fluctuations will reduce λ_s and make $\lambda_p > \lambda_p$ therefore unconventional superconductivity may indeed be realized here.**
- **Discussed effects have nothing to do with topological aspect of the problem, may be found in other doped band insulators.**